



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:41 AM EDT

PDB ID : 1JRP / pdb_00001jrp
Title : Crystal Structure of Xanthine Dehydrogenase inhibited by alloxanthine from *Rhodobacter capsulatus*
Authors : Truglio, J.J.; Theis, K.; Leimkuhler, S.; Rappa, R.; Rajagopalan, K.V.; Kisker, C.
Deposited on : 2001-08-14
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

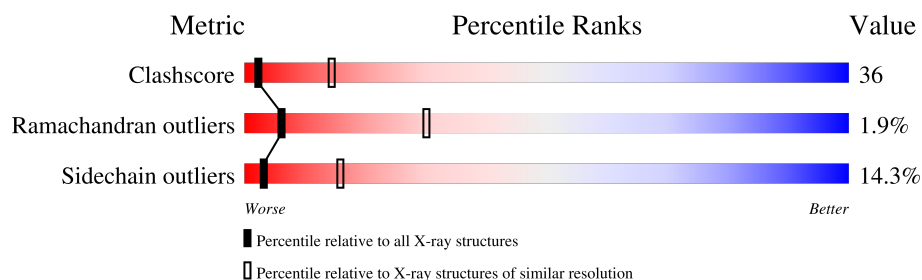
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	462	37% 42% 18% ..
1	C	462	42% 40% 14% ..
1	E	462	32% 45% 18% ..
1	G	462	32% 43% 19% ..
2	B	777	37% 43% 15% ..
2	D	777	37% 42% 16% ..
2	F	777	33% 45% 17% ..
2	H	777	33% 48% 15% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	E	3002	-	-	X	-
3	FES	G	3001	-	-	X	-
6	MTE	F	3003	-	-	X	-
6	MTE	H	3003	-	-	X	-
7	MOS	B	3004	-	-	X	-
7	MOS	D	3004	-	-	X	-
7	MOS	F	3004	-	-	X	-
7	MOS	H	3004	-	-	X	-
8	141	B	4000	-	-	X	-
8	141	D	4000	-	-	X	-
8	141	F	4000	-	-	X	-
8	141	H	4000	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36748 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called xanthine dehydrogenase, chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			

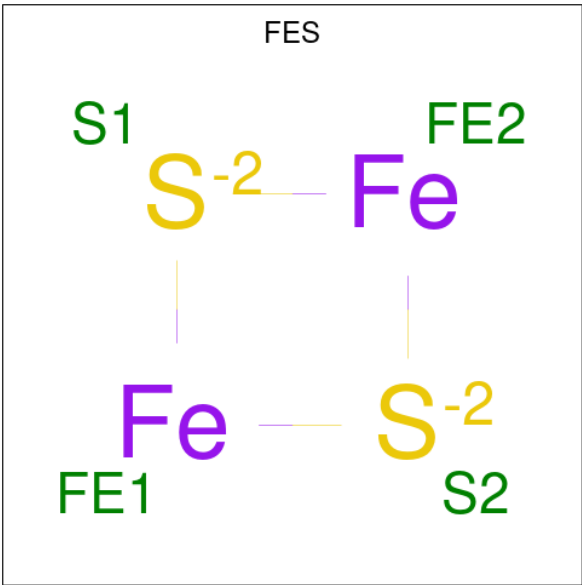
- Molecule 2 is a protein called xanthine dehydrogenase, chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	D	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	F	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	H	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			

There are 4 discrepancies between the modelled and reference sequences:

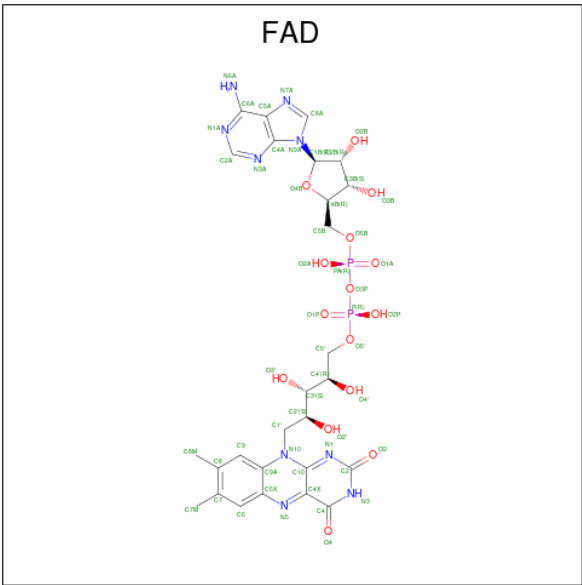
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	EMBL 13397863
D	772	ARG	GLY	conflict	EMBL 13397863
F	772	ARG	GLY	conflict	EMBL 13397863
H	772	ARG	GLY	conflict	EMBL 13397863

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

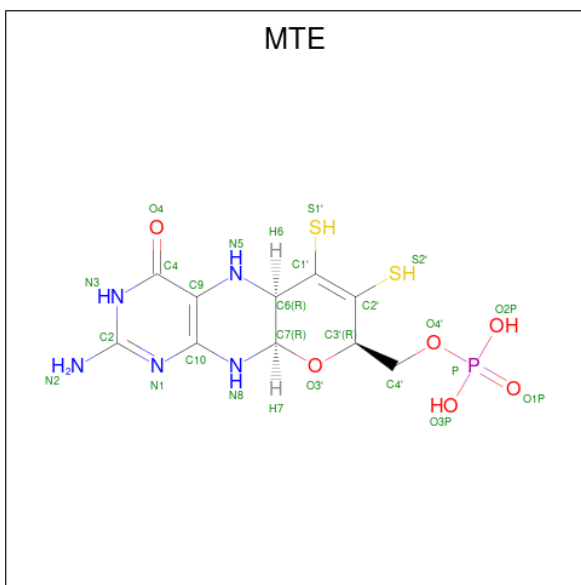


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

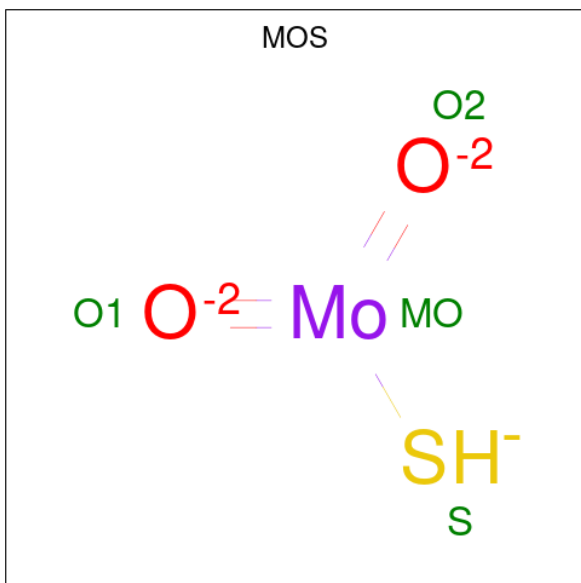
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).



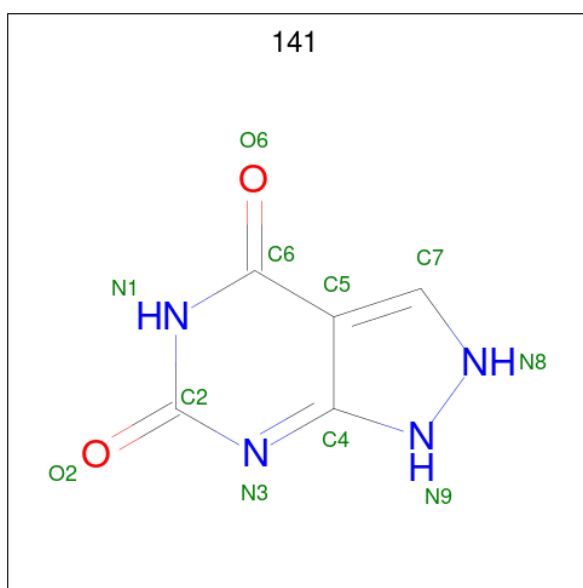
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	D	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	F	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	H	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_2S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	Mo	O	S	0	0
			3	1	1	1		
7	D	1	Total	Mo	O	S	0	0
			3	1	1	1		
7	F	1	Total	Mo	O	S	0	0
			3	1	1	1		
7	H	1	Total	Mo	O	S	0	0
			3	1	1	1		

- Molecule 8 is Oxypurinol (CCD ID: 141) (formula: $C_5H_4N_4O_2$).



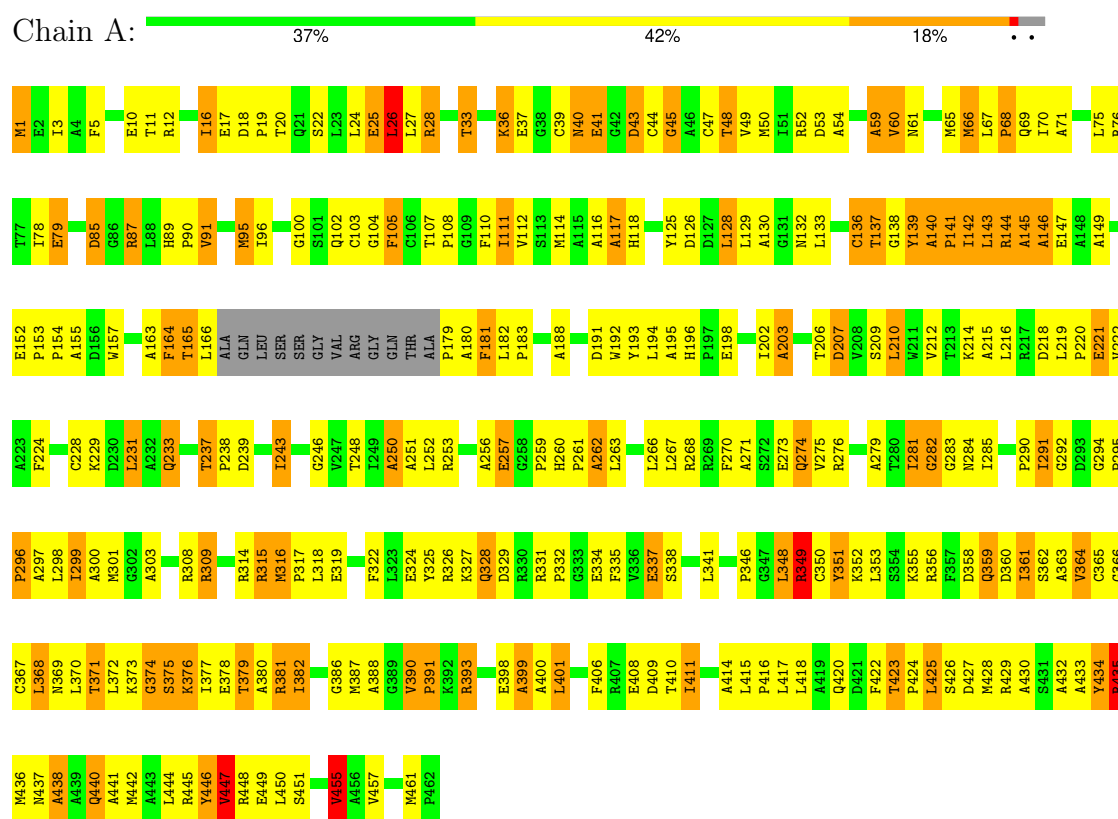
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	5	4	2		
8	D	1	Total	C	N	O	0	0
			11	5	4	2		
8	F	1	Total	C	N	O	0	0
			11	5	4	2		
8	H	1	Total	C	N	O	0	0
			11	5	4	2		

3 Residue-property plots

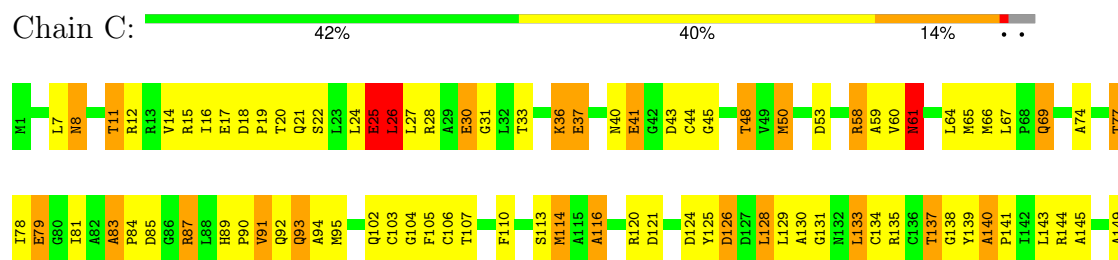
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

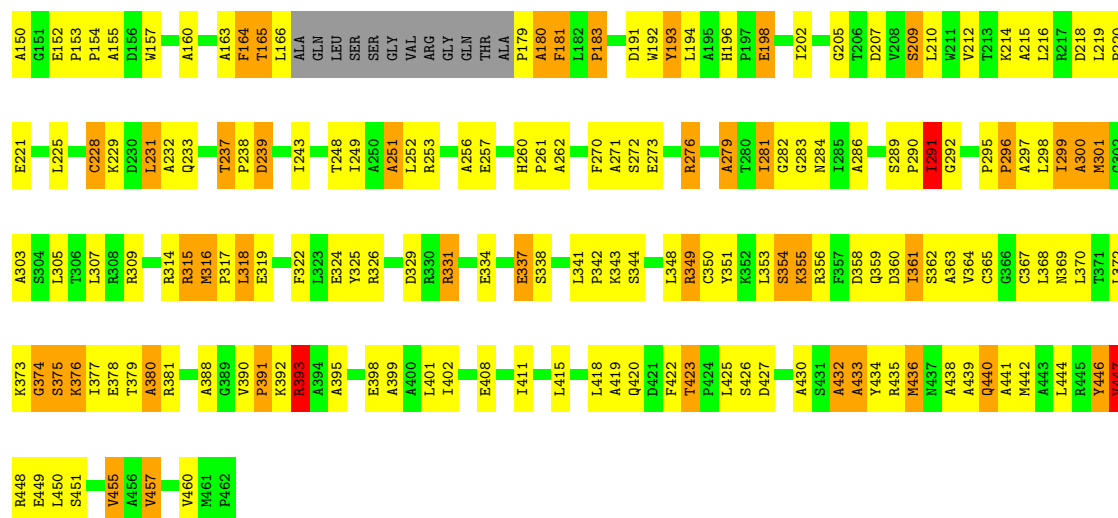
Note EDS was not executed.

• Molecule 1: xanthine dehydrogenase, chain A



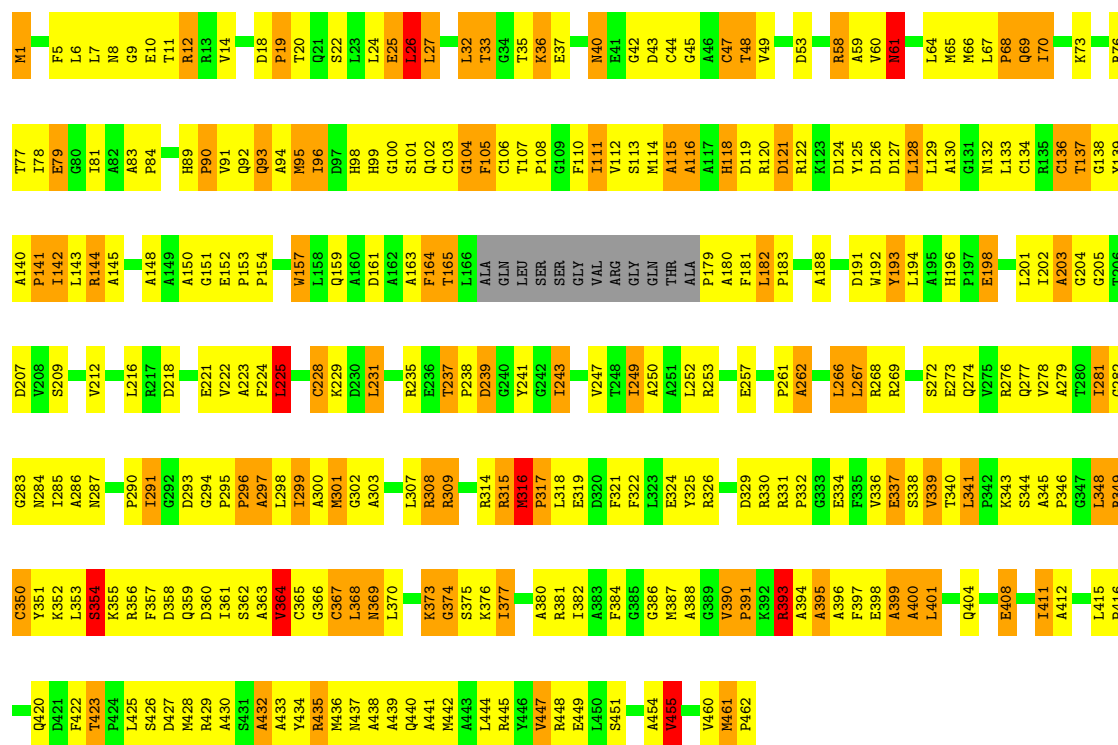
• Molecule 1: xanthine dehydrogenase, chain A





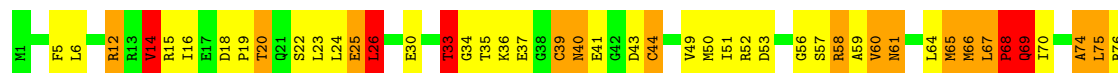
• Molecule 1: xanthine dehydrogenase, chain A

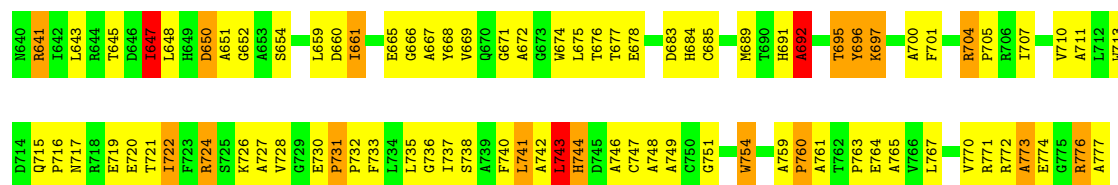
Chain E: 32% 45% 18%



• Molecule 1: xanthine dehydrogenase, chain A

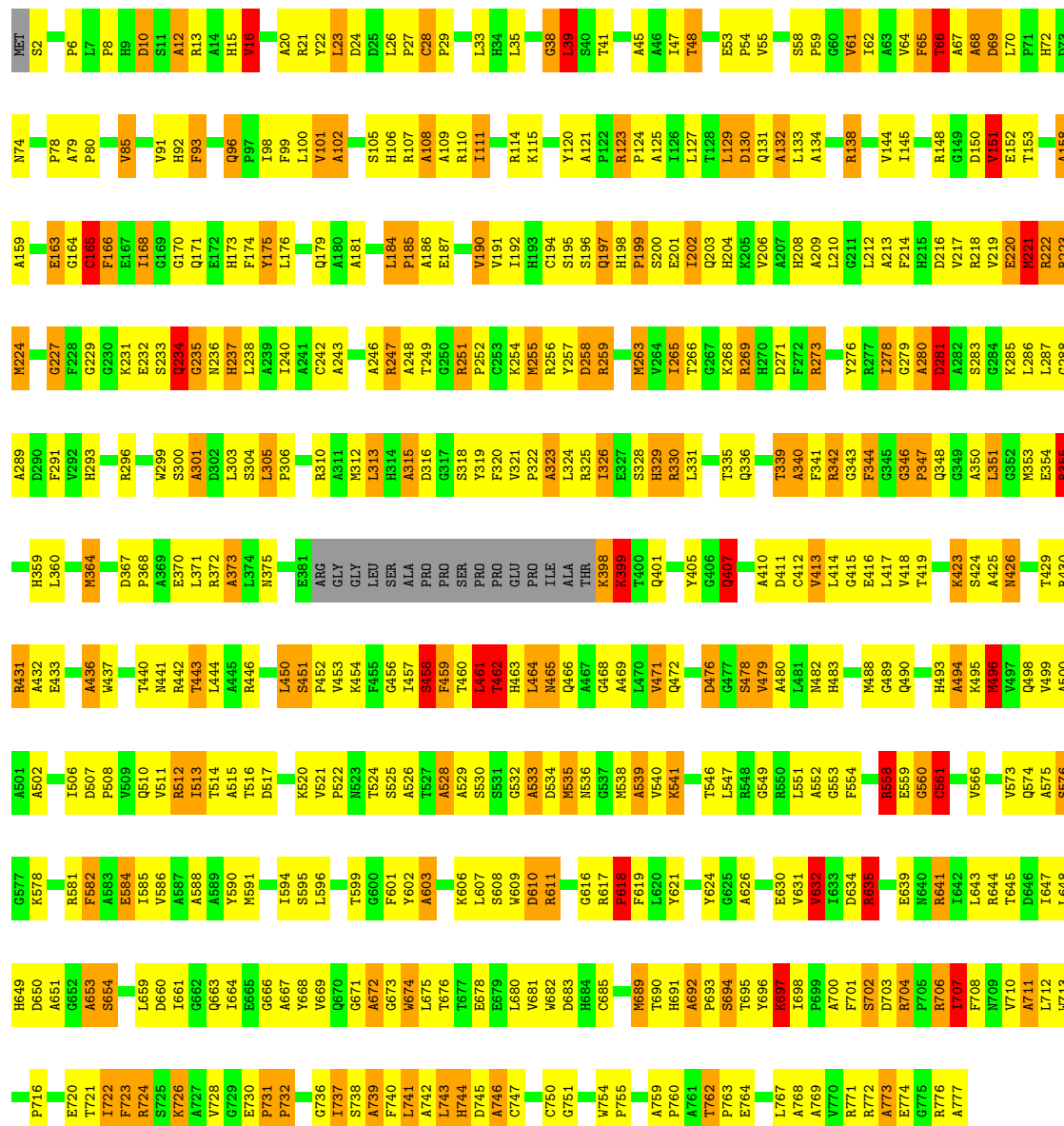
Chain G: 32% 43% 19%





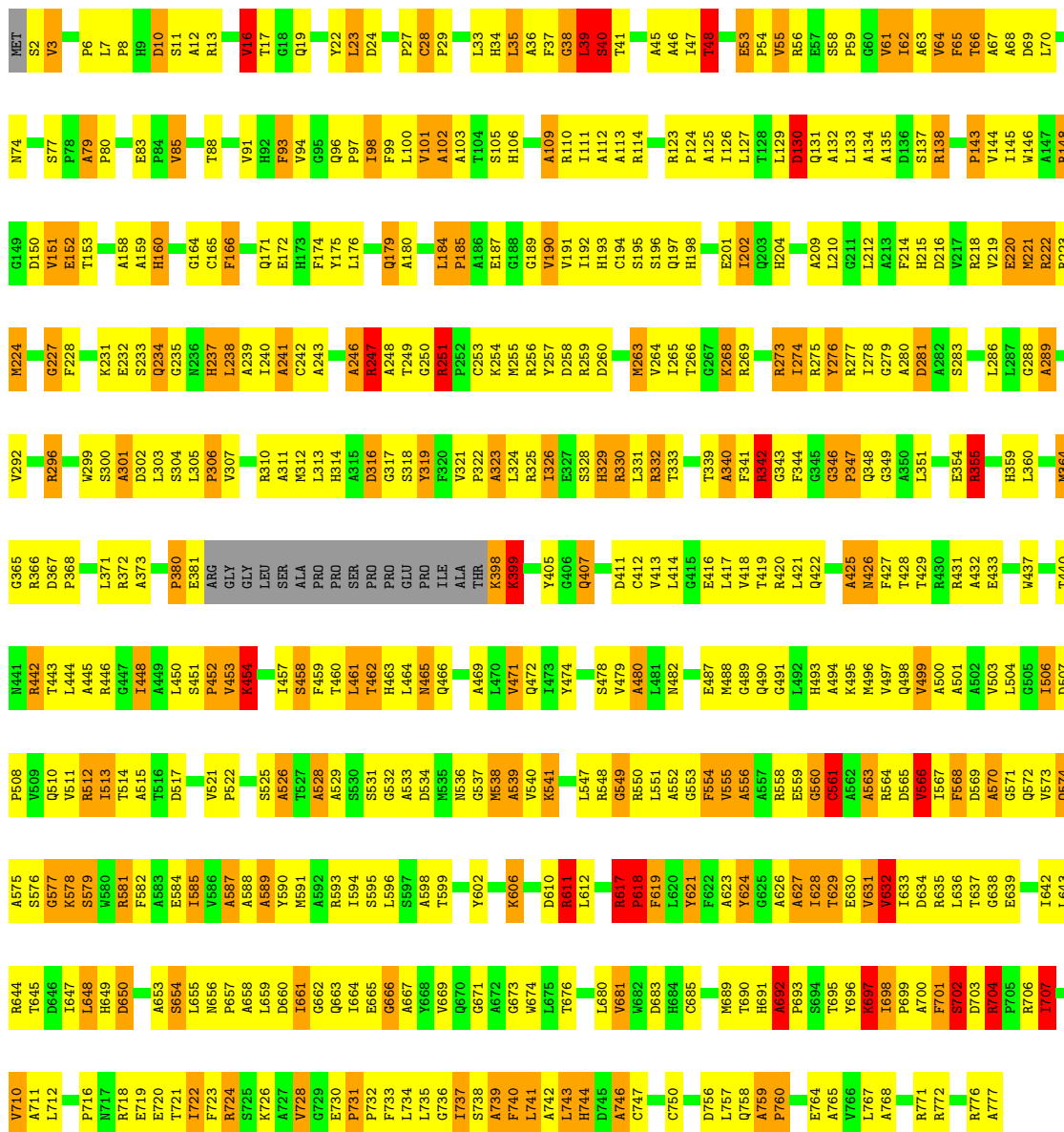
• Molecule 2: xanthine dehydrogenase, chain B

Chain D: 37% 42% 16% . .

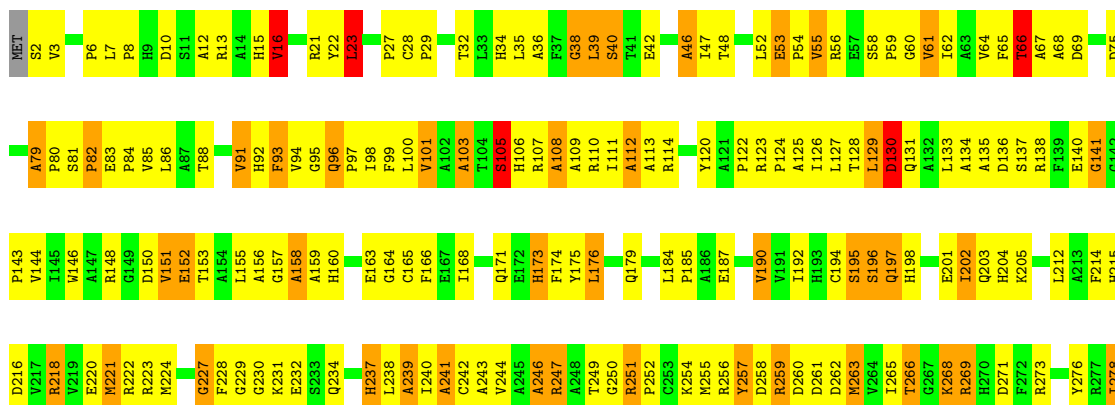


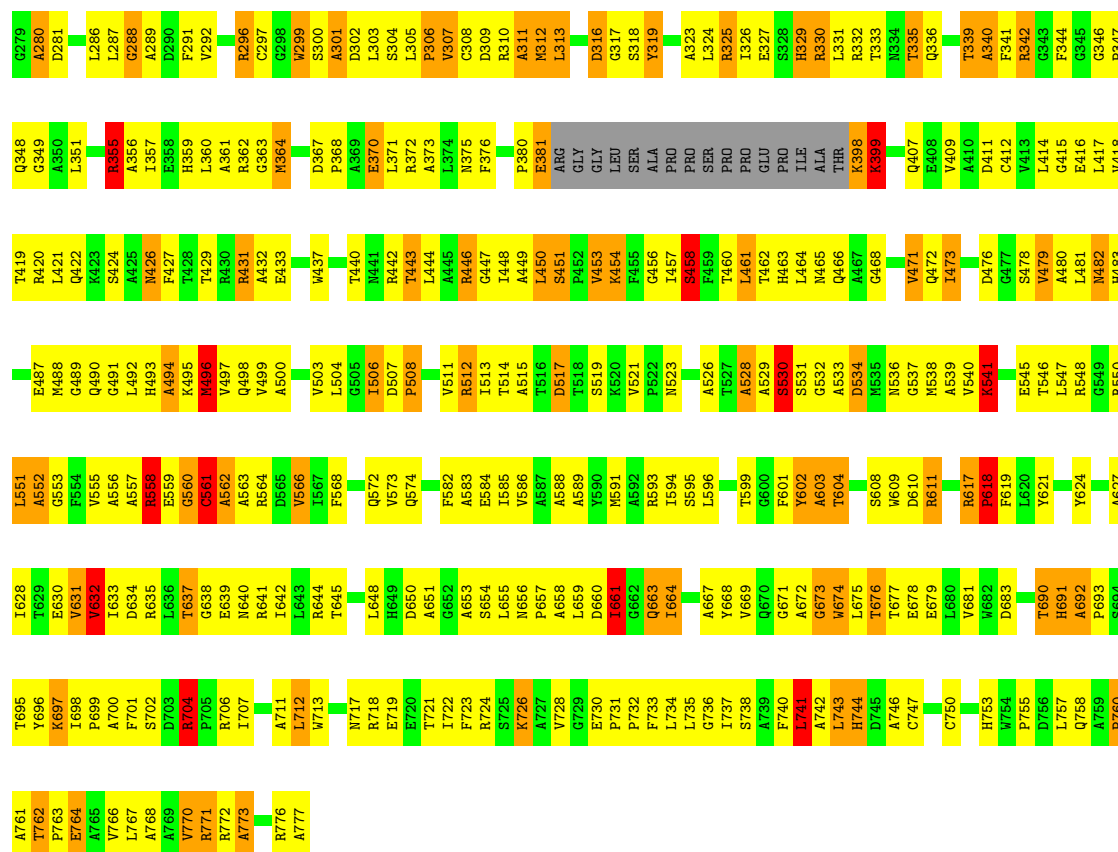
• Molecule 2: xanthine dehydrogenase, chain B

Chain F: 33% 45% 17% . .



- Molecule 2: xanthine dehydrogenase, chain B





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.62Å 140.73Å 157.66Å 109.59° 105.84° 101.25°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.1 (30.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.193 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36748	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MOS, 141, MTE, CA, FAD, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.60	43/3431 (1.3%)	1.72	64/4647 (1.4%)
1	C	1.98	74/3431 (2.2%)	1.72	67/4647 (1.4%)
1	E	1.64	40/3431 (1.2%)	1.77	62/4647 (1.3%)
1	G	1.50	31/3431 (0.9%)	1.76	73/4647 (1.6%)
2	B	1.88	115/5845 (2.0%)	1.87	146/7942 (1.8%)
2	D	2.02	159/5845 (2.7%)	1.87	124/7942 (1.6%)
2	F	1.85	111/5845 (1.9%)	1.88	145/7942 (1.8%)
2	H	1.75	82/5845 (1.4%)	1.85	146/7942 (1.8%)
All	All	1.81	655/37104 (1.8%)	1.82	827/50356 (1.6%)

All (655) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	521	VAL	CA-CB	-14.39	1.41	1.54
2	D	759	ALA	CA-CB	-12.55	1.36	1.53
2	B	16	VAL	CA-CB	-12.25	1.40	1.54
2	D	669	VAL	CA-CB	-11.86	1.41	1.54
2	B	321	VAL	CA-CB	-11.71	1.45	1.54
1	E	203	ALA	CA-C	-10.96	1.45	1.52
1	C	50	MET	SD-CE	-10.86	1.52	1.79
1	C	116	ALA	CA-CB	-10.78	1.35	1.53
1	A	140	ALA	CA-CB	-10.74	1.44	1.54
2	F	64	VAL	CA-CB	-10.69	1.40	1.54
2	B	312	MET	SD-CE	-10.53	1.53	1.79
2	D	364	MET	SD-CE	-10.43	1.53	1.79
2	D	219	VAL	CA-CB	-10.28	1.42	1.54
2	D	108	ALA	CA-CB	-10.00	1.37	1.53
2	D	689	MET	SD-CE	9.88	2.04	1.79
2	F	61	VAL	CA-CB	-9.66	1.42	1.54
2	B	3	VAL	CA-CB	-9.62	1.44	1.54
1	E	291	ILE	CA-CB	-9.61	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	528	ALA	CA-CB	-9.50	1.39	1.53
2	H	126	ILE	CA-CB	-9.36	1.42	1.53
2	H	307	VAL	CA-CB	-9.10	1.44	1.54
1	C	74	ALA	CA-CB	-9.05	1.40	1.53
1	A	355	LYS	CA-C	-9.01	1.41	1.52
2	B	515	ALA	CA-CB	-8.98	1.38	1.53
1	C	48	THR	C-O	-8.79	1.13	1.23
2	D	471	VAL	CA-CB	-8.77	1.42	1.54
1	G	361	ILE	CA-CB	-8.73	1.43	1.54
2	D	591	MET	C-O	-8.70	1.13	1.24
2	H	16	VAL	CA-CB	-8.67	1.42	1.54
1	A	107	THR	CA-CB	-8.66	1.39	1.53
2	D	255	MET	SD-CE	-8.65	1.57	1.79
1	C	442	MET	SD-CE	-8.61	1.58	1.79
2	B	219	VAL	C-O	-8.61	1.14	1.24
2	D	769	ALA	CA-CB	-8.59	1.39	1.53
2	D	515	ALA	CA-CB	-8.52	1.39	1.53
2	F	555	VAL	CA-CB	-8.49	1.43	1.54
2	H	259	ARG	CA-C	-8.49	1.41	1.52
2	F	55	VAL	CA-CB	-8.48	1.44	1.54
2	H	335	THR	CA-CB	-8.44	1.41	1.53
1	C	202	ILE	CA-CB	-8.43	1.43	1.54
2	D	109	ALA	CA-CB	-8.42	1.40	1.53
2	B	340	ALA	CA-CB	-8.40	1.40	1.53
2	D	12	ALA	CA-CB	-8.39	1.40	1.53
1	E	111	ILE	CA-CB	-8.37	1.43	1.54
2	D	10	ASP	C-O	-8.36	1.13	1.24
1	C	299	ILE	C-O	-8.35	1.14	1.24
1	C	262	ALA	CA-CB	-8.34	1.40	1.53
2	B	528	ALA	CA-CB	-8.30	1.40	1.53
1	C	202	ILE	C-O	-8.28	1.15	1.24
1	C	303	ALA	CA-C	-8.25	1.42	1.52
2	H	333	THR	CA-C	-8.25	1.42	1.52
2	F	224	MET	SD-CE	-8.22	1.58	1.79
2	D	224	MET	SD-CE	-8.15	1.59	1.79
1	E	461	MET	SD-CE	8.14	2.00	1.79
2	D	746	ALA	CA-CB	-8.13	1.40	1.53
2	F	585	ILE	CA-CB	-8.11	1.44	1.54
1	E	150	ALA	CA-CB	-8.09	1.40	1.53
2	H	651	ALA	CA-CB	-8.08	1.42	1.53
2	B	297	CYS	CA-C	-8.04	1.42	1.52
2	D	521	VAL	CA-CB	-8.03	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	98	ILE	C-O	-8.01	1.14	1.23
2	F	46	ALA	CA-CB	-8.01	1.41	1.53
1	C	137	THR	CA-CB	-7.99	1.42	1.54
2	H	604	THR	CA-CB	-7.97	1.38	1.53
2	F	48	THR	CA-CB	-7.93	1.42	1.54
2	F	219	VAL	CA-CB	-7.89	1.45	1.54
2	F	246	ALA	CA-CB	-7.81	1.41	1.53
2	B	108	ALA	CA-CB	-7.81	1.40	1.53
2	D	91	VAL	C-O	-7.81	1.16	1.24
2	B	61	VAL	CA-CB	-7.77	1.44	1.54
1	C	243	ILE	CA-CB	-7.75	1.45	1.54
2	B	586	VAL	CA-CB	-7.72	1.45	1.54
2	D	739	ALA	CA-CB	-7.72	1.41	1.53
2	D	535	MET	SD-CE	-7.71	1.60	1.79
2	F	65	PHE	CA-C	-7.71	1.43	1.52
2	F	525	SER	CA-C	-7.67	1.43	1.53
2	H	503	VAL	CA-CB	-7.64	1.44	1.54
2	H	32	THR	C-O	-7.64	1.14	1.23
2	H	311	ALA	CA-CB	-7.63	1.41	1.53
2	H	664	ILE	CA-CB	-7.62	1.45	1.54
1	G	114	MET	SD-CE	-7.62	1.60	1.79
2	H	471	VAL	CA-CB	-7.60	1.44	1.54
2	B	486	THR	CA-C	-7.60	1.43	1.52
2	B	409	VAL	CA-CB	-7.58	1.44	1.53
2	D	702	SER	C-O	-7.58	1.14	1.24
2	B	568	PHE	CA-C	-7.57	1.43	1.52
2	F	626	ALA	CA-CB	-7.56	1.40	1.53
2	F	28	CYS	N-CA	7.55	1.53	1.45
1	E	384	PHE	CA-C	-7.51	1.43	1.52
2	F	240	ILE	CA-CB	-7.50	1.45	1.54
2	D	246	ALA	CA-CB	-7.50	1.41	1.53
2	B	30	ALA	CA-CB	-7.48	1.41	1.53
2	B	240	ILE	CA-CB	-7.48	1.45	1.54
2	D	55	VAL	CA-CB	-7.47	1.45	1.54
2	F	499	VAL	CA-CB	-7.47	1.44	1.54
2	D	546	THR	CA-CB	-7.45	1.41	1.53
1	A	91	VAL	CA-CB	-7.43	1.45	1.54
2	D	61	VAL	CA-CB	-7.43	1.44	1.54
1	C	441	ALA	CA-CB	-7.43	1.41	1.53
2	D	243	ALA	CA-CB	-7.41	1.41	1.53
2	B	502	ALA	CA-CB	-7.41	1.41	1.53
2	D	339	THR	CA-CB	-7.39	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	669	VAL	CA-CB	-7.39	1.45	1.54
1	C	249	ILE	CA-CB	-7.39	1.45	1.54
1	C	150	ALA	CA-CB	-7.37	1.41	1.53
2	F	511	VAL	CA-CB	-7.36	1.45	1.54
2	B	156	ALA	CA-CB	-7.33	1.41	1.53
1	A	291	ILE	CA-CB	-7.32	1.46	1.54
2	B	357	ILE	CA-CB	-7.31	1.45	1.54
2	B	572	GLN	CA-C	-7.31	1.43	1.52
1	C	114	MET	SD-CE	-7.31	1.61	1.79
1	E	116	ALA	CA-CB	-7.30	1.41	1.53
2	D	20	ALA	CA-C	-7.30	1.43	1.52
2	B	192	ILE	CA-CB	-7.29	1.45	1.54
2	B	556	ALA	CA-CB	-7.29	1.42	1.53
2	F	340	ALA	CA-CB	-7.29	1.41	1.53
2	D	530	SER	CA-C	-7.26	1.43	1.53
2	B	573	VAL	CA-CB	-7.26	1.45	1.54
2	B	543	ALA	CA-CB	-7.25	1.41	1.53
1	A	5	PHE	CA-C	-7.22	1.44	1.52
1	A	149	ALA	CA-CB	-7.21	1.41	1.53
2	B	677	THR	CA-CB	-7.21	1.42	1.53
2	D	101	VAL	CA-CB	-7.20	1.45	1.54
2	F	202	ILE	CA-CB	-7.20	1.44	1.54
2	D	120	TYR	C-O	-7.20	1.14	1.23
2	H	594	ILE	CA-CB	-7.19	1.45	1.54
2	B	85	VAL	CA-CB	-7.19	1.45	1.54
2	H	220	GLU	CA-C	-7.19	1.43	1.52
2	D	499	VAL	CA-CB	-7.18	1.44	1.54
2	D	184	LEU	C-O	-7.18	1.18	1.25
2	F	85	VAL	CA-CB	-7.17	1.45	1.54
2	F	103	ALA	CA-CB	-7.17	1.42	1.53
1	A	28	ARG	CA-C	-7.14	1.43	1.52
2	H	146	TRP	CA-C	-7.14	1.44	1.52
2	B	257	TYR	C-O	-7.14	1.15	1.24
2	F	623	ALA	CA-C	-7.14	1.43	1.52
2	D	502	ALA	CA-CB	-7.11	1.41	1.53
1	E	115	ALA	CA-CB	-7.09	1.42	1.53
2	F	746	ALA	CA-CB	-7.07	1.42	1.53
2	B	132	ALA	CA-CB	-7.07	1.42	1.53
1	C	364	VAL	CA-CB	-7.03	1.45	1.54
1	G	81	ILE	CA-CB	-7.02	1.45	1.54
1	C	299	ILE	CA-CB	-7.02	1.46	1.54
2	F	742	ALA	CA-CB	-7.02	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	528	ALA	CA-CB	-7.02	1.42	1.53
2	B	585	ILE	CA-CB	-7.01	1.46	1.54
1	E	460	VAL	CA-CB	-7.00	1.45	1.54
1	C	228	CYS	CA-C	-7.00	1.45	1.53
2	D	190	VAL	CA-C	-6.99	1.44	1.52
1	E	49	VAL	C-O	6.98	1.31	1.23
2	D	762	THR	CA-CB	-6.98	1.42	1.53
2	B	94	VAL	CA-C	-6.97	1.44	1.52
2	B	109	ALA	CA-CB	-6.97	1.42	1.53
2	B	202	ILE	CA-CB	-6.92	1.45	1.54
2	F	731	PRO	CA-CB	-6.92	1.44	1.54
2	B	64	VAL	C-O	-6.91	1.17	1.24
2	D	710	VAL	CA-CB	-6.91	1.46	1.54
2	B	570	ALA	CA-CB	-6.91	1.42	1.53
1	G	411	ILE	CA-CB	-6.90	1.46	1.54
1	E	48	THR	CA-CB	-6.90	1.42	1.53
2	B	168	ILE	CA-CB	-6.89	1.45	1.54
2	D	221	MET	SD-CE	-6.89	1.62	1.79
2	F	697	LYS	C-O	6.87	1.31	1.23
2	H	289	ALA	CA-CB	-6.85	1.42	1.53
2	B	647	ILE	CA-C	-6.85	1.44	1.52
2	F	239	ALA	CA-CB	-6.84	1.42	1.53
2	D	323	ALA	CA-CB	-6.83	1.40	1.53
1	E	91	VAL	CA-CB	-6.83	1.46	1.54
2	D	528	ALA	CA-CB	-6.82	1.43	1.53
2	B	146	TRP	CA-C	-6.80	1.44	1.52
2	D	413	VAL	CA-CB	-6.80	1.45	1.54
2	D	731	PRO	CA-CB	-6.79	1.44	1.54
2	B	20	ALA	CA-CB	-6.77	1.42	1.53
2	H	515	ALA	CA-CB	-6.77	1.42	1.53
2	D	85	VAL	CA-CB	-6.76	1.45	1.54
2	H	541	LYS	CA-C	-6.76	1.44	1.52
2	B	773	ALA	CA-CB	-6.73	1.42	1.53
2	F	47	ILE	CA-CB	-6.73	1.46	1.54
2	B	408	GLU	C-O	-6.72	1.15	1.23
2	H	677	THR	CA-CB	-6.71	1.43	1.54
2	D	340	ALA	CA-CB	-6.70	1.42	1.53
1	G	95	MET	SD-CE	-6.69	1.62	1.79
2	F	16	VAL	CA-CB	-6.68	1.45	1.54
1	A	140	ALA	N-CA	-6.68	1.39	1.46
2	F	425	ALA	CA-CB	-6.66	1.41	1.53
2	H	94	VAL	CA-C	-6.66	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	483	HIS	CA-CB	-6.66	1.45	1.53
2	B	184	LEU	C-O	-6.66	1.19	1.25
2	B	552	ALA	CA-CB	-6.66	1.42	1.53
2	D	708	PHE	CA-C	-6.65	1.45	1.53
2	B	221	MET	SD-CE	-6.64	1.62	1.79
1	A	66	MET	SD-CE	-6.64	1.62	1.79
2	D	539	ALA	CA-CB	-6.64	1.42	1.53
1	C	433	ALA	CA-CB	-6.64	1.43	1.53
1	G	249	ILE	CA-CB	-6.63	1.46	1.54
2	D	240	ILE	CA-CB	-6.63	1.46	1.54
1	C	253	ARG	CA-C	-6.62	1.44	1.52
1	A	299	ILE	CA-CB	-6.62	1.46	1.54
1	C	380	ALA	CA-CB	-6.62	1.43	1.52
2	F	326	ILE	CA-CB	-6.61	1.46	1.54
2	B	540	VAL	CA-CB	-6.61	1.46	1.54
1	C	232	ALA	CA-CB	-6.61	1.44	1.53
2	D	28	CYS	C-O	-6.59	1.17	1.24
2	D	344	PHE	C-O	-6.59	1.15	1.24
2	H	631	VAL	CA-CB	-6.59	1.46	1.54
2	D	443	THR	CA-CB	-6.59	1.44	1.53
1	E	316	MET	SD-CE	6.58	1.96	1.79
2	H	108	ALA	CA-CB	-6.58	1.42	1.53
2	H	109	ALA	CA-CB	-6.56	1.43	1.53
2	D	64	VAL	C-O	-6.56	1.17	1.24
1	E	202	ILE	CA-CB	-6.55	1.46	1.54
2	D	460	THR	C-O	-6.55	1.15	1.24
2	F	689	MET	SD-CE	6.55	1.96	1.79
2	D	305	LEU	N-CA	-6.53	1.41	1.46
2	F	151	VAL	CA-CB	-6.52	1.46	1.54
2	B	692	ALA	CA-CB	-6.50	1.43	1.53
2	D	123	ARG	CA-CB	-6.50	1.46	1.53
1	C	290	PRO	CA-C	-6.50	1.46	1.52
2	B	134	ALA	CA-CB	-6.49	1.43	1.53
2	D	263	MET	SD-CE	-6.49	1.63	1.79
2	F	125	ALA	CA-CB	-6.48	1.42	1.53
2	B	418	VAL	CA-CB	-6.48	1.46	1.54
2	H	55	VAL	CA-CB	-6.48	1.46	1.54
2	D	502	ALA	CA-C	-6.47	1.44	1.52
2	F	45	ALA	CA-CB	-6.47	1.42	1.53
1	C	180	ALA	CA-CB	-6.46	1.42	1.53
2	F	739	ALA	CA-CB	-6.45	1.43	1.53
1	C	291	ILE	CA-CB	-6.44	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	74	ALA	CA-CB	-6.44	1.41	1.53
2	B	467	ALA	CA-CB	-6.44	1.42	1.53
1	A	116	ALA	CA-CB	-6.42	1.42	1.53
2	F	728	VAL	CA-CB	-6.42	1.45	1.54
1	E	361	ILE	CA-CB	-6.41	1.46	1.54
2	B	206	VAL	CA-CB	-6.41	1.46	1.54
2	D	168	ILE	CA-CB	-6.41	1.46	1.54
2	D	209	ALA	CA-C	-6.41	1.44	1.52
1	C	91	VAL	CA-CB	-6.40	1.46	1.54
1	C	423	THR	CA-CB	-6.40	1.44	1.53
2	D	460	THR	CA-C	-6.40	1.44	1.52
2	D	573	VAL	CA-CB	-6.39	1.46	1.54
2	H	61	VAL	CA-CB	-6.39	1.46	1.54
2	F	759	ALA	CA-CB	-6.38	1.40	1.54
2	H	712	LEU	CA-C	-6.38	1.44	1.52
2	D	209	ALA	C-O	-6.38	1.15	1.24
2	B	475	THR	C-O	-6.38	1.15	1.24
2	B	533	ALA	CA-CB	-6.38	1.43	1.53
1	C	107	THR	CA-CB	-6.38	1.43	1.53
2	F	184	LEU	C-O	-6.38	1.19	1.25
1	C	37	GLU	C-O	-6.38	1.16	1.24
2	B	711	ALA	CA-CB	-6.37	1.41	1.54
2	H	79	ALA	CA-CB	-6.37	1.46	1.53
2	D	217	VAL	C-O	-6.36	1.17	1.24
2	F	12	ALA	CA-CB	-6.36	1.43	1.53
2	F	453	VAL	CA-CB	-6.36	1.45	1.54
1	A	59	ALA	CA-CB	-6.35	1.42	1.53
2	D	524	THR	CA-CB	-6.35	1.43	1.53
1	G	441	ALA	CA-CB	-6.34	1.43	1.53
1	C	251	ALA	CA-CB	-6.34	1.43	1.53
2	B	453	VAL	CA-C	-6.33	1.44	1.52
1	A	50	MET	SD-CE	-6.33	1.63	1.79
1	C	438	ALA	CA-CB	-6.33	1.43	1.53
2	D	202	ILE	CA-CB	-6.32	1.46	1.54
2	D	213	ALA	CA-CB	-6.31	1.43	1.53
2	F	499	VAL	CA-C	-6.31	1.44	1.52
1	C	440	GLN	N-CA	-6.29	1.38	1.46
2	F	599	THR	CA-CB	-6.29	1.44	1.53
1	A	382	ILE	CA-CB	-6.28	1.46	1.54
2	B	64	VAL	CA-CB	-6.27	1.44	1.55
2	F	737	ILE	CA-CB	-6.26	1.46	1.54
1	A	71	ALA	CA-CB	-6.25	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	473	ILE	CA-CB	-6.24	1.46	1.53
2	D	711	ALA	CA-CB	-6.23	1.41	1.54
1	E	136	CYS	CA-C	6.23	1.60	1.52
2	B	307	VAL	CA-CB	-6.22	1.47	1.54
1	A	352	LYS	CA-C	-6.22	1.45	1.52
1	E	243	ILE	CA-CB	-6.21	1.46	1.53
1	C	140	ALA	CA-CB	-6.21	1.43	1.53
2	H	246	ALA	CA-CB	-6.21	1.43	1.53
1	C	61	ASN	C-O	-6.20	1.16	1.24
1	E	411	ILE	CA-CB	-6.20	1.47	1.54
2	F	563	ALA	CA-CB	-6.20	1.43	1.53
2	F	692	ALA	CA-CB	-6.19	1.43	1.53
2	F	568	PHE	CA-C	-6.19	1.45	1.52
1	A	351	TYR	C-O	6.19	1.31	1.24
2	F	364	MET	SD-CE	-6.18	1.64	1.79
2	D	220	GLU	CA-C	-6.18	1.45	1.52
1	A	111	ILE	CA-CB	-6.17	1.47	1.54
1	A	70	ILE	CA-C	-6.17	1.44	1.52
2	F	265	ILE	CA-CB	-6.17	1.45	1.54
2	H	212	LEU	CA-C	-6.16	1.45	1.52
2	H	263	MET	SD-CE	-6.14	1.64	1.79
2	F	3	VAL	CA-CB	-6.13	1.47	1.54
1	E	364	VAL	CA-CB	-6.13	1.46	1.54
1	C	362	SER	CA-C	-6.13	1.44	1.52
1	C	355	LYS	CA-C	-6.12	1.44	1.52
2	D	419	THR	C-O	-6.12	1.17	1.24
1	A	438	ALA	CA-CB	-6.11	1.43	1.53
2	F	506	ILE	C-O	-6.11	1.16	1.24
1	A	219	LEU	CA-C	-6.11	1.46	1.52
2	D	480	ALA	CA-C	-6.10	1.45	1.52
2	F	101	VAL	CA-CB	-6.10	1.46	1.54
2	F	135	ALA	CA-CB	-6.10	1.43	1.53
2	H	64	VAL	CA-CB	-6.10	1.44	1.55
2	H	339	THR	CA-CB	-6.09	1.46	1.54
2	H	47	ILE	CA-C	-6.09	1.45	1.52
1	C	411	ILE	CA-CB	-6.09	1.46	1.54
2	D	258	ASP	CB-CG	-6.08	1.36	1.52
2	D	672	ALA	CA-CB	-6.07	1.43	1.53
1	G	145	ALA	CA-CB	6.06	1.62	1.53
2	H	292	VAL	CA-CB	-6.06	1.46	1.54
2	D	305	LEU	C-O	-6.05	1.19	1.24
1	E	281	ILE	CA-CB	-6.05	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	486	THR	C-O	-6.05	1.16	1.23
1	E	282	GLY	C-O	6.04	1.32	1.23
2	B	707	ILE	CA-CB	-6.04	1.46	1.54
2	D	654	SER	C-O	-6.02	1.16	1.23
2	H	243	ALA	CA-CB	-6.01	1.44	1.53
1	A	146	ALA	CA-CB	-6.01	1.44	1.53
2	H	3	VAL	CA-CB	-6.00	1.48	1.54
1	G	291	ILE	CA-CB	-6.00	1.47	1.54
2	B	47	ILE	CA-CB	-5.99	1.46	1.54
2	B	334	ASN	CA-C	-5.99	1.46	1.53
2	H	479	VAL	CA-CB	-5.98	1.46	1.54
2	F	710	VAL	CA-CB	-5.98	1.47	1.54
1	C	77	THR	CA-CB	-5.97	1.44	1.53
2	B	98	ILE	CA-C	-5.97	1.46	1.53
2	H	15	HIS	N-CA	-5.97	1.39	1.46
2	B	126	ILE	CA-CB	-5.97	1.46	1.53
2	B	546	THR	CA-CB	-5.97	1.44	1.53
2	D	111	ILE	N-CA	-5.96	1.39	1.46
2	B	325	ARG	CA-C	5.94	1.59	1.52
2	B	289	ALA	CA-CB	-5.94	1.43	1.53
1	C	430	ALA	CA-CB	-5.94	1.43	1.53
2	F	469	ALA	CA-C	-5.94	1.45	1.52
1	C	270	PHE	CA-C	-5.93	1.45	1.52
2	D	459	PHE	C-O	-5.92	1.16	1.23
2	F	480	ALA	CA-C	-5.92	1.45	1.52
2	B	67	ALA	CA-CB	-5.92	1.44	1.53
2	D	242	CYS	N-CA	-5.91	1.39	1.46
2	D	754	TRP	CA-C	-5.91	1.45	1.52
1	E	47	CYS	CA-C	-5.91	1.45	1.52
2	D	145	ILE	CA-CB	-5.91	1.47	1.54
2	D	186	ALA	CA-CB	-5.89	1.43	1.52
2	F	11	SER	C-O	5.88	1.32	1.23
2	H	451	SER	CA-C	-5.88	1.46	1.52
1	A	48	THR	C-O	-5.87	1.16	1.23
2	H	91	VAL	CA-CB	-5.86	1.46	1.54
2	H	453	VAL	CA-CB	-5.86	1.46	1.54
1	A	142	ILE	CA-CB	-5.85	1.46	1.54
2	F	16	VAL	C-O	5.85	1.31	1.24
2	D	558	ARG	C-O	-5.84	1.17	1.24
2	F	263	MET	SD-CE	-5.84	1.65	1.79
2	D	410	ALA	CA-C	-5.83	1.45	1.52
2	D	469	ALA	CA-C	-5.83	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	79	ALA	C-O	-5.82	1.18	1.24
2	D	41	THR	CA-C	-5.81	1.45	1.52
2	H	506	ILE	CA-CB	-5.81	1.46	1.54
2	F	248	ALA	C-O	-5.81	1.17	1.24
1	G	39	CYS	CA-C	-5.81	1.45	1.52
1	G	5	PHE	CA-C	-5.80	1.45	1.52
2	B	217	VAL	CA-CB	-5.80	1.47	1.54
1	C	110	PHE	C-O	-5.80	1.17	1.24
2	F	654	SER	C-O	-5.80	1.16	1.23
2	D	694	SER	C-O	-5.80	1.16	1.24
1	G	116	ALA	CA-CB	-5.80	1.43	1.53
2	F	102	ALA	CA-CB	-5.79	1.44	1.53
2	B	514	THR	CA-CB	-5.79	1.44	1.53
2	D	726	LYS	C-O	-5.79	1.16	1.23
2	D	248	ALA	C-O	-5.76	1.17	1.24
1	C	16	ILE	C-O	-5.75	1.18	1.24
1	C	380	ALA	CA-C	-5.75	1.47	1.53
1	C	18	ASP	C-O	-5.74	1.19	1.25
2	H	266	THR	CA-C	-5.74	1.45	1.53
2	H	292	VAL	C-O	5.74	1.30	1.24
2	B	408	GLU	CA-C	-5.72	1.45	1.52
2	B	695	THR	C-O	-5.72	1.16	1.24
1	E	59	ALA	CA-CB	-5.71	1.44	1.53
2	B	369	ALA	CA-CB	-5.71	1.44	1.53
2	H	62	ILE	CA-CB	-5.71	1.47	1.54
1	E	299	ILE	C-O	-5.69	1.17	1.24
2	B	111	ILE	CA-CB	-5.69	1.46	1.54
1	A	435	ARG	N-CA	-5.69	1.39	1.46
2	H	511	VAL	CA-CB	-5.69	1.47	1.54
2	D	626	ALA	CA-CB	-5.68	1.43	1.53
2	F	333	THR	CA-C	-5.67	1.45	1.52
2	B	43	ALA	CA-CB	-5.67	1.44	1.53
2	B	514	THR	CA-C	-5.66	1.45	1.52
2	D	47	ILE	CA-C	-5.66	1.45	1.52
2	D	65	PHE	CA-C	-5.66	1.45	1.52
2	B	566	VAL	CA-CB	-5.65	1.47	1.54
2	D	737	ILE	CA-CB	-5.64	1.46	1.54
2	F	251	ARG	N-CA	-5.64	1.42	1.46
1	G	348	LEU	CA-C	-5.64	1.45	1.52
2	F	249	THR	CA-CB	-5.64	1.43	1.53
2	D	208	HIS	N-CA	-5.63	1.39	1.46
1	A	363	ALA	CA-C	-5.63	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	326	ILE	CA-CB	-5.62	1.47	1.54
2	H	340	ALA	CA-CB	-5.62	1.44	1.53
1	A	262	ALA	CA-CB	-5.62	1.44	1.53
1	E	428	MET	SD-CE	5.62	1.93	1.79
2	F	323	ALA	CA-CB	-5.62	1.42	1.53
2	H	98	ILE	C-O	-5.62	1.17	1.24
2	H	447	GLY	C-O	5.62	1.31	1.23
2	B	478	SER	CA-C	-5.61	1.45	1.53
2	B	550	ARG	NE-CZ	-5.61	1.26	1.33
2	B	98	ILE	CA-CB	-5.61	1.47	1.54
1	G	383	ALA	CA-CB	-5.61	1.44	1.53
1	C	286	ALA	CA-CB	-5.60	1.44	1.53
1	C	361	ILE	CA-CB	-5.60	1.47	1.54
2	B	540	VAL	N-CA	-5.60	1.39	1.46
2	B	759	ALA	CA-C	-5.60	1.46	1.52
1	C	457	VAL	CA-CB	-5.60	1.46	1.54
1	C	299	ILE	CA-C	-5.60	1.46	1.52
2	F	460	THR	C-O	-5.59	1.16	1.24
2	B	453	VAL	CA-CB	-5.59	1.47	1.54
2	B	502	ALA	CA-C	-5.59	1.45	1.52
2	F	474	TYR	CA-C	5.59	1.60	1.53
2	B	103	ALA	CA-CB	-5.58	1.45	1.53
1	G	142	ILE	CA-CB	-5.58	1.46	1.54
2	H	691	HIS	C-O	5.58	1.29	1.23
2	B	105	SER	CA-C	5.57	1.59	1.52
1	E	262	ALA	CA-CB	-5.57	1.44	1.53
2	D	566	VAL	CA-CB	-5.57	1.47	1.54
1	C	395	ALA	CA-CB	-5.56	1.44	1.53
2	F	598	ALA	N-CA	5.56	1.52	1.45
2	B	339	THR	CA-CB	-5.56	1.47	1.54
2	B	134	ALA	CA-C	-5.55	1.45	1.52
2	D	482	ASN	CA-C	-5.55	1.45	1.52
2	D	48	THR	CA-CB	-5.54	1.45	1.53
1	C	402	ILE	CA-CB	-5.54	1.48	1.54
2	F	109	ALA	CA-CB	-5.54	1.44	1.53
2	H	599	THR	CA-C	-5.54	1.46	1.52
2	F	490	GLN	CA-C	-5.53	1.44	1.52
2	D	68	ALA	CA-CB	-5.53	1.44	1.53
1	A	60	VAL	CA-CB	-5.53	1.46	1.54
2	F	289	ALA	CA-CB	-5.53	1.44	1.53
2	F	36	ALA	CA-CB	-5.52	1.44	1.53
2	F	191	VAL	CA-CB	-5.52	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411	ILE	CA-CB	-5.51	1.48	1.54
1	C	438	ALA	CA-C	-5.51	1.45	1.52
1	G	19	PRO	CA-C	-5.50	1.47	1.52
2	D	316	ASP	CA-C	-5.50	1.45	1.52
2	F	238	LEU	C-O	5.50	1.30	1.24
1	A	16	ILE	C-O	-5.50	1.18	1.24
2	D	8	PRO	C-O	-5.49	1.17	1.23
2	D	373	ALA	CA-C	-5.49	1.45	1.52
1	G	60	VAL	CA-CB	-5.49	1.45	1.55
2	F	190	VAL	CA-C	-5.48	1.46	1.52
2	F	623	ALA	CA-CB	-5.48	1.45	1.53
1	C	261	PRO	C-O	-5.47	1.17	1.24
2	D	773	ALA	CA-CB	-5.47	1.44	1.53
2	B	525	SER	CA-C	-5.47	1.45	1.53
2	D	364	MET	CG-SD	5.46	1.94	1.80
1	G	90	PRO	CA-C	-5.46	1.44	1.52
2	B	511	VAL	C-O	-5.46	1.18	1.24
2	B	512	ARG	NE-CZ	-5.46	1.27	1.33
2	H	36	ALA	CA-CB	-5.46	1.44	1.53
2	D	96	GLN	CA-C	-5.45	1.46	1.53
2	D	287	LEU	CA-C	-5.44	1.47	1.52
2	D	768	ALA	CA-CB	-5.44	1.44	1.53
2	F	40	SER	C-O	-5.43	1.17	1.23
2	H	103	ALA	CA-CB	-5.43	1.45	1.53
1	A	133	LEU	CA-C	-5.43	1.45	1.52
2	F	248	ALA	CA-CB	-5.42	1.44	1.53
2	D	269	ARG	CA-C	-5.42	1.46	1.52
2	F	454	LYS	N-CA	-5.42	1.39	1.46
2	D	16	VAL	CA-CB	-5.41	1.47	1.54
2	B	212	LEU	C-O	-5.41	1.17	1.24
2	B	451	SER	CA-C	-5.41	1.47	1.52
2	H	603	ALA	CA-C	-5.41	1.46	1.52
1	C	149	ALA	CA-C	-5.40	1.45	1.52
1	E	356	ARG	NE-CZ	-5.38	1.27	1.33
2	B	672	ALA	CA-CB	-5.38	1.45	1.53
2	D	15	HIS	N-CA	-5.37	1.40	1.46
1	G	65	MET	SD-CE	5.37	1.93	1.79
1	C	276	ARG	NE-CZ	-5.37	1.27	1.33
2	B	567	ILE	CA-CB	-5.37	1.47	1.54
2	F	587	ALA	CA-CB	-5.36	1.45	1.53
2	D	48	THR	CA-C	-5.36	1.45	1.52
2	H	168	ILE	CA-CB	-5.36	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	654	SER	C-O	-5.36	1.17	1.23
2	D	468	GLY	C-O	-5.36	1.15	1.23
1	G	271	ALA	C-O	5.35	1.29	1.24
1	C	48	THR	CA-C	-5.34	1.45	1.52
1	A	137	THR	CA-CB	-5.34	1.45	1.54
1	G	363	ALA	CA-C	-5.34	1.46	1.52
2	H	278	ILE	CA-CB	-5.33	1.47	1.55
2	F	702	SER	C-O	-5.33	1.17	1.24
1	E	301	MET	CG-SD	5.32	1.94	1.80
2	D	607	LEU	CA-C	-5.32	1.46	1.52
2	B	632	VAL	CA-C	-5.32	1.46	1.52
1	C	66	MET	SD-CE	-5.32	1.66	1.79
1	C	301	MET	C-O	-5.32	1.17	1.24
2	D	703	ASP	CA-C	-5.32	1.45	1.52
2	F	48	THR	CA-C	-5.32	1.45	1.52
1	G	382	ILE	CA-CB	-5.32	1.47	1.54
2	H	409	VAL	CA-CB	-5.32	1.47	1.54
2	D	132	ALA	CA-CB	-5.31	1.44	1.53
1	A	145	ALA	C-O	-5.31	1.18	1.24
2	F	190	VAL	CA-CB	-5.31	1.46	1.54
2	F	469	ALA	CA-CB	-5.31	1.44	1.53
1	A	282	GLY	C-O	5.30	1.29	1.23
1	C	83	ALA	CA-CB	-5.30	1.45	1.53
2	D	424	SER	C-O	-5.30	1.17	1.24
1	G	455	VAL	CA-CB	-5.30	1.47	1.54
1	E	367	CYS	CA-C	-5.30	1.46	1.52
2	D	26	LEU	C-O	-5.30	1.17	1.24
2	D	496	MET	SD-CE	-5.30	1.66	1.79
2	B	241	ALA	C-O	-5.30	1.18	1.24
2	D	125	ALA	CA-CB	-5.29	1.41	1.53
2	H	599	THR	CA-CB	-5.29	1.45	1.53
1	A	455	VAL	CA-CB	-5.29	1.47	1.54
1	E	32	LEU	C-O	5.28	1.30	1.23
1	A	203	ALA	CA-C	-5.28	1.45	1.52
1	C	243	ILE	CA-C	-5.28	1.46	1.52
2	D	181	ALA	CA-C	-5.28	1.46	1.52
1	C	289	SER	C-O	-5.28	1.17	1.23
2	H	762	THR	CA-CB	-5.28	1.45	1.53
2	D	102	ALA	CA-CB	-5.27	1.45	1.53
2	D	249	THR	CA-CB	-5.27	1.44	1.53
2	D	653	ALA	CA-CB	-5.27	1.45	1.52
2	F	209	ALA	C-O	-5.27	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PHE	C-O	-5.27	1.17	1.23
1	C	155	ALA	CA-CB	-5.26	1.45	1.53
1	C	364	VAL	CA-C	-5.26	1.46	1.52
2	D	66	THR	C-O	-5.26	1.17	1.23
2	D	33	LEU	C-O	5.26	1.30	1.23
1	G	338	SER	CA-C	-5.26	1.46	1.52
2	B	330	ARG	C-O	5.24	1.29	1.23
2	F	160	HIS	CA-C	-5.24	1.46	1.52
1	C	152	GLU	CA-C	-5.24	1.46	1.52
1	C	436	MET	SD-CE	-5.23	1.66	1.79
2	F	589	ALA	C-O	5.23	1.30	1.24
2	D	326	ILE	N-CA	-5.23	1.40	1.46
1	E	81	ILE	C-O	-5.23	1.17	1.24
2	F	253	CYS	CA-C	-5.23	1.46	1.52
1	G	70	ILE	CA-C	-5.23	1.45	1.52
1	A	461	MET	SD-CE	5.23	1.92	1.79
2	H	443	THR	CA-CB	-5.22	1.46	1.53
2	B	190	VAL	CA-CB	-5.22	1.46	1.54
1	E	365	CYS	C-O	-5.22	1.17	1.24
2	D	21	ARG	CA-C	-5.21	1.46	1.52
2	H	496	MET	SD-CE	-5.21	1.66	1.79
1	E	148	ALA	C-O	-5.21	1.17	1.24
1	E	281	ILE	CA-C	-5.20	1.45	1.52
1	G	262	ALA	CA-CB	-5.20	1.45	1.53
2	H	523	ASN	CA-C	-5.20	1.46	1.53
2	F	445	ALA	CA-CB	-5.20	1.44	1.53
2	F	566	VAL	CA-CB	-5.20	1.47	1.54
1	A	243	ILE	CA-CB	-5.20	1.47	1.54
1	C	365	CYS	C-O	-5.19	1.18	1.24
2	H	134	ALA	CA-CB	-5.19	1.45	1.53
2	D	619	PHE	C-O	-5.19	1.17	1.24
2	D	767	LEU	CA-C	-5.19	1.46	1.52
2	H	604	THR	CA-C	-5.19	1.47	1.52
1	G	137	THR	CA-CB	-5.19	1.47	1.54
2	D	293	HIS	N-CA	-5.18	1.39	1.46
2	B	754	TRP	CA-C	-5.18	1.46	1.52
2	H	490	GLN	CA-C	-5.18	1.45	1.52
2	B	79	ALA	CA-CB	-5.18	1.45	1.53
2	H	552	ALA	CA-CB	-5.18	1.45	1.53
1	C	291	ILE	N-CA	-5.17	1.40	1.46
2	B	770	VAL	CA-CB	-5.17	1.48	1.54
2	D	462	THR	CA-CB	-5.17	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	26	LEU	CG-CD2	5.17	1.69	1.52
2	B	246	ALA	CA-CB	-5.17	1.45	1.53
2	D	493	HIS	CA-C	5.17	1.59	1.52
1	A	285	ILE	CA-CB	-5.17	1.48	1.54
2	D	525	SER	CA-C	-5.17	1.45	1.53
1	G	243	ILE	CA-C	-5.17	1.46	1.52
2	D	165	CYS	N-CA	-5.16	1.39	1.45
2	F	134	ALA	CA-CB	-5.16	1.45	1.53
2	B	48	THR	CA-CB	-5.16	1.46	1.53
2	B	190	VAL	CA-C	-5.16	1.46	1.52
1	E	228	CYS	CA-C	-5.16	1.47	1.53
2	H	500	ALA	CA-CB	-5.16	1.45	1.53
2	D	85	VAL	C-O	-5.16	1.18	1.23
2	D	511	VAL	C-O	-5.16	1.18	1.24
2	H	773	ALA	CA-CB	-5.16	1.45	1.53
2	D	722	ILE	CA-CB	-5.15	1.47	1.54
1	C	300	ALA	C-O	-5.14	1.18	1.24
1	E	354	SER	CA-C	-5.14	1.46	1.53
2	H	288	GLY	C-O	5.14	1.29	1.24
2	D	121	ALA	CA-C	-5.14	1.47	1.52
2	B	727	ALA	CA-CB	-5.14	1.45	1.53
2	D	127	LEU	CA-C	-5.14	1.46	1.52
1	A	303	ALA	CA-C	-5.14	1.45	1.53
2	F	617	ARG	C-N	-5.14	1.29	1.34
2	F	759	ALA	CA-C	-5.14	1.46	1.52
2	H	42	GLU	C-O	-5.13	1.17	1.23
2	B	45	ALA	CA-CB	-5.13	1.45	1.53
2	H	742	ALA	CA-CB	-5.13	1.45	1.53
2	B	114	ARG	C-O	-5.13	1.17	1.24
2	H	572	GLN	CA-C	-5.12	1.46	1.52
2	H	482	ASN	CA-CB	-5.12	1.45	1.53
2	H	112	ALA	CA-CB	-5.12	1.45	1.53
2	F	648	LEU	N-CA	-5.11	1.40	1.46
2	B	441	ASN	CA-C	-5.11	1.46	1.52
1	C	415	LEU	C-O	-5.11	1.19	1.24
1	E	301	MET	SD-CE	5.11	1.92	1.79
2	H	93	PHE	CA-C	-5.10	1.46	1.52
2	D	265	ILE	CA-CB	-5.10	1.47	1.54
2	D	240	ILE	C-O	-5.09	1.18	1.24
1	C	279	ALA	CA-C	-5.09	1.46	1.52
2	D	533	ALA	C-O	-5.09	1.17	1.24
2	F	300	SER	CA-C	-5.08	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	692	ALA	CA-CB	-5.08	1.45	1.53
2	D	674	TRP	CB-CG	-5.08	1.34	1.50
2	D	423	LYS	C-O	-5.08	1.17	1.24
1	G	349	ARG	CA-C	5.08	1.58	1.52
2	B	446	ARG	N-CA	-5.07	1.40	1.45
2	F	159	ALA	CA-CB	-5.07	1.44	1.53
1	A	3	ILE	CA-CB	-5.07	1.47	1.54
2	D	695	THR	CA-CB	-5.07	1.47	1.54
1	G	51	ILE	CA-CB	-5.07	1.47	1.54
2	D	599	THR	CA-CB	-5.07	1.46	1.53
1	C	19	PRO	CA-C	-5.07	1.45	1.52
2	D	339	THR	C-O	-5.06	1.20	1.24
1	C	419	ALA	CA-CB	-5.05	1.44	1.53
2	D	706	ARG	C-O	-5.05	1.17	1.24
2	D	506	ILE	CA-CB	-5.05	1.47	1.54
2	D	315	ALA	CA-CB	-5.05	1.45	1.53
2	F	209	ALA	CA-C	-5.05	1.46	1.52
2	F	448	ILE	CA-CB	-5.05	1.48	1.54
2	F	707	ILE	N-CA	-5.05	1.39	1.46
2	D	582	PHE	CA-CB	-5.05	1.45	1.53
1	E	426	SER	CA-C	-5.04	1.46	1.52
1	E	27	LEU	C-O	5.04	1.29	1.24
1	A	352	LYS	C-O	-5.04	1.18	1.24
2	B	759	ALA	CA-CB	-5.04	1.43	1.54
2	F	179	GLN	CA-C	-5.04	1.46	1.52
2	B	77	SER	CA-C	-5.03	1.47	1.53
1	C	253	ARG	C-O	-5.03	1.18	1.24
2	F	274	ILE	CA-C	-5.03	1.46	1.52
2	B	219	VAL	CA-CB	-5.03	1.48	1.54
2	D	322	PRO	C-O	-5.03	1.17	1.24
2	D	745	ASP	C-O	-5.03	1.18	1.24
2	F	716	PRO	C-O	-5.03	1.17	1.23
2	D	603	ALA	C-O	-5.03	1.18	1.23
2	D	464	LEU	CA-C	-5.03	1.45	1.52
1	C	233	GLN	C-O	-5.03	1.18	1.23
2	F	220	GLU	CD-OE2	5.02	1.34	1.25
2	H	726	LYS	CA-C	-5.02	1.46	1.52
2	H	192	ILE	CA-C	-5.01	1.46	1.52
2	F	698	ILE	CA-CB	-5.01	1.47	1.54
2	D	407	GLN	CA-C	-5.01	1.46	1.52
2	F	132	ALA	CA-CB	-5.01	1.45	1.53
2	D	479	VAL	CA-CB	-5.01	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	690	THR	CA-CB	-5.01	1.46	1.52
2	B	14	ALA	CA-CB	-5.01	1.45	1.53
2	F	248	ALA	CA-C	-5.01	1.46	1.52
2	B	85	VAL	C-O	-5.00	1.18	1.23
2	D	682	TRP	C-O	-5.00	1.17	1.24
2	F	145	ILE	CA-CB	-5.00	1.48	1.54
2	D	462	THR	CA-C	-5.00	1.46	1.52

All (827) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	632	VAL	CB-CA-C	-11.48	92.82	110.50
2	B	151	VAL	N-CA-C	11.00	121.91	110.36
2	D	521	VAL	CB-CA-C	-10.89	98.44	110.52
1	E	136	CYS	N-CA-C	10.53	122.51	111.14
2	B	462	THR	N-CA-C	10.41	123.60	111.11
2	D	632	VAL	CB-CA-C	-10.24	92.99	110.71
2	B	151	VAL	CB-CA-C	-10.24	98.77	111.88
2	H	151	VAL	CB-CA-C	-10.03	99.13	111.97
2	B	190	VAL	CB-CA-C	-9.66	95.86	110.55
2	B	85	VAL	N-CA-C	-9.57	102.55	111.45
1	G	207	ASP	N-CA-C	-9.50	101.58	113.55
1	G	141	PRO	N-CA-C	-9.43	101.22	113.57
1	A	363	ALA	N-CA-C	-9.33	101.19	111.36
1	C	207	ASP	N-CA-C	-9.13	102.65	113.88
1	E	150	ALA	N-CA-C	-8.86	101.07	112.23
1	A	364	VAL	CB-CA-C	-8.82	98.22	111.80
2	H	151	VAL	N-CA-C	8.75	118.82	110.42
2	B	632	VAL	CB-CA-C	-8.71	95.12	110.71
1	C	26	LEU	N-CA-C	-8.67	100.71	111.11
2	F	453	VAL	CB-CA-C	-8.64	97.20	110.50
2	F	329	HIS	CA-C-N	-8.59	111.67	122.84
2	F	329	HIS	C-N-CA	-8.59	111.67	122.84
2	D	199	PRO	N-CD-CG	-8.55	90.37	103.20
2	F	151	VAL	N-CA-C	8.46	118.55	110.42
2	H	62	ILE	N-CA-C	8.45	118.74	111.90
2	D	346	GLY	O-C-N	8.39	124.09	121.07
2	F	6	PRO	CB-CA-C	-8.39	100.64	112.64
2	D	85	VAL	N-CA-C	-8.38	103.66	111.45
2	F	62	ILE	N-CA-C	8.32	118.64	111.90
2	H	251	ARG	N-CA-C	8.28	121.47	108.55
2	F	138	ARG	N-CA-C	8.19	120.03	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	GLN	N-CA-C	-8.17	102.33	111.07
1	A	447	VAL	CB-CA-C	-8.16	101.62	111.81
2	D	138	ARG	N-CA-C	8.12	119.34	108.38
1	A	398	GLU	N-CA-C	-8.12	102.38	111.07
2	D	351	LEU	N-CA-C	-8.08	102.45	111.82
2	F	185	PRO	N-CD-CG	-8.01	91.18	103.20
2	H	355	ARG	N-CA-C	-8.01	102.50	111.07
2	D	511	VAL	CB-CA-C	-7.99	99.42	110.77
2	H	479	VAL	CB-CA-C	-7.98	96.91	110.71
2	H	521	VAL	CB-CA-C	-7.97	101.68	110.52
2	B	676	THR	CA-C-N	-7.95	110.16	122.49
2	B	676	THR	C-N-CA	-7.95	110.16	122.49
2	B	510	GLN	CA-C-N	-7.93	112.75	123.14
2	B	510	GLN	C-N-CA	-7.93	112.75	123.14
2	D	192	ILE	CB-CA-C	-7.84	99.14	110.83
2	B	353	MET	N-CA-C	-7.84	102.73	111.82
2	F	101	VAL	CB-CA-C	-7.82	99.95	110.98
2	F	6	PRO	CA-C-O	-7.81	112.86	121.77
2	D	265	ILE	CB-CA-C	-7.78	101.81	112.24
2	B	641	ARG	N-CA-C	7.77	120.39	108.42
2	B	94	VAL	CB-CA-C	-7.76	101.57	110.96
1	E	64	LEU	CA-C-N	-7.76	112.04	122.99
1	E	64	LEU	C-N-CA	-7.76	112.04	122.99
2	F	695	THR	OG1-CB-CG2	-7.76	93.78	109.30
2	H	192	ILE	CB-CA-C	-7.73	99.19	110.63
2	H	85	VAL	N-CA-C	-7.70	103.36	110.82
2	H	551	LEU	N-CA-C	-7.69	102.84	111.14
2	H	661	ILE	N-CA-C	-7.68	102.79	110.62
2	D	158	ALA	N-CA-C	7.67	121.75	109.24
1	E	364	VAL	CB-CA-C	-7.67	98.72	111.29
2	D	707	ILE	N-CA-C	-7.65	96.45	107.77
2	H	152	GLU	N-CA-C	-7.64	102.90	111.07
2	F	351	LEU	N-CA-C	-7.63	102.96	111.82
2	D	619	PHE	N-CA-C	7.63	121.83	109.40
1	C	137	THR	CB-CA-C	-7.61	96.29	109.07
2	H	471	VAL	N-CA-C	7.58	119.39	108.48
2	B	586	VAL	N-CA-C	7.54	118.27	110.36
1	C	30	GLU	N-CA-C	-7.53	104.07	113.18
2	D	316	ASP	N-CA-C	-7.52	103.22	113.30
2	F	61	VAL	N-CA-C	7.48	119.39	109.21
2	H	197	GLN	CA-C-N	-7.47	114.63	122.85
2	H	197	GLN	C-N-CA	-7.47	114.63	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	19	PRO	N-CA-C	-7.47	106.91	114.68
2	F	710	VAL	CB-CA-C	-7.44	99.53	110.62
1	E	363	ALA	N-CA-C	-7.42	102.89	112.23
2	F	38	GLY	N-CA-C	-7.40	97.53	110.71
1	G	259	PRO	CA-C-N	-7.40	114.38	122.59
1	G	259	PRO	C-N-CA	-7.40	114.38	122.59
2	H	190	VAL	CB-CA-C	-7.39	97.48	110.71
2	B	534	ASP	N-CA-C	-7.37	102.94	110.97
2	F	704	ARG	NE-CZ-NH1	-7.36	114.14	121.50
2	F	599	THR	CB-CA-C	-7.36	96.89	111.60
1	E	460	VAL	CB-CA-C	-7.35	101.79	110.91
2	B	476	ASP	N-CA-C	-7.34	103.89	112.92
1	G	363	ALA	N-CA-C	-7.34	103.21	111.14
2	B	359	HIS	N-CA-C	-7.32	103.24	111.07
2	D	405	TYR	N-CA-C	-7.28	103.49	112.88
2	D	151	VAL	CB-CA-C	-7.28	102.66	111.97
2	B	479	VAL	CB-CA-C	-7.26	97.72	110.71
2	D	355	ARG	N-CA-C	-7.24	102.99	111.03
2	F	666	GLY	CA-C-N	-7.20	108.44	120.68
2	F	666	GLY	C-N-CA	-7.20	108.44	120.68
2	B	192	ILE	CB-CA-C	-7.18	100.13	110.83
2	F	619	PHE	N-CA-C	7.17	121.22	109.24
2	H	566	VAL	CA-C-N	-7.16	113.04	122.99
2	H	566	VAL	C-N-CA	-7.16	113.04	122.99
2	D	291	PHE	CA-C-N	-7.14	113.79	123.14
2	D	291	PHE	C-N-CA	-7.14	113.79	123.14
1	G	422	PHE	N-CA-C	7.12	120.27	109.23
1	G	30	GLU	N-CA-C	-7.12	104.33	113.16
1	E	193	TYR	N-CA-C	-7.12	103.45	111.14
2	F	189	GLY	CA-C-N	-7.11	112.68	122.92
2	F	189	GLY	C-N-CA	-7.11	112.68	122.92
2	D	166	PHE	N-CA-C	7.09	119.96	108.76
1	A	69	GLN	CA-C-N	-7.07	111.66	122.76
1	A	69	GLN	C-N-CA	-7.07	111.66	122.76
2	F	521	VAL	CB-CA-C	-7.07	102.67	110.52
1	C	116	ALA	N-CA-C	-7.07	103.62	111.82
1	A	117	ALA	N-CA-C	-7.06	102.78	111.40
2	F	249	THR	CB-CA-C	-7.06	97.31	110.01
1	A	95	MET	CA-C-N	-7.04	111.69	120.56
1	A	95	MET	C-N-CA	-7.04	111.69	120.56
1	C	363	ALA	N-CA-C	-7.03	103.04	111.69
2	D	462	THR	N-CA-C	7.03	125.78	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	23	LEU	N-CA-C	7.03	118.59	111.07
2	H	562	ALA	N-CA-C	7.03	121.48	110.17
2	F	273	ARG	N-CA-C	-7.00	97.49	108.90
2	H	163	GLU	N-CA-C	-7.00	98.83	109.95
2	H	351	LEU	N-CA-C	-7.00	103.66	111.28
2	F	355	ARG	N-CA-C	-6.99	103.59	111.14
2	H	15	HIS	N-CA-C	-6.96	103.38	110.97
2	B	15	HIS	N-CA-C	-6.95	103.78	111.36
2	B	235	GLY	N-CA-C	-6.95	106.04	114.66
2	B	158	ALA	N-CA-C	6.94	119.84	108.52
2	B	567	ILE	N-CA-C	6.94	117.83	108.11
2	B	173	HIS	N-CA-C	6.94	119.44	111.11
1	G	208	VAL	N-CA-C	6.94	117.70	110.62
1	G	132	ASN	CA-C-N	-6.92	110.87	122.64
1	G	132	ASN	C-N-CA	-6.92	110.87	122.64
2	F	158	ALA	N-CA-C	6.92	120.95	109.46
2	D	273	ARG	NE-CZ-NH1	-6.89	114.61	121.50
2	H	130	ASP	CA-C-N	-6.87	110.97	120.38
2	H	130	ASP	C-N-CA	-6.87	110.97	120.38
2	D	685	CYS	CB-CA-C	-6.87	97.65	110.01
2	H	318	SER	CA-C-N	-6.86	111.82	122.59
2	H	318	SER	C-N-CA	-6.86	111.82	122.59
2	H	464	LEU	CA-C-N	-6.86	111.87	122.16
2	H	464	LEU	C-N-CA	-6.86	111.87	122.16
2	F	16	VAL	N-CA-C	6.82	123.53	109.34
2	D	516	THR	OG1-CB-CG2	-6.81	95.68	109.30
2	H	676	THR	CA-C-N	-6.81	111.43	122.26
2	H	676	THR	C-N-CA	-6.81	111.43	122.26
2	H	494	ALA	N-CA-C	-6.81	103.79	111.14
2	B	251	ARG	N-CA-C	6.78	120.88	109.09
1	E	26	LEU	N-CA-CB	6.76	120.01	109.94
1	E	420	GLN	N-CA-C	-6.75	104.68	113.12
1	G	94	ALA	N-CA-C	-6.74	103.93	111.28
1	G	188	ALA	N-CA-C	-6.73	103.97	111.71
2	B	185	PRO	N-CD-CG	-6.72	93.12	103.20
1	G	70	ILE	CB-CA-C	-6.72	103.32	111.85
2	F	151	VAL	CB-CA-C	-6.71	103.38	111.97
2	F	681	VAL	N-CA-C	6.70	117.69	107.77
2	F	13	ARG	N-CA-C	-6.70	104.06	111.36
1	A	422	PHE	N-CA-C	6.68	119.87	109.52
1	C	393	ARG	N-CA-C	-6.67	101.93	110.53
1	A	207	ASP	N-CA-C	-6.67	105.68	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	251	ARG	N-CA-C	6.66	120.68	109.09
1	A	43	ASP	N-CA-C	6.64	121.13	112.89
2	D	190	VAL	CB-CA-C	-6.64	100.45	110.55
1	A	270	PHE	N-CA-C	-6.64	96.24	107.99
1	G	391	PRO	CA-C-O	-6.64	113.57	121.67
2	F	510	GLN	CA-C-N	-6.63	114.45	123.14
2	F	510	GLN	C-N-CA	-6.63	114.45	123.14
2	D	206	VAL	N-CA-C	-6.63	104.02	110.72
1	E	388	ALA	N-CA-C	6.62	116.61	107.73
1	G	193	TYR	N-CA-C	-6.62	103.99	111.07
2	B	499	VAL	CB-CA-C	-6.61	103.21	112.14
2	H	3	VAL	N-CA-C	-6.61	100.11	109.63
2	B	61	VAL	CB-CA-C	-6.61	101.83	111.68
1	C	377	ILE	N-CA-C	6.59	116.73	107.37
2	D	265	ILE	N-CA-C	6.59	118.18	111.00
2	B	130	ASP	N-CA-C	-6.58	104.03	111.07
2	F	676	THR	CA-C-N	-6.58	110.54	121.92
2	F	676	THR	C-N-CA	-6.58	110.54	121.92
1	E	422	PHE	N-CA-C	6.58	119.42	109.23
2	F	526	ALA	N-CA-C	-6.56	102.06	110.53
2	D	676	THR	CA-C-N	-6.56	110.91	122.26
2	D	676	THR	C-N-CA	-6.56	110.91	122.26
2	B	259	ARG	CB-CA-C	-6.55	100.32	110.81
2	D	35	LEU	N-CA-C	6.55	119.84	109.81
1	E	8	ASN	CB-CA-C	-6.55	102.58	111.89
1	C	391	PRO	CA-C-O	-6.55	113.45	121.31
1	G	283	GLY	CA-C-N	-6.54	111.43	120.38
1	G	283	GLY	C-N-CA	-6.54	111.43	120.38
2	B	321	VAL	CB-CA-C	-6.53	103.56	110.16
2	B	85	VAL	CB-CA-C	-6.52	103.38	111.92
1	A	141	PRO	N-CA-C	-6.49	105.07	113.57
1	A	137	THR	CA-C-N	-6.49	111.89	122.20
1	A	137	THR	C-N-CA	-6.49	111.89	122.20
2	H	281	ASP	N-CA-CB	-6.48	99.53	110.49
2	F	462	THR	N-CA-C	6.48	122.06	111.37
2	D	610	ASP	N-CA-C	6.48	119.36	108.02
2	B	101	VAL	CB-CA-C	-6.47	101.06	110.63
2	B	579	SER	CA-CB-OG	-6.46	98.18	111.10
2	B	27	PRO	CA-C-O	-6.46	113.79	121.67
2	B	593	ARG	CA-C-N	-6.46	114.51	123.10
2	B	593	ARG	C-N-CA	-6.46	114.51	123.10
2	F	685	CYS	CB-CA-C	-6.44	97.13	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	157	GLY	CA-C-N	-6.44	114.11	123.00
2	H	157	GLY	C-N-CA	-6.44	114.11	123.00
2	D	697	LYS	N-CA-C	6.43	120.28	107.62
2	H	316	ASP	N-CA-C	-6.43	105.44	113.28
2	D	737	ILE	CA-C-N	-6.42	111.04	120.28
2	D	737	ILE	C-N-CA	-6.42	111.04	120.28
1	E	141	PRO	N-CA-C	-6.42	105.16	113.57
2	B	174	PHE	CB-CA-C	-6.42	102.43	111.80
1	C	135	ARG	NE-CZ-NH2	6.42	124.98	119.20
2	D	151	VAL	N-CA-C	6.42	116.58	110.42
2	B	266	THR	OG1-CB-CG2	-6.41	96.47	109.30
2	F	94	VAL	CB-CA-C	-6.41	103.20	110.96
2	B	370	GLU	N-CA-C	-6.41	104.38	111.36
1	A	274	GLN	CA-C-N	-6.40	114.80	122.35
1	A	274	GLN	C-N-CA	-6.40	114.80	122.35
2	H	663	GLN	N-CA-C	-6.40	104.23	111.14
2	F	191	VAL	CB-CA-C	-6.40	100.99	110.33
2	D	281	ASP	N-CA-CB	-6.40	99.68	110.49
2	F	618	PRO	N-CA-C	-6.39	103.88	114.75
1	E	144	ARG	CA-C-N	-6.39	111.71	120.28
1	E	144	ARG	C-N-CA	-6.39	111.71	120.28
2	F	740	PHE	N-CA-C	-6.39	104.01	110.97
2	F	62	ILE	CB-CA-C	-6.39	105.17	111.30
2	H	446	ARG	N-CA-C	-6.39	99.79	109.95
2	F	316	ASP	N-CA-C	-6.38	105.53	113.38
1	C	25	GLU	N-CA-C	6.38	118.03	111.14
1	A	391	PRO	N-CA-C	-6.38	101.03	111.68
2	F	405	TYR	N-CA-C	-6.38	103.95	112.94
1	G	364	VAL	CB-CA-C	-6.38	100.83	111.29
1	C	303	ALA	N-CA-C	-6.37	100.78	110.14
1	E	317	PRO	CB-CA-C	-6.36	104.63	111.56
2	F	631	VAL	CB-CA-C	-6.36	101.41	110.82
2	D	606	LYS	CA-C-N	-6.36	113.71	122.93
2	D	606	LYS	C-N-CA	-6.36	113.71	122.93
2	F	690	THR	OG1-CB-CG2	-6.36	96.58	109.30
1	G	296	PRO	CA-C-N	-6.36	111.96	120.54
1	G	296	PRO	C-N-CA	-6.36	111.96	120.54
1	C	282	GLY	N-CA-C	-6.35	105.14	112.50
2	H	764	GLU	N-CA-C	-6.34	103.28	111.02
1	G	96	ILE	CB-CA-C	-6.34	103.58	112.14
1	E	96	ILE	N-CA-C	6.34	116.50	110.42
1	E	343	LYS	N-CA-C	-6.34	104.47	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	PHE	N-CA-C	6.33	118.99	111.71
2	D	101	VAL	CB-CA-C	-6.33	101.19	110.81
1	C	290	PRO	CA-C-N	-6.32	113.93	122.72
1	C	290	PRO	C-N-CA	-6.32	113.93	122.72
2	H	610	ASP	CA-C-N	6.32	128.65	120.44
2	H	610	ASP	C-N-CA	6.32	128.65	120.44
2	D	561	CYS	CA-C-N	-6.30	111.92	122.64
2	D	561	CYS	C-N-CA	-6.30	111.92	122.64
2	F	555	VAL	CB-CA-C	-6.30	103.63	112.14
2	B	776	ARG	CB-CA-C	-6.30	103.47	111.22
1	E	188	ALA	N-CA-C	-6.30	103.70	111.33
2	F	166	PHE	N-CA-C	6.30	118.64	109.07
2	D	249	THR	N-CA-C	-6.29	105.64	113.38
1	E	14	VAL	N-CA-C	6.29	117.84	108.46
1	A	26	LEU	N-CA-C	-6.29	103.56	111.11
2	F	606	LYS	CA-C-N	-6.29	114.04	122.72
2	F	606	LYS	C-N-CA	-6.29	114.04	122.72
2	F	23	LEU	N-CA-C	6.28	118.65	111.11
1	G	144	ARG	CA-C-N	-6.28	111.86	120.28
1	G	144	ARG	C-N-CA	-6.28	111.86	120.28
1	E	391	PRO	CA-C-O	-6.28	113.63	120.97
2	H	462	THR	N-CA-C	6.28	124.17	110.80
1	A	420	GLN	N-CA-C	-6.27	106.16	113.88
1	E	61	ASN	N-CA-C	6.27	118.38	108.67
1	C	193	TYR	N-CA-C	-6.26	104.37	111.07
2	D	85	VAL	CB-CA-C	-6.26	103.72	111.92
2	B	405	TYR	N-CA-C	-6.25	104.92	113.30
1	E	104	GLY	CA-C-O	6.25	125.00	119.56
1	G	137	THR	CA-C-N	-6.25	112.70	122.51
1	G	137	THR	C-N-CA	-6.25	112.70	122.51
2	F	241	ALA	N-CA-C	-6.24	104.16	110.97
2	F	39	LEU	N-CA-C	6.23	119.34	109.81
2	B	318	SER	CA-C-N	-6.22	112.92	122.62
2	B	318	SER	C-N-CA	-6.22	112.92	122.62
2	F	280	ALA	CA-C-N	6.22	133.41	121.54
2	F	280	ALA	C-N-CA	6.22	133.41	121.54
2	H	94	VAL	CB-CA-C	-6.22	103.07	111.15
1	C	446	TYR	CA-C-N	-6.21	112.94	120.70
1	C	446	TYR	C-N-CA	-6.21	112.94	120.70
2	F	250	GLY	CA-C-N	-6.19	115.05	123.96
2	F	250	GLY	C-N-CA	-6.19	115.05	123.96
2	B	39	LEU	N-CA-C	6.19	119.79	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	562	ALA	N-CA-C	6.18	119.89	109.76
2	H	713	TRP	N-CA-C	-6.18	99.80	109.25
2	B	516	THR	OG1-CB-CG2	-6.17	96.95	109.30
1	A	193	TYR	N-CA-C	-6.15	104.49	111.07
2	D	6	PRO	CB-CA-C	-6.15	104.18	112.97
1	G	43	ASP	N-CA-C	6.15	120.51	112.89
1	C	228	CYS	CB-CA-C	-6.14	102.72	112.05
2	F	152	GLU	N-CA-C	-6.14	104.28	110.97
1	C	318	LEU	N-CA-C	6.14	118.47	111.11
2	H	241	ALA	CA-C-N	-6.14	111.58	120.29
2	H	241	ALA	C-N-CA	-6.14	111.58	120.29
2	F	190	VAL	CB-CA-C	-6.13	101.75	110.82
1	G	91	VAL	N-CA-C	6.13	116.30	110.42
2	D	549	GLY	CA-C-N	-6.11	111.03	120.31
2	D	549	GLY	C-N-CA	-6.11	111.03	120.31
2	D	168	ILE	CA-C-N	-6.11	115.01	122.15
2	D	168	ILE	C-N-CA	-6.11	115.01	122.15
1	A	296	PRO	CA-C-N	-6.10	112.50	120.44
1	A	296	PRO	C-N-CA	-6.10	112.50	120.44
2	B	464	LEU	CA-C-N	-6.09	113.04	122.05
2	B	464	LEU	C-N-CA	-6.09	113.04	122.05
2	F	130	ASP	CA-C-N	-6.09	112.32	120.54
2	F	130	ASP	C-N-CA	-6.09	112.32	120.54
1	A	60	VAL	CA-C-O	-6.08	115.68	121.64
1	E	157	TRP	N-CA-C	6.08	118.70	111.71
2	F	41	THR	N-CA-C	-6.08	105.18	112.59
2	D	219	VAL	CB-CA-C	-6.06	101.80	110.83
1	A	164	PHE	N-CA-C	6.06	119.69	109.76
2	F	663	GLN	N-CA-C	-6.05	104.76	111.36
2	H	101	VAL	CB-CA-C	-6.05	101.68	110.63
2	F	627	ALA	CA-C-N	-6.04	115.70	123.19
2	F	627	ALA	C-N-CA	-6.04	115.70	123.19
2	B	325	ARG	CA-C-N	-6.04	114.55	122.94
2	B	325	ARG	C-N-CA	-6.04	114.55	122.94
2	D	259	ARG	N-CA-C	6.03	118.35	111.11
2	H	325	ARG	CA-C-N	-6.03	114.02	122.71
2	H	325	ARG	C-N-CA	-6.03	114.02	122.71
2	H	499	VAL	CB-CA-C	-6.02	104.16	112.04
2	D	38	GLY	N-CA-C	-6.01	100.02	110.71
2	B	197	GLN	CA-C-N	-6.00	116.25	122.85
2	B	197	GLN	C-N-CA	-6.00	116.25	122.85
1	G	271	ALA	CB-CA-C	-6.00	109.64	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	27	PRO	CA-C-O	-6.00	114.35	121.67
1	E	291	ILE	N-CA-C	-5.99	107.28	113.10
2	H	158	ALA	N-CA-C	5.99	118.71	109.07
2	B	524	THR	N-CA-C	5.98	118.63	110.55
2	B	377	TYR	N-CA-C	-5.98	102.59	110.43
2	D	713	TRP	CA-C-N	-5.98	114.29	123.14
2	D	713	TRP	C-N-CA	-5.98	114.29	123.14
1	E	393	ARG	N-CA-C	-5.98	102.82	110.53
1	C	183	PRO	N-CD-CG	-5.97	94.24	103.20
2	H	504	LEU	N-CA-C	-5.97	105.99	113.28
2	D	618	PRO	N-CA-C	-5.97	106.21	114.27
2	F	661	ILE	N-CA-C	-5.97	104.53	110.62
2	B	281	ASP	N-CA-CB	-5.96	100.41	110.49
2	D	494	ALA	N-CA-C	-5.96	104.70	111.14
2	H	127	LEU	CA-C-N	-5.96	113.32	122.62
2	H	127	LEU	C-N-CA	-5.96	113.32	122.62
2	D	584	GLU	CA-C-N	-5.95	112.97	120.77
2	D	584	GLU	C-N-CA	-5.95	112.97	120.77
2	B	584	GLU	CA-C-N	-5.95	113.06	120.56
2	B	584	GLU	C-N-CA	-5.95	113.06	120.56
1	C	179	PRO	CA-C-N	5.95	132.90	121.54
1	C	179	PRO	C-N-CA	5.95	132.90	121.54
1	A	91	VAL	N-CA-C	5.95	116.68	110.62
2	D	760	PRO	N-CD-CG	-5.94	96.67	103.80
1	G	389	GLY	N-CA-C	-5.94	107.81	114.40
1	E	105	PHE	N-CA-C	5.94	118.54	111.71
2	H	38	GLY	CA-C-N	-5.94	113.31	122.87
2	H	38	GLY	C-N-CA	-5.94	113.31	122.87
2	F	301	ALA	N-CA-C	5.94	117.75	111.28
2	B	280	ALA	CA-C-N	5.93	132.87	121.54
2	B	280	ALA	C-N-CA	5.93	132.87	121.54
2	B	499	VAL	CA-C-N	-5.93	111.87	120.29
2	B	499	VAL	C-N-CA	-5.93	111.87	120.29
2	D	471	VAL	N-CA-C	5.93	117.90	108.89
1	E	207	ASP	N-CA-C	-5.93	106.21	113.50
2	H	329	HIS	CA-C-N	-5.92	114.38	123.14
2	H	329	HIS	C-N-CA	-5.92	114.38	123.14
2	B	3	VAL	N-CA-C	-5.90	101.14	109.63
2	F	143	PRO	CA-C-O	-5.89	114.38	122.15
2	D	266	THR	CA-C-N	-5.88	117.19	122.43
2	D	266	THR	C-N-CA	-5.88	117.19	122.43
2	D	453	VAL	N-CA-C	5.88	116.58	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	673	GLY	N-CA-C	-5.88	105.66	112.83
2	F	554	PHE	CA-C-N	-5.87	112.41	120.46
2	F	554	PHE	C-N-CA	-5.87	112.41	120.46
1	A	26	LEU	N-CA-CB	5.87	118.69	109.94
1	E	249	ILE	CA-C-N	-5.87	112.91	120.65
1	E	249	ILE	C-N-CA	-5.87	112.91	120.65
2	H	280	ALA	CA-C-N	5.87	132.74	121.54
2	H	280	ALA	C-N-CA	5.87	132.74	121.54
1	A	250	ALA	N-CA-C	-5.86	104.80	111.07
1	C	364	VAL	CB-CA-C	-5.86	100.46	111.30
2	H	21	ARG	CB-CA-C	-5.86	99.59	109.72
2	B	98	ILE	CB-CA-C	-5.85	105.91	111.06
2	F	549	GLY	CA-C-N	-5.85	111.99	120.29
2	F	549	GLY	C-N-CA	-5.85	111.99	120.29
2	H	244	VAL	N-CA-C	5.85	116.31	110.23
2	D	453	VAL	CB-CA-C	-5.84	101.80	110.33
1	G	350	CYS	N-CA-C	5.84	118.43	108.90
2	B	328	SER	CA-C-N	-5.84	113.94	122.65
2	B	328	SER	C-N-CA	-5.84	113.94	122.65
1	G	19	PRO	CA-C-N	-5.84	112.97	122.26
1	G	19	PRO	C-N-CA	-5.84	112.97	122.26
2	B	611	ARG	CG-CD-NE	-5.84	99.16	112.00
2	H	105	SER	N-CA-C	5.84	117.28	108.46
2	B	8	PRO	CB-CA-C	-5.83	103.31	110.95
2	F	276	TYR	N-CA-C	5.83	118.27	109.23
1	G	366	GLY	O-C-N	-5.83	119.68	123.35
2	F	365	GLY	N-CA-C	-5.83	106.91	115.30
2	H	46	ALA	N-CA-C	-5.82	101.06	110.32
1	A	17	GLU	N-CA-C	-5.82	106.52	113.97
2	H	534	ASP	N-CA-C	-5.82	104.13	111.11
2	D	493	HIS	CA-C-N	-5.82	112.53	120.44
2	D	493	HIS	C-N-CA	-5.82	112.53	120.44
1	A	33	THR	N-CA-CB	-5.81	100.67	110.49
1	A	447	VAL	N-CA-CB	5.81	116.95	110.62
2	B	282	ALA	N-CA-C	-5.81	106.03	113.23
1	C	44	CYS	N-CA-C	5.81	120.50	113.41
2	H	673	GLY	CA-C-O	5.80	126.37	120.45
2	H	125	ALA	CA-C-N	-5.79	115.34	122.93
2	H	125	ALA	C-N-CA	-5.79	115.34	122.93
1	A	136	CYS	N-CA-C	5.79	120.50	112.45
1	C	135	ARG	NE-CZ-NH1	-5.79	115.71	121.50
2	B	468	GLY	O-C-N	-5.79	118.15	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	606	LYS	N-CA-C	5.79	119.64	112.47
2	B	259	ARG	N-CA-C	5.79	118.05	111.11
2	D	522	PRO	CB-CA-C	-5.78	102.02	111.56
1	G	33	THR	N-CA-CB	-5.78	100.72	110.49
1	E	118	HIS	N-CA-C	-5.77	105.07	111.36
1	G	100	GLY	CA-C-N	-5.76	112.78	122.29
1	G	100	GLY	C-N-CA	-5.76	112.78	122.29
2	B	453	VAL	CB-CA-C	-5.76	100.51	110.65
1	G	134	CYS	N-CA-C	-5.76	99.62	109.24
1	C	69	GLN	CA-C-N	-5.76	114.10	122.28
1	C	69	GLN	C-N-CA	-5.76	114.10	122.28
1	E	350	CYS	N-CA-C	5.76	117.79	108.34
1	G	164	PHE	N-CA-C	5.76	119.44	110.17
2	B	329	HIS	CA-C-N	-5.75	114.62	123.14
2	B	329	HIS	C-N-CA	-5.75	114.62	123.14
2	B	495	LYS	N-CA-C	-5.75	105.01	111.28
2	B	618	PRO	N-CA-C	-5.75	106.18	114.18
2	B	237	HIS	CA-C-N	-5.75	112.97	120.44
2	B	237	HIS	C-N-CA	-5.75	112.97	120.44
1	C	26	LEU	N-CA-CB	5.75	118.50	109.94
1	C	11	THR	OG1-CB-CG2	-5.75	97.81	109.30
2	H	681	VAL	N-CA-C	5.75	116.56	108.17
2	D	588	ALA	CA-C-N	-5.74	112.02	120.28
2	D	588	ALA	C-N-CA	-5.74	112.02	120.28
2	F	453	VAL	N-CA-C	5.74	117.00	108.46
1	C	43	ASP	N-CA-C	5.73	119.99	112.89
1	A	335	PHE	N-CA-C	5.72	118.10	109.23
2	H	306	PRO	CA-C-N	-5.72	113.55	120.70
2	H	306	PRO	C-N-CA	-5.72	113.55	120.70
1	G	146	ALA	N-CA-C	-5.72	105.13	111.36
2	F	277	ARG	CA-C-N	-5.72	113.60	122.69
2	F	277	ARG	C-N-CA	-5.72	113.60	122.69
2	H	632	VAL	CB-CA-C	-5.71	100.82	110.71
1	E	377	ILE	N-CA-C	5.71	116.60	107.98
1	G	43	ASP	CA-C-N	-5.71	112.74	122.11
1	G	43	ASP	C-N-CA	-5.71	112.74	122.11
2	B	611	ARG	CB-CA-C	-5.70	101.28	110.74
2	H	602	TYR	N-CA-C	5.70	117.93	108.99
1	G	116	ALA	CA-C-N	-5.69	112.20	120.29
1	G	116	ALA	C-N-CA	-5.69	112.20	120.29
2	D	666	GLY	CA-C-N	-5.69	112.21	120.29
2	D	666	GLY	C-N-CA	-5.69	112.21	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	280	ALA	CA-C-N	5.69	132.40	121.54
2	D	280	ALA	C-N-CA	5.69	132.40	121.54
2	F	742	ALA	N-CA-C	-5.68	105.16	111.36
2	B	185	PRO	CB-CA-C	-5.68	104.42	111.64
2	D	590	TYR	N-CA-C	-5.68	105.09	111.28
1	E	183	PRO	N-CD-CG	-5.68	94.68	103.20
2	F	629	THR	OG1-CB-CG2	-5.67	97.95	109.30
2	D	235	GLY	N-CA-C	-5.67	99.74	113.18
2	D	586	VAL	N-CA-C	5.67	117.08	110.62
2	H	741	LEU	CA-CB-CG	-5.67	96.46	116.30
1	C	164	PHE	N-CA-C	5.67	119.29	110.17
1	A	100	GLY	CA-C-N	-5.66	113.03	122.21
1	A	100	GLY	C-N-CA	-5.66	113.03	122.21
2	D	15	HIS	N-CA-C	-5.66	105.02	111.14
1	C	17	GLU	N-CA-C	-5.66	106.92	113.88
2	B	338	ASN	N-CA-C	5.66	117.63	110.33
2	B	661	ILE	N-CA-C	-5.66	104.85	110.62
2	F	342	ARG	NE-CZ-NH1	-5.66	115.84	121.50
2	F	380	PRO	CA-C-O	-5.66	115.11	122.12
2	B	62	ILE	N-CA-C	5.65	116.87	112.12
2	H	23	LEU	N-CA-C	5.65	117.89	111.11
1	E	70	ILE	CB-CA-C	-5.65	105.69	112.19
2	D	301	ALA	N-CA-C	5.65	117.89	111.11
2	H	96	GLN	CA-C-N	5.64	125.41	119.76
2	H	96	GLN	C-N-CA	5.64	125.41	119.76
2	F	707	ILE	N-CA-C	-5.64	99.42	107.77
2	H	637	THR	CB-CA-C	-5.64	99.84	109.65
2	H	299	TRP	N-CA-C	5.63	120.02	113.20
2	B	749	ALA	CA-C-N	-5.63	113.76	122.49
2	B	749	ALA	C-N-CA	-5.63	113.76	122.49
2	H	453	VAL	CB-CA-C	-5.63	101.83	110.50
1	G	252	LEU	CA-C-N	-5.63	112.30	120.29
1	G	252	LEU	C-N-CA	-5.63	112.30	120.29
2	H	679	GLU	CA-C-N	-5.63	113.76	122.09
2	H	679	GLU	C-N-CA	-5.63	113.76	122.09
2	F	314	HIS	N-CA-C	5.62	119.84	112.92
1	A	137	THR	CB-CA-C	-5.62	100.11	109.55
2	F	566	VAL	CA-C-N	-5.62	115.17	122.99
2	F	566	VAL	C-N-CA	-5.62	115.17	122.99
2	H	265	ILE	CB-CA-C	-5.62	103.72	111.65
2	B	265	ILE	CB-CA-C	-5.62	104.68	112.04
1	E	35	THR	N-CA-C	-5.62	101.53	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	417	LEU	CA-CB-CG	-5.61	96.65	116.30
2	H	220	GLU	N-CA-C	-5.61	99.87	109.24
1	E	228	CYS	CA-CB-SG	-5.61	101.50	114.40
2	F	93	PHE	CA-C-N	-5.61	115.36	122.37
2	F	93	PHE	C-N-CA	-5.61	115.36	122.37
2	F	332	ARG	NE-CZ-NH1	-5.60	115.90	121.50
2	H	85	VAL	CB-CA-C	-5.60	104.70	112.04
2	B	512	ARG	CA-C-N	-5.60	112.30	122.43
2	B	512	ARG	C-N-CA	-5.60	112.30	122.43
2	H	292	VAL	CB-CA-C	-5.59	102.16	110.33
2	F	88	THR	OG1-CB-CG2	-5.58	98.14	109.30
2	B	696	TYR	N-CA-C	-5.58	100.09	109.07
1	C	150	ALA	N-CA-C	-5.58	105.35	111.82
2	B	252	PRO	CA-C-O	-5.57	115.06	121.36
2	F	570	ALA	CA-C-N	-5.57	111.12	121.93
2	F	570	ALA	C-N-CA	-5.57	111.12	121.93
2	F	85	VAL	N-CA-C	-5.57	105.67	110.74
2	B	426	ASN	N-CA-C	-5.56	103.73	111.52
1	C	225	LEU	N-CA-C	5.56	119.91	113.18
2	F	47	ILE	CB-CA-C	-5.56	104.01	110.91
2	D	413	VAL	N-CA-CB	-5.56	105.88	112.39
1	E	182	LEU	N-CA-C	5.55	118.72	108.94
2	B	152	GLU	N-CA-C	-5.55	105.23	111.28
1	C	290	PRO	N-CA-C	-5.55	108.91	114.68
1	C	14	VAL	N-CA-C	5.55	116.47	108.48
1	E	19	PRO	N-CA-C	-5.55	108.91	114.68
2	H	259	ARG	CB-CA-C	-5.54	101.94	110.81
2	D	281	ASP	CB-CA-C	-5.54	99.39	110.42
2	F	61	VAL	CB-CA-C	-5.54	103.47	111.34
1	E	95	MET	CA-C-N	-5.54	113.58	120.56
1	E	95	MET	C-N-CA	-5.54	113.58	120.56
2	D	39	LEU	N-CA-C	5.54	118.72	110.14
2	D	713	TRP	N-CA-C	-5.53	100.17	108.96
1	A	292	GLY	N-CA-C	-5.53	105.57	111.93
1	C	343	LYS	N-CA-C	-5.53	106.03	112.89
2	D	732	PRO	N-CD-CG	-5.53	94.91	103.20
1	G	372	LEU	N-CA-C	5.52	118.48	109.59
2	H	38	GLY	N-CA-C	-5.52	101.35	110.95
2	F	165	CYS	CA-CB-SG	-5.51	101.72	114.40
2	B	510	GLN	CB-CA-C	-5.51	100.16	110.36
2	D	318	SER	CA-C-N	-5.51	114.16	122.81
2	D	318	SER	C-N-CA	-5.51	114.16	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	476	ASP	N-CA-C	-5.50	106.24	113.17
2	F	346	GLY	O-C-N	5.50	123.05	121.07
1	C	276	ARG	NE-CZ-NH1	-5.50	116.00	121.50
2	H	82	PRO	N-CD-CG	-5.49	94.96	103.20
2	H	674	TRP	CA-C-N	-5.49	113.94	122.67
2	H	674	TRP	C-N-CA	-5.49	113.94	122.67
1	G	69	GLN	CA-C-N	-5.49	114.14	122.76
1	G	69	GLN	C-N-CA	-5.49	114.14	122.76
1	E	368	LEU	N-CA-C	5.48	118.34	109.40
2	H	376	PHE	N-CA-C	-5.47	103.26	110.43
2	H	88	THR	OG1-CB-CG2	-5.47	98.36	109.30
2	F	251	ARG	N-CA-C	5.47	118.80	109.06
2	F	27	PRO	CA-C-O	-5.47	115.00	121.67
1	C	447	VAL	CB-CA-C	-5.47	104.98	111.81
2	B	705	PRO	CA-C-O	-5.46	115.36	121.32
1	E	96	ILE	CB-CA-C	-5.46	104.98	111.97
1	G	279	ALA	CA-C-N	-5.46	114.23	122.81
1	G	279	ALA	C-N-CA	-5.46	114.23	122.81
1	A	349	ARG	N-CA-C	-5.46	99.70	108.55
2	B	126	ILE	N-CA-CB	-5.46	104.59	111.41
1	E	423	THR	O-C-N	5.46	125.63	121.27
2	B	223	ARG	NE-CZ-NH2	5.45	124.11	119.20
2	F	658	ALA	N-CA-C	-5.45	105.25	111.14
2	B	20	ALA	CA-C-N	-5.45	114.53	122.65
2	B	20	ALA	C-N-CA	-5.45	114.53	122.65
2	D	510	GLN	CA-C-N	-5.45	115.85	123.10
2	D	510	GLN	C-N-CA	-5.45	115.85	123.10
2	F	37	PHE	N-CA-C	-5.45	102.46	110.52
2	B	347	PRO	CA-C-N	-5.44	113.37	120.44
2	B	347	PRO	C-N-CA	-5.44	113.37	120.44
2	B	759	ALA	N-CA-C	-5.44	101.92	110.14
2	B	265	ILE	N-CA-C	5.44	116.09	110.82
1	A	215	ALA	N-CA-C	-5.44	106.42	113.16
1	C	432	ALA	CA-C-N	-5.43	113.38	120.44
1	C	432	ALA	C-N-CA	-5.43	113.38	120.44
2	H	300	SER	CA-CB-OG	-5.43	100.23	111.10
1	G	215	ALA	N-CA-C	-5.42	106.44	113.16
1	C	291	ILE	N-CA-C	-5.42	107.84	113.10
2	F	347	PRO	CA-C-N	-5.42	113.40	120.44
2	F	347	PRO	C-N-CA	-5.42	113.40	120.44
1	C	460	VAL	CB-CA-C	-5.42	104.19	110.91
2	D	78	PRO	N-CA-C	-5.42	109.05	114.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ARG	N-CA-C	-5.42	105.46	111.36
1	E	137	THR	CA-C-N	-5.41	112.25	122.05
1	E	137	THR	C-N-CA	-5.41	112.25	122.05
2	F	513	ILE	CB-CA-C	-5.41	103.79	111.21
2	H	229	GLY	N-CA-C	-5.41	107.46	113.79
1	A	91	VAL	CB-CA-C	-5.41	104.84	112.14
1	E	373	LYS	N-CA-C	-5.40	101.44	109.11
2	F	145	ILE	N-CA-C	5.40	115.67	108.11
1	E	356	ARG	NE-CZ-NH1	-5.40	116.10	121.50
2	F	273	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	C	372	LEU	N-CA-C	5.39	118.18	109.40
1	G	252	LEU	N-CA-C	-5.39	105.51	111.71
2	H	269	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	H	702	SER	CA-C-N	-5.38	113.30	122.56
2	H	702	SER	C-N-CA	-5.38	113.30	122.56
2	H	251	ARG	O-C-N	-5.38	118.27	121.71
2	B	774	GLU	N-CA-C	-5.37	106.23	112.89
1	G	75	LEU	CA-C-N	-5.37	115.41	122.99
1	G	75	LEU	C-N-CA	-5.37	115.41	122.99
2	H	66	THR	N-CA-CB	-5.37	102.69	111.66
2	F	318	SER	CB-CA-C	-5.36	101.53	110.81
1	G	357	PHE	N-CA-C	5.36	117.56	111.02
1	A	434	TYR	CA-C-N	-5.36	113.10	120.28
1	A	434	TYR	C-N-CA	-5.36	113.10	120.28
2	H	534	ASP	CB-CA-C	-5.36	102.24	110.81
2	B	125	ALA	CA-C-N	-5.36	115.91	122.93
2	B	125	ALA	C-N-CA	-5.36	115.91	122.93
1	E	137	THR	CB-CA-C	-5.36	100.33	109.65
2	B	277	ARG	CA-C-N	-5.35	113.68	122.67
2	B	277	ARG	C-N-CA	-5.35	113.68	122.67
2	F	193	HIS	N-CA-C	-5.35	100.98	109.59
1	E	225	LEU	N-CA-C	5.35	119.06	112.54
2	B	599	THR	CB-CA-C	-5.34	101.20	110.45
2	F	471	VAL	CB-CA-C	-5.34	102.59	110.82
2	D	635	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	G	26	LEU	N-CA-CB	5.34	119.52	110.49
2	H	202	ILE	N-CA-C	-5.34	104.38	111.05
1	G	44	CYS	CA-CB-SG	-5.33	102.13	114.40
1	A	188	ALA	N-CA-C	-5.33	105.47	111.28
2	B	66	THR	N-CA-CB	-5.33	102.76	111.66
1	C	181	PHE	N-CA-C	5.33	118.62	110.20
2	H	176	LEU	CA-C-N	-5.33	114.67	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	176	LEU	C-N-CA	-5.33	114.67	122.19
1	G	204	GLY	N-CA-C	-5.33	105.95	112.77
2	F	347	PRO	N-CA-C	-5.33	105.85	113.47
1	G	164	PHE	CA-C-N	5.33	130.12	122.40
1	G	164	PHE	C-N-CA	5.33	130.12	122.40
2	H	771	ARG	CA-C-N	-5.33	113.14	120.28
2	H	771	ARG	C-N-CA	-5.33	113.14	120.28
2	D	191	VAL	CB-CA-C	-5.33	102.75	110.63
1	A	446	TYR	CA-C-N	-5.32	114.05	120.70
1	A	446	TYR	C-N-CA	-5.32	114.05	120.70
1	C	422	PHE	N-CA-C	5.32	117.47	109.23
2	D	61	VAL	N-CA-C	5.32	116.95	108.87
1	C	107	THR	N-CA-C	5.31	121.55	109.81
2	F	538	MET	CB-CA-C	-5.31	102.47	110.92
2	B	88	THR	CB-CA-C	-5.31	103.59	111.72
2	B	347	PRO	N-CA-C	-5.30	106.16	113.53
2	F	8	PRO	CB-CA-C	-5.30	104.28	111.12
2	F	556	ALA	N-CA-C	5.30	117.06	111.28
2	H	558	ARG	N-CA-C	-5.30	105.41	111.14
2	H	584	GLU	CA-C-N	-5.30	113.20	120.46
2	H	584	GLU	C-N-CA	-5.30	113.20	120.46
2	H	677	THR	N-CA-C	-5.29	106.84	113.72
2	D	185	PRO	N-CD-CG	-5.29	95.26	103.20
2	H	257	TYR	CB-CA-C	-5.29	101.03	109.75
2	F	612	LEU	CA-C-N	-5.28	112.29	120.31
2	F	612	LEU	C-N-CA	-5.28	112.29	120.31
1	G	179	PRO	CA-C-N	5.27	131.61	121.54
1	G	179	PRO	C-N-CA	5.27	131.61	121.54
2	B	440	THR	N-CA-CB	-5.27	102.38	110.44
2	F	98	ILE	N-CA-C	5.27	116.17	111.90
1	C	164	PHE	CA-C-N	5.27	129.82	122.08
1	C	164	PHE	C-N-CA	5.27	129.82	122.08
2	F	584	GLU	CA-C-N	-5.27	112.94	120.42
2	F	584	GLU	C-N-CA	-5.27	112.94	120.42
2	H	704	ARG	NE-CZ-NH1	-5.27	116.23	121.50
2	F	126	ILE	N-CA-CB	-5.26	104.84	111.41
2	H	218	ARG	CA-C-N	-5.26	115.81	123.06
2	H	218	ARG	C-N-CA	-5.26	115.81	123.06
1	A	195	ALA	CA-C-N	-5.25	116.37	123.46
1	A	195	ALA	C-N-CA	-5.25	116.37	123.46
1	A	328	GLN	N-CA-C	5.25	117.39	109.41
2	B	710	VAL	CA-C-N	-5.25	113.70	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	710	VAL	C-N-CA	-5.25	113.70	122.21
2	D	61	VAL	CA-C-N	-5.25	117.26	122.77
2	D	61	VAL	C-N-CA	-5.25	117.26	122.77
2	D	528	ALA	CA-C-N	-5.25	115.44	123.47
2	D	528	ALA	C-N-CA	-5.25	115.44	123.47
2	H	312	MET	N-CA-C	-5.25	105.56	111.28
1	E	455	VAL	N-CA-CB	-5.25	102.58	111.23
2	F	522	PRO	CB-CA-C	-5.24	102.91	111.56
2	H	599	THR	N-CA-C	-5.24	102.43	110.14
2	F	662	GLY	CA-C-O	5.24	126.15	120.75
2	H	618	PRO	N-CA-C	-5.24	106.90	114.18
1	C	114	MET	N-CA-C	-5.24	105.65	111.36
2	H	370	GLU	N-CA-C	-5.24	105.57	111.28
2	D	93	PHE	CA-C-N	-5.23	114.47	121.80
2	D	93	PHE	C-N-CA	-5.23	114.47	121.80
1	G	391	PRO	N-CA-C	-5.23	103.06	111.38
2	B	318	SER	CB-CA-C	-5.23	103.17	111.17
2	B	497	VAL	CB-CA-C	-5.23	105.19	111.88
2	B	624	TYR	N-CA-C	5.23	116.61	109.18
1	E	202	ILE	N-CA-C	5.23	115.49	108.17
2	B	351	LEU	N-CA-C	-5.23	105.70	111.71
1	G	105	PHE	N-CA-C	5.23	117.38	111.11
2	F	192	ILE	CB-CA-C	-5.23	103.04	110.83
2	D	69	ASP	CA-C-N	-5.22	113.54	120.65
2	D	69	ASP	C-N-CA	-5.22	113.54	120.65
2	H	768	ALA	CA-C-N	-5.22	112.01	121.14
2	H	768	ALA	C-N-CA	-5.22	112.01	121.14
1	A	28	ARG	N-CA-C	-5.22	105.66	112.23
2	B	494	ALA	CA-C-N	-5.22	113.29	120.28
2	B	494	ALA	C-N-CA	-5.22	113.29	120.28
1	C	93	GLN	N-CA-C	-5.21	105.60	111.28
2	D	115	LYS	CA-C-N	-5.21	112.75	120.94
2	D	115	LYS	C-N-CA	-5.21	112.75	120.94
1	G	181	PHE	N-CA-C	5.21	118.11	109.46
1	C	26	LEU	CB-CG-CD2	5.21	126.33	110.70
2	B	202	ILE	N-CA-C	-5.21	105.31	110.62
1	E	369	ASN	N-CA-C	5.21	116.67	107.61
1	C	25	GLU	N-CA-CB	5.21	117.62	110.07
1	E	336	VAL	CA-C-O	-5.21	115.10	121.04
2	F	281	ASP	N-CA-CB	-5.21	101.69	110.49
1	A	10	GLU	CA-CB-CG	5.20	124.51	114.10
1	A	45	GLY	CA-C-O	5.20	124.77	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	CYS	N-CA-C	5.20	117.55	108.76
2	F	587	ALA	CA-C-N	-5.20	113.68	120.44
2	F	587	ALA	C-N-CA	-5.20	113.68	120.44
2	D	731	PRO	CB-CA-C	-5.20	104.58	110.92
1	A	368	LEU	N-CA-C	5.19	117.86	109.40
2	B	619	PHE	N-CA-C	5.19	118.02	109.72
2	D	6	PRO	CA-C-O	-5.19	114.48	122.57
1	C	296	PRO	CA-C-N	-5.18	113.70	120.44
1	C	296	PRO	C-N-CA	-5.18	113.70	120.44
2	H	6	PRO	CA-C-O	-5.18	115.65	121.97
2	H	301	ALA	N-CA-C	5.18	117.01	111.36
1	G	107	THR	N-CA-C	5.18	121.26	109.81
2	D	716	PRO	CA-C-O	-5.17	115.56	121.56
1	G	83	ALA	CA-C-N	5.17	125.47	119.47
1	G	83	ALA	C-N-CA	5.17	125.47	119.47
2	B	321	VAL	CA-C-O	-5.17	117.25	119.94
2	F	247	ARG	N-CA-C	-5.17	105.77	111.71
2	D	347	PRO	CA-C-N	-5.16	113.57	120.54
2	D	347	PRO	C-N-CA	-5.16	113.57	120.54
1	C	126	ASP	CA-C-N	-5.16	111.76	120.58
1	C	126	ASP	C-N-CA	-5.16	111.76	120.58
2	H	195	SER	CA-C-N	-5.16	114.49	122.59
2	H	195	SER	C-N-CA	-5.16	114.49	122.59
2	B	743	LEU	N-CA-C	-5.16	105.15	111.75
2	F	577	GLY	CA-C-N	-5.16	113.35	122.74
2	F	577	GLY	C-N-CA	-5.16	113.35	122.74
1	C	420	GLN	N-CA-C	-5.16	106.67	113.12
2	B	23	LEU	CB-CA-C	-5.16	102.56	110.81
2	B	506	ILE	N-CA-CB	-5.16	106.68	112.45
1	C	8	ASN	CB-CA-C	-5.15	104.22	111.95
2	H	249	THR	CB-CA-C	-5.15	99.22	109.99
1	E	164	PHE	N-CA-C	5.15	118.46	110.17
2	H	291	PHE	CA-C-N	-5.15	115.83	122.99
2	H	291	PHE	C-N-CA	-5.15	115.83	122.99
1	C	354	SER	N-CA-C	5.15	115.08	108.34
1	E	291	ILE	CB-CA-C	-5.14	105.27	110.93
2	F	561	CYS	CA-CB-SG	-5.14	102.57	114.40
2	H	173	HIS	N-CA-C	5.14	117.28	111.11
2	H	239	ALA	CA-C-N	-5.14	114.08	120.56
2	H	239	ALA	C-N-CA	-5.14	114.08	120.56
2	H	483	HIS	N-CA-C	5.14	115.07	108.34
2	F	185	PRO	N-CA-C	-5.13	103.04	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	468	GLY	O-C-N	-5.13	118.80	123.57
2	B	224	MET	N-CA-C	-5.13	101.51	109.72
1	E	339	VAL	N-CA-C	-5.13	100.49	108.95
2	D	460	THR	N-CA-C	-5.13	107.03	113.28
2	D	502	ALA	N-CA-C	-5.12	105.15	111.40
2	D	740	PHE	N-CA-C	-5.12	105.61	111.14
1	C	296	PRO	N-CD-CG	-5.12	95.52	103.20
2	F	35	LEU	N-CA-C	5.12	117.66	110.14
1	C	58	ARG	CA-C-N	-5.12	115.03	122.65
1	C	58	ARG	C-N-CA	-5.12	115.03	122.65
2	F	760	PRO	N-CD-CG	-5.12	97.66	103.80
2	H	460	THR	N-CA-C	-5.12	106.55	112.89
2	B	311	ALA	N-CA-C	-5.11	105.89	111.82
2	B	760	PRO	N-CD-CG	-5.11	97.67	103.80
1	C	133	LEU	CA-C-O	-5.11	115.59	121.47
2	B	273	ARG	CA-C-N	-5.11	116.44	123.14
2	B	273	ARG	C-N-CA	-5.11	116.44	123.14
2	F	621	TYR	N-CA-C	5.11	115.79	108.74
2	B	264	VAL	N-CA-C	-5.11	106.17	111.58
2	B	576	SER	CB-CA-C	-5.11	104.35	111.80
1	A	144	ARG	CA-C-N	-5.10	113.81	120.44
1	A	144	ARG	C-N-CA	-5.10	113.81	120.44
2	D	461	LEU	CA-CB-CG	5.10	134.16	116.30
2	B	355	ARG	N-CA-C	-5.10	105.72	111.28
2	F	306	PRO	CA-C-N	-5.10	114.32	120.70
2	F	306	PRO	C-N-CA	-5.10	114.32	120.70
1	C	342	PRO	N-CD-CG	-5.10	95.56	103.20
2	B	223	ARG	NE-CZ-NH1	-5.09	116.41	121.50
2	D	223	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	H	241	ALA	N-CA-C	-5.09	105.73	111.28
2	B	147	ALA	CA-C-N	-5.08	115.82	122.99
2	B	147	ALA	C-N-CA	-5.08	115.82	122.99
1	A	44	CYS	N-CA-C	5.08	119.56	112.90
2	B	82	PRO	N-CD-CG	-5.08	95.58	103.20
1	A	181	PHE	N-CA-C	5.08	117.90	109.46
2	H	426	ASN	N-CA-C	-5.08	104.29	111.56
2	D	27	PRO	CA-C-O	-5.08	115.67	121.86
2	D	436	ALA	N-CA-C	-5.08	105.43	110.97
2	F	539	ALA	CA-C-N	-5.08	114.16	120.56
2	F	539	ALA	C-N-CA	-5.08	114.16	120.56
2	F	10	ASP	CA-C-N	-5.08	114.67	123.25
2	F	10	ASP	C-N-CA	-5.08	114.67	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	363	GLY	CA-C-N	-5.08	114.56	122.73
2	H	363	GLY	C-N-CA	-5.08	114.56	122.73
2	D	500	ALA	CA-C-N	-5.07	112.25	120.72
2	D	500	ALA	C-N-CA	-5.07	112.25	120.72
1	A	346	PRO	N-CA-C	-5.07	107.25	113.84
1	E	243	ILE	N-CA-C	5.07	114.87	107.37
2	F	19	GLN	CA-C-N	-5.07	113.86	120.95
2	F	19	GLN	C-N-CA	-5.07	113.86	120.95
2	H	631	VAL	N-CA-C	5.07	114.71	108.53
1	G	14	VAL	N-CA-C	5.06	117.11	108.86
2	H	770	VAL	N-CA-C	-5.06	105.56	110.42
2	D	329	HIS	CA-C-N	-5.06	115.65	123.14
2	D	329	HIS	C-N-CA	-5.06	115.65	123.14
2	D	197	GLN	N-CA-C	-5.06	106.89	113.16
2	D	163	GLU	N-CA-C	-5.06	101.91	109.95
1	G	208	VAL	CB-CA-C	-5.05	105.31	112.14
2	H	564	ARG	CA-C-N	-5.05	114.63	122.67
2	H	564	ARG	C-N-CA	-5.05	114.63	122.67
2	H	508	PRO	CB-CA-C	-5.05	103.23	111.56
2	B	239	ALA	CA-C-N	-5.05	114.20	120.56
2	B	239	ALA	C-N-CA	-5.05	114.20	120.56
1	E	432	ALA	CA-C-N	-5.05	113.77	120.79
1	E	432	ALA	C-N-CA	-5.05	113.77	120.79
2	F	146	TRP	N-CA-C	-5.05	101.52	109.50
1	A	70	ILE	CB-CA-C	-5.05	105.44	111.85
1	E	296	PRO	N-CD-CG	-5.04	95.64	103.20
2	B	586	VAL	CB-CA-C	-5.04	105.43	111.88
2	H	250	GLY	CA-C-N	-5.04	114.09	123.11
2	H	250	GLY	C-N-CA	-5.04	114.09	123.11
2	B	230	GLY	N-CA-C	-5.04	108.81	114.40
1	A	164	PHE	CA-C-N	5.03	129.28	122.19
1	A	164	PHE	C-N-CA	5.03	129.28	122.19
2	H	83	GLU	N-CA-C	-5.02	98.71	109.81
2	B	446	ARG	N-CA-C	-5.01	102.65	110.42
2	F	27	PRO	N-CA-C	-5.01	103.41	111.38
2	B	566	VAL	CA-C-N	-5.01	116.58	123.14
2	B	566	VAL	C-N-CA	-5.01	116.58	123.14
2	D	353	MET	N-CA-C	-5.01	105.90	111.36
2	B	299	TRP	N-CA-C	5.00	119.25	113.20
1	G	82	ALA	N-CA-C	-5.00	103.12	110.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3370	0	3368	272	0
1	C	3370	0	3368	184	0
1	E	3370	0	3370	319	1
1	G	3370	0	3370	323	1
2	B	5717	0	5630	362	0
2	D	5717	0	5631	343	0
2	F	5717	0	5631	422	0
2	H	5717	0	5630	454	0
3	A	8	0	0	1	0
3	C	8	0	0	0	0
3	E	8	0	0	6	0
3	G	8	0	0	3	0
4	A	53	0	31	10	0
4	C	53	0	30	3	0
4	E	53	0	30	10	0
4	G	53	0	31	9	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	B	24	0	10	4	0
6	D	24	0	10	4	0
6	F	24	0	11	7	0
6	H	24	0	10	7	0
7	B	3	0	0	4	0
7	D	3	0	0	7	0
7	F	3	0	0	8	0
7	H	3	0	0	5	0
8	B	11	0	3	9	0
8	D	11	0	3	5	0
8	F	11	0	3	5	0
8	H	11	0	3	4	0
All	All	36748	0	36173	2615	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (2615) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:689:MET:CE	2:D:689:MET:SD	2.04	1.46
1:E:95:MET:SD	1:E:114:MET:HE1	1.62	1.36
1:E:381:ARG:HH21	1:E:393:ARG:NH2	1.30	1.28
1:A:425:LEU:CD1	2:F:579:SER:HB3	1.62	1.27
2:D:496:MET:HE2	2:D:496:MET:CA	1.68	1.20
1:A:425:LEU:HD12	2:F:579:SER:HB3	1.22	1.14
1:E:301:MET:HE3	1:E:341:LEU:HB3	1.29	1.13
1:A:348:LEU:HD12	1:A:349:ARG:N	1.62	1.13
2:D:339:THR:HG23	2:D:340:ALA:N	1.56	1.12
2:H:312:MET:HE2	2:H:330:ARG:HH12	0.94	1.10
2:B:339:THR:HG23	2:B:340:ALA:N	1.59	1.10
1:G:325:TYR:O	1:G:326:ARG:HB2	1.52	1.09
2:D:496:MET:HA	2:D:496:MET:CE	1.83	1.08
1:A:348:LEU:HD12	1:A:349:ARG:H	1.10	1.07
2:B:560:GLY:O	2:B:561:CYS:HB3	1.48	1.07
2:D:507:ASP:OD1	2:D:508:PRO:HD2	1.55	1.07
2:B:704:ARG:HG2	2:B:704:ARG:HH11	0.98	1.06
1:A:138:GLY:O	1:A:139:TYR:HB2	1.53	1.06
1:C:133:LEU:HD13	2:D:698:ILE:HD11	1.37	1.06
2:F:657:PRO:O	2:F:661:ILE:HG12	1.56	1.05
2:H:496:MET:HE2	2:H:496:MET:HA	1.34	1.05
2:B:704:ARG:HH11	2:B:704:ARG:CG	1.65	1.04
2:H:631:VAL:HG12	2:H:642:ILE:HA	1.33	1.04
1:G:455:VAL:HG22	2:H:443:THR:HG21	1.38	1.04
1:G:390:VAL:HG22	1:G:391:PRO:HD2	1.38	1.03
1:G:301:MET:HE3	1:G:341:LEU:HB3	1.41	1.02
2:F:621:TYR:CE1	2:F:726:LYS:HG2	1.95	1.02
2:H:312:MET:HE2	2:H:330:ARG:NH1	1.74	1.01
2:H:446:ARG:HG2	2:H:632:VAL:CG1	1.91	1.01
1:A:301:MET:HE3	1:A:341:LEU:HB3	1.40	1.00
1:G:353:LEU:HD21	1:G:434:TYR:OH	1.62	1.00
2:H:296:ARG:HG3	2:H:296:ARG:NH1	1.74	0.99
2:H:138:ARG:NH2	2:H:329:HIS:ND1	2.07	0.99
2:D:312:MET:HE2	2:D:330:ARG:HH12	1.27	0.99
1:A:95:MET:SD	1:A:114:MET:HE1	2.03	0.99
1:G:50:MET:CE	1:G:116:ALA:HA	1.93	0.98
1:E:325:TYR:O	1:E:326:ARG:HB2	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:408:GLU:OE1	2:H:442:ARG:NH2	1.96	0.98
2:H:339:THR:HG23	2:H:340:ALA:N	1.73	0.98
1:E:381:ARG:HH21	1:E:393:ARG:CZ	1.78	0.97
2:H:560:GLY:O	2:H:561:CYS:HB3	1.63	0.97
1:A:301:MET:HE2	1:A:341:LEU:HD22	1.46	0.96
2:H:621:TYR:HE1	2:H:726:LYS:HG2	1.27	0.96
2:B:558:ARG:HD3	2:B:559:GLU:OE2	1.64	0.96
2:B:704:ARG:HG2	2:B:704:ARG:NH1	1.78	0.95
2:D:138:ARG:NH2	2:D:329:HIS:ND1	2.14	0.95
1:C:301:MET:HE2	1:C:341:LEU:HD22	1.49	0.95
1:G:237:THR:HG23	1:G:238:PRO:CD	1.96	0.95
1:E:301:MET:CE	1:E:341:LEU:HB3	1.95	0.95
1:E:381:ARG:NH2	1:E:393:ARG:NH2	2.14	0.95
2:F:305:LEU:HB3	2:F:306:PRO:HD3	1.49	0.94
2:H:731:PRO:N	2:H:732:PRO:HD2	1.79	0.94
1:E:368:LEU:HD12	1:E:368:LEU:N	1.81	0.94
1:G:50:MET:HE3	1:G:116:ALA:HB2	1.50	0.94
2:H:66:THR:HG22	2:H:68:ALA:H	1.31	0.93
1:G:368:LEU:N	1:G:368:LEU:HD12	1.81	0.93
1:A:390:VAL:HG22	1:A:391:PRO:HD2	1.49	0.93
1:C:301:MET:HE3	1:C:341:LEU:HB3	1.51	0.93
2:H:561:CYS:SG	2:H:562:ALA:N	2.42	0.93
1:E:102:GLN:HB3	2:F:489:GLY:O	1.68	0.93
2:H:198:HIS:CG	2:H:526:ALA:HB2	2.02	0.92
1:G:210:LEU:N	1:G:210:LEU:HD23	1.83	0.92
2:B:446:ARG:HG2	2:B:632:VAL:HG13	1.50	0.92
2:F:538:MET:HG3	2:F:602:TYR:CE1	2.05	0.92
2:F:339:THR:HG23	2:F:340:ALA:N	1.84	0.91
1:E:266:LEU:O	1:E:268:ARG:N	2.04	0.91
1:E:301:MET:HE2	1:E:341:LEU:HD22	1.50	0.91
2:H:303:LEU:O	2:H:306:PRO:HD2	1.70	0.91
2:D:360:LEU:HG	2:D:364:MET:HE3	1.53	0.91
1:G:50:MET:HE3	1:G:116:ALA:CB	2.00	0.91
2:F:312:MET:HE2	2:F:330:ARG:HH12	1.36	0.91
2:B:319:TYR:OH	2:B:372:ARG:HD3	1.70	0.91
1:E:6:LEU:HD12	1:E:10:GLU:O	1.70	0.91
1:E:314:ARG:HD3	1:E:334:GLU:OE1	1.71	0.91
2:D:528:ALA:O	2:D:529:ALA:HB3	1.68	0.90
2:D:144:VAL:HG11	2:D:312:MET:HE1	1.54	0.90
2:F:66:THR:HG22	2:F:68:ALA:H	1.34	0.90
2:F:621:TYR:HE1	2:F:726:LYS:HG2	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:296:ARG:HG3	2:H:296:ARG:HH11	1.28	0.90
2:D:496:MET:CA	2:D:496:MET:CE	2.46	0.90
1:C:237:THR:HG23	1:C:238:PRO:CD	2.01	0.90
2:H:621:TYR:CE1	2:H:726:LYS:HG2	2.06	0.90
1:G:106:CYS:HG	3:G:3001:FES:FE2	0.68	0.89
1:G:301:MET:CE	1:G:341:LEU:HB3	2.01	0.89
1:C:314:ARG:O	1:C:315:ARG:HB2	1.70	0.89
1:E:225:LEU:N	1:E:225:LEU:HD23	1.87	0.89
1:G:138:GLY:O	1:G:139:TYR:HB2	1.73	0.89
2:B:560:GLY:O	2:B:561:CYS:CB	2.21	0.88
1:G:50:MET:HE3	1:G:116:ALA:CA	2.01	0.88
2:H:319:TYR:OH	2:H:372:ARG:HD3	1.72	0.88
2:D:58:SER:OG	2:D:59:PRO:HD2	1.72	0.88
1:E:95:MET:SD	1:E:114:MET:CE	2.58	0.88
2:H:457:ILE:O	2:H:458:SER:HB2	1.72	0.88
1:A:425:LEU:HD12	2:F:579:SER:CB	2.02	0.88
2:B:731:PRO:HB2	2:B:732:PRO:HD3	1.53	0.88
1:G:364:VAL:CG2	1:G:435:ARG:HG2	2.03	0.88
1:C:41:GLU:HG3	1:C:214:LYS:HE3	1.55	0.87
1:E:6:LEU:HD12	1:E:10:GLU:C	1.98	0.87
2:D:538:MET:HG3	2:D:602:TYR:CE1	2.09	0.87
1:A:325:TYR:O	1:A:326:ARG:HB2	1.73	0.87
2:B:66:THR:HG22	2:B:68:ALA:H	1.40	0.87
2:H:517:ASP:OD2	2:H:519:SER:N	2.07	0.87
1:A:237:THR:HG23	1:A:238:PRO:CD	2.04	0.87
2:D:560:GLY:O	2:D:561:CYS:HB3	1.73	0.87
1:E:367:CYS:C	1:E:368:LEU:HD12	1.99	0.87
2:H:446:ARG:HG2	2:H:632:VAL:HG12	1.56	0.87
1:E:399:ALA:O	1:E:401:LEU:N	2.07	0.86
2:F:247:ARG:HG2	2:F:247:ARG:HH11	1.38	0.86
2:F:507:ASP:OD1	2:F:508:PRO:HD2	1.75	0.86
2:H:195:SER:O	2:H:231:LYS:HD3	1.75	0.86
2:H:496:MET:HE2	2:H:496:MET:CA	2.05	0.86
2:F:218:ARG:NE	2:F:220:GLU:OE2	2.06	0.86
1:E:237:THR:HG23	1:E:238:PRO:CD	2.06	0.86
2:D:247:ARG:HG2	2:D:247:ARG:HH11	1.39	0.86
1:G:58:ARG:HD3	1:G:277:GLN:OE1	1.76	0.86
2:H:312:MET:CE	2:H:330:ARG:HH12	1.84	0.86
1:G:348:LEU:HD12	1:G:349:ARG:H	1.40	0.86
1:G:322:PHE:HB3	1:G:390:VAL:CG2	2.05	0.85
2:B:496:MET:HE2	2:B:496:MET:HA	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301:MET:HE2	1:G:341:LEU:HD22	1.56	0.85
1:A:26:LEU:HD13	1:A:67:LEU:HD11	1.57	0.85
1:G:364:VAL:HG22	1:G:435:ARG:HG2	1.59	0.84
2:H:538:MET:HG3	2:H:602:TYR:CE1	2.12	0.84
1:E:44:CYS:HG	3:E:3002:FES:FE2	0.58	0.84
2:D:339:THR:CG2	2:D:340:ALA:N	2.35	0.84
2:H:247:ARG:HG2	2:H:247:ARG:HH11	1.42	0.84
2:D:496:MET:HE2	2:D:496:MET:HA	0.90	0.84
1:E:349:ARG:HD3	1:E:449:GLU:OE2	1.76	0.84
1:C:301:MET:CE	1:C:341:LEU:HB3	2.08	0.84
2:F:138:ARG:NH2	2:F:329:HIS:ND1	2.26	0.84
2:D:528:ALA:HB1	8:D:4000:141:C7	2.08	0.83
1:C:237:THR:HG23	1:C:238:PRO:HD2	1.60	0.83
2:D:24:ASP:OD2	2:D:254:LYS:NZ	2.10	0.83
2:F:559:GLU:OE1	2:F:578:LYS:NZ	2.11	0.83
1:G:390:VAL:HG22	1:G:391:PRO:CD	2.07	0.83
6:H:3003:MTE:S1'	7:H:3004:MOS:S	2.77	0.83
2:F:319:TYR:OH	2:F:372:ARG:HD3	1.77	0.83
2:D:731:PRO:N	2:D:732:PRO:HD2	1.92	0.83
1:G:348:LEU:HD12	1:G:349:ARG:N	1.93	0.83
1:A:18:ASP:OD2	1:A:19:PRO:HD2	1.79	0.83
2:H:79:ALA:HB1	2:H:80:PRO:HD2	1.60	0.82
2:H:731:PRO:CD	2:H:732:PRO:HD2	2.09	0.82
2:F:58:SER:OG	2:F:59:PRO:HD2	1.77	0.82
2:B:138:ARG:NH2	2:B:329:HIS:ND1	2.26	0.82
2:B:704:ARG:CG	2:B:704:ARG:NH1	2.28	0.82
2:H:60:GLY:O	2:H:103:ALA:HB1	1.80	0.82
2:B:684:HIS:CE1	2:F:567:ILE:HD11	2.15	0.82
2:D:179:GLN:HB3	2:D:238:LEU:HD13	1.61	0.82
1:A:425:LEU:HD11	2:F:579:SER:HB3	1.58	0.82
1:G:390:VAL:CG2	1:G:391:PRO:HD2	2.10	0.82
1:G:314:ARG:HD3	1:G:334:GLU:OE1	1.80	0.82
1:E:399:ALA:C	1:E:401:LEU:H	1.88	0.82
2:F:528:ALA:HB1	8:F:4000:141:C7	2.10	0.82
1:G:102:GLN:HB3	2:H:489:GLY:O	1.80	0.81
1:A:368:LEU:N	1:A:368:LEU:HD12	1.94	0.81
1:E:83:ALA:HB2	1:E:157:TRP:CD2	2.15	0.81
2:F:573:VAL:HG21	2:F:585:ILE:HG13	1.60	0.81
2:D:507:ASP:OD1	2:D:508:PRO:CD	2.27	0.81
1:A:24:LEU:HD21	1:A:37:GLU:HB2	1.62	0.81
2:H:198:HIS:ND1	2:H:526:ALA:HB2	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:ARG:HD3	1:G:449:GLU:OE2	1.81	0.81
1:G:373:LYS:HB2	1:G:378:GLU:HG2	1.62	0.81
2:H:305:LEU:HD23	2:H:305:LEU:C	2.06	0.80
4:A:3005:FAD:H8A	4:A:3005:FAD:H51A	1.63	0.80
2:F:632:VAL:HG22	2:F:643:LEU:HD11	1.63	0.80
1:A:399:ALA:O	1:A:401:LEU:N	2.13	0.80
2:B:558:ARG:CD	2:B:559:GLU:OE2	2.29	0.80
2:D:513:ILE:HG13	2:D:514:THR:N	1.97	0.80
1:E:22:SER:OG	1:E:25:GLU:HG2	1.80	0.80
2:F:221:MET:HE1	2:F:224:MET:HG3	1.61	0.80
2:B:513:ILE:HG13	2:B:514:THR:N	1.97	0.80
2:B:684:HIS:ND1	2:F:567:ILE:HD11	1.97	0.80
2:F:216:ASP:OD1	2:H:512:ARG:HD2	1.81	0.80
1:A:351:TYR:HB3	1:A:442:MET:HE2	1.64	0.79
1:E:366:GLY:HA3	1:E:442:MET:SD	2.22	0.79
1:G:134:CYS:SG	1:G:137:THR:HG23	2.22	0.79
1:G:237:THR:CG2	1:G:239:ASP:H	1.95	0.79
1:E:44:CYS:SG	3:E:3002:FES:FE2	1.72	0.79
1:A:367:CYS:C	1:A:368:LEU:HD12	2.06	0.79
2:F:665:GLU:HG2	2:F:710:VAL:HG21	1.64	0.79
2:F:720:GLU:HG2	2:F:724:ARG:NH2	1.96	0.79
1:C:349:ARG:HD3	1:C:449:GLU:OE2	1.82	0.79
2:D:621:TYR:CE1	2:D:726:LYS:HG2	2.18	0.79
1:A:252:LEU:CD2	1:A:281:ILE:HD13	2.13	0.78
1:A:390:VAL:HG22	1:A:391:PRO:CD	2.13	0.78
6:F:3003:MTE:SI'	7:F:3004:MOS:O2	2.42	0.78
2:D:278:ILE:HD11	2:D:286:LEU:HD22	1.64	0.78
1:A:390:VAL:HG13	1:A:391:PRO:O	1.84	0.78
1:C:314:ARG:HD3	1:C:334:GLU:OE1	1.84	0.78
2:D:635:ARG:HD3	2:D:750:CYS:SG	2.23	0.78
1:E:237:THR:CG2	1:E:239:ASP:H	1.96	0.78
2:B:496:MET:HE2	2:B:496:MET:CA	2.14	0.77
1:E:127:ASP:OD2	1:E:268:ARG:HD2	1.84	0.77
1:A:301:MET:CE	1:A:341:LEU:HB3	2.15	0.77
1:A:432:ALA:O	1:A:433:ALA:C	2.24	0.77
2:F:197:GLN:HG2	2:F:224:MET:HE1	1.65	0.77
2:B:492:LEU:C	2:B:492:LEU:HD12	2.07	0.77
2:B:731:PRO:HB2	2:B:732:PRO:CD	2.15	0.77
1:E:302:GLY:HA2	1:E:381:ARG:HH11	1.48	0.77
2:H:635:ARG:HD3	2:H:750:CYS:SG	2.24	0.77
2:D:319:TYR:OH	2:D:372:ARG:HD3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:263:MET:HE3	2:H:692:ALA:HA	1.65	0.77
2:B:531:SER:HB2	2:B:535:MET:HE2	1.67	0.77
1:C:316:MET:HB2	1:C:317:PRO:HD2	1.66	0.77
2:D:632:VAL:HG22	2:D:643:LEU:HD11	1.67	0.77
1:E:381:ARG:NH2	1:E:393:ARG:CZ	2.46	0.77
2:F:563:ALA:O	2:F:566:VAL:HG23	1.83	0.77
2:D:621:TYR:HE1	2:D:726:LYS:HG2	1.49	0.77
1:E:316:MET:HB2	1:E:317:PRO:HD2	1.66	0.77
2:B:221:MET:O	2:B:221:MET:HG3	1.81	0.76
4:C:3005:FAD:N1	4:C:3005:FAD:H2'	1.99	0.76
1:G:50:MET:HE3	1:G:116:ALA:HA	1.62	0.76
2:F:720:GLU:HG2	2:F:724:ARG:HH21	1.48	0.76
2:D:224:MET:HE3	2:D:488:MET:HB3	1.67	0.76
1:E:32:LEU:HD22	1:E:79:GLU:HG3	1.66	0.76
1:G:373:LYS:O	1:G:374:GLY:O	2.04	0.76
1:C:165:THR:C	1:C:166:LEU:HD23	2.09	0.76
2:F:65:PHE:HB2	2:F:100:LEU:HB3	1.67	0.76
2:H:691:HIS:O	2:H:692:ALA:HB2	1.84	0.76
1:G:115:ALA:O	1:G:116:ALA:C	2.27	0.76
1:G:237:THR:HG23	1:G:238:PRO:HD2	1.68	0.76
1:E:192:TRP:O	1:E:196:HIS:HD2	1.69	0.76
2:B:40:SER:HB2	2:B:91:VAL:HG11	1.67	0.75
2:F:538:MET:HG3	2:F:602:TYR:CD1	2.20	0.75
2:B:674:TRP:CE3	2:B:675:LEU:HD21	2.21	0.75
4:A:3005:FAD:H51A	4:A:3005:FAD:C8A	2.16	0.75
2:H:123:ARG:HB3	2:H:124:PRO:HD2	1.68	0.75
2:B:42:GLU:OE1	2:F:564:ARG:NH2	2.19	0.75
2:H:559:GLU:O	2:H:560:GLY:O	2.03	0.75
1:G:418:LEU:HB3	1:G:436:MET:HE1	1.69	0.75
2:H:224:MET:HE3	2:H:488:MET:HB3	1.68	0.75
1:A:351:TYR:CB	1:A:442:MET:HE2	2.17	0.75
1:G:367:CYS:C	1:G:368:LEU:HD12	2.11	0.74
1:A:399:ALA:C	1:A:401:LEU:H	1.95	0.74
2:D:325:ARG:C	2:D:326:ILE:HG13	2.11	0.74
1:A:301:MET:CE	1:A:341:LEU:HD22	2.17	0.74
2:D:303:LEU:O	2:D:306:PRO:HD2	1.87	0.74
1:E:381:ARG:HH21	1:E:393:ARG:HH21	1.35	0.74
1:C:325:TYR:O	1:C:326:ARG:HB2	1.85	0.74
2:B:517:ASP:OD2	2:B:519:SER:OG	2.05	0.74
2:D:407:GLN:OE1	2:D:618:PRO:HD2	1.87	0.74
2:B:530:SER:OG	2:B:730:GLU:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ALA:HB2	1:E:157:TRP:CE3	2.23	0.74
2:F:296:ARG:HG3	2:F:296:ARG:NH1	2.03	0.74
6:F:3003:MTE:S1'	7:F:3004:MOS:S	2.83	0.74
2:H:674:TRP:CE3	2:H:675:LEU:HD21	2.23	0.74
2:H:701:PHE:O	2:H:704:ARG:HG2	1.88	0.73
1:G:237:THR:HG23	1:G:238:PRO:CG	2.18	0.73
2:H:247:ARG:HG2	2:H:247:ARG:NH1	2.01	0.73
1:A:233:GLN:OE1	1:A:233:GLN:HA	1.87	0.73
2:B:728:VAL:O	2:B:728:VAL:HG22	1.88	0.73
1:C:50:MET:HE3	1:C:116:ALA:HA	1.68	0.73
1:G:41:GLU:HG3	1:G:214:LYS:HE3	1.68	0.73
2:H:367:ASP:OD2	2:H:431:ARG:NH1	2.17	0.73
2:D:247:ARG:HG2	2:D:247:ARG:NH1	2.01	0.73
1:E:133:LEU:HD13	2:F:698:ILE:HD11	1.71	0.73
1:C:367:CYS:C	1:C:368:LEU:HD12	2.14	0.73
1:A:314:ARG:HD3	1:A:334:GLU:OE1	1.88	0.73
1:G:366:GLY:HA3	1:G:442:MET:SD	2.28	0.73
2:H:105:SER:O	2:H:106:HIS:C	2.30	0.73
2:H:296:ARG:HH11	2:H:296:ARG:CG	1.96	0.73
1:A:128:LEU:C	1:A:129:LEU:HD23	2.14	0.73
1:C:279:ALA:HB1	4:C:3005:FAD:H4'	1.69	0.73
1:C:360:ASP:OD1	2:D:697:LYS:HE3	1.88	0.73
2:H:58:SER:OG	2:H:59:PRO:HD2	1.88	0.73
2:H:412:CYS:HA	2:H:624:TYR:CZ	2.24	0.73
1:G:432:ALA:O	1:G:433:ALA:C	2.27	0.72
2:F:720:GLU:CG	2:F:724:ARG:HH21	2.01	0.72
1:E:337:GLU:O	1:E:338:SER:HB3	1.87	0.72
2:D:730:GLU:C	2:D:732:PRO:HD2	2.13	0.72
2:H:507:ASP:OD1	2:H:508:PRO:CD	2.37	0.72
1:A:128:LEU:O	1:A:129:LEU:HD23	1.89	0.72
1:A:271:ALA:HA	1:A:359:GLN:NE2	2.05	0.72
2:B:621:TYR:CE1	2:B:726:LYS:HG2	2.24	0.72
1:C:12:ARG:NH2	1:C:30:GLU:OE1	2.20	0.72
1:E:319:GLU:OE2	1:E:319:GLU:N	2.22	0.72
1:G:353:LEU:HD21	1:G:434:TYR:HH	1.53	0.72
1:A:237:THR:HG23	1:A:238:PRO:HD2	1.72	0.72
1:E:83:ALA:HB2	1:E:157:TRP:CE2	2.25	0.72
7:B:3004:MOS:MO	7:B:3004:MOS:S	2.01	0.72
2:D:232:GLU:OE2	8:D:4000:141:H1	1.89	0.72
2:D:631:VAL:HG21	2:D:743:LEU:CD1	2.20	0.72
1:E:390:VAL:HG23	1:E:391:PRO:HD2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:ALA:HA	1:G:359:GLN:NE2	2.05	0.72
2:H:417:LEU:HG	2:H:648:LEU:HD23	1.71	0.72
2:B:303:LEU:O	2:B:306:PRO:HD2	1.89	0.71
1:E:266:LEU:O	1:E:267:LEU:C	2.32	0.71
2:H:731:PRO:HB2	2:H:732:PRO:CD	2.20	0.71
1:C:60:VAL:HG21	1:C:65:MET:HE1	1.71	0.71
2:B:561:CYS:SG	2:B:562:ALA:N	2.63	0.71
1:E:58:ARG:HG2	1:E:277:GLN:OE1	1.90	0.71
1:E:358:ASP:OD2	2:F:702:SER:HB3	1.90	0.71
1:A:41:GLU:HG3	1:A:214:LYS:HE3	1.72	0.71
2:D:731:PRO:CD	2:D:732:PRO:HD2	2.19	0.71
1:E:89:HIS:O	1:E:90:PRO:C	2.29	0.71
1:C:319:GLU:N	1:C:319:GLU:OE2	2.22	0.71
2:D:329:HIS:HB3	2:D:331:LEU:HD21	1.71	0.71
2:F:221:MET:CE	2:F:224:MET:HG3	2.20	0.71
1:A:373:LYS:HB2	1:A:378:GLU:HG2	1.72	0.71
1:E:37:GLU:CD	2:F:256:ARG:NH2	2.49	0.71
1:E:314:ARG:HH22	1:E:329:ASP:CG	1.97	0.71
2:D:360:LEU:CG	2:D:364:MET:HE3	2.19	0.71
1:E:316:MET:HE1	1:E:329:ASP:OD2	1.90	0.71
1:C:301:MET:HE1	1:C:341:LEU:HD13	1.71	0.71
1:E:360:ASP:OD1	2:F:697:LYS:HE3	1.91	0.71
1:G:115:ALA:O	1:G:118:HIS:N	2.24	0.71
1:G:252:LEU:CD2	1:G:281:ILE:HD13	2.19	0.71
2:H:280:ALA:C	2:H:287:LEU:HD12	2.16	0.71
2:H:673:GLY:O	2:H:678:GLU:HB2	1.91	0.71
1:A:110:PHE:HB3	1:A:114:MET:HE2	1.73	0.71
1:A:322:PHE:HB3	1:A:390:VAL:CG2	2.21	0.71
2:D:198:HIS:CG	2:D:526:ALA:HB2	2.26	0.71
2:H:595:SER:O	2:H:596:LEU:HD23	1.91	0.70
2:B:691:HIS:O	2:B:692:ALA:HB2	1.91	0.70
2:F:635:ARG:HD3	2:F:750:CYS:SG	2.31	0.70
2:B:744:HIS:C	2:B:744:HIS:CD2	2.70	0.70
2:H:671:GLY:O	2:H:674:TRP:HB3	1.90	0.70
2:B:360:LEU:HG	2:B:364:MET:HE3	1.74	0.70
2:H:448:ILE:HG13	2:H:630:GLU:HB2	1.73	0.70
7:D:3004:MOS:S	7:D:3004:MOS:MO	2.03	0.70
2:F:144:VAL:HG11	2:F:312:MET:HE1	1.72	0.70
7:F:3004:MOS:S	7:F:3004:MOS:MO	2.01	0.70
1:C:373:LYS:O	1:C:374:GLY:O	2.10	0.70
1:E:237:THR:HG22	1:E:239:ASP:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:HIS:C	2:B:35:LEU:HD23	2.16	0.70
1:E:129:LEU:O	1:E:130:ALA:C	2.32	0.70
2:F:367:ASP:OD2	2:F:431:ARG:NH1	2.21	0.70
2:B:617:ARG:HD3	2:B:619:PHE:O	1.92	0.69
1:G:37:GLU:OE1	2:H:256:ARG:NH2	2.25	0.69
1:G:314:ARG:HH22	1:G:329:ASP:CG	2.00	0.69
2:H:776:ARG:O	2:H:777:ALA:HB3	1.92	0.69
2:B:325:ARG:C	2:B:326:ILE:HG13	2.17	0.69
2:D:559:GLU:OE1	2:D:578:LYS:NZ	2.15	0.69
1:E:243:ILE:CD1	1:E:341:LEU:HD11	2.21	0.69
2:B:457:ILE:O	2:B:458:SER:HB2	1.93	0.69
2:F:303:LEU:O	2:F:306:PRO:HD2	1.93	0.69
2:H:507:ASP:OD1	2:H:508:PRO:HD2	1.92	0.69
2:F:66:THR:HG22	2:F:68:ALA:N	2.08	0.69
2:F:498:GLN:O	2:F:499:VAL:C	2.35	0.69
1:A:359:GLN:HG3	1:A:359:GLN:O	1.93	0.69
2:B:107:ARG:O	2:B:108:ALA:C	2.33	0.69
2:B:296:ARG:HG3	2:B:296:ARG:NH1	2.08	0.69
2:B:367:ASP:OD1	2:B:368:PRO:HD2	1.93	0.69
1:E:445:ARG:NH2	2:F:634:ASP:OD2	2.26	0.69
2:F:247:ARG:HG2	2:F:247:ARG:NH1	2.05	0.69
2:H:757:LEU:HD12	2:H:758:GLN:N	2.07	0.69
1:A:446:TYR:CE2	1:A:450:LEU:HD12	2.28	0.69
2:B:150:ASP:C	2:B:150:ASP:OD1	2.35	0.69
1:E:349:ARG:HG2	1:E:351:TYR:OH	1.93	0.68
1:C:368:LEU:HD12	1:C:368:LEU:N	2.08	0.68
2:D:631:VAL:HG21	2:D:743:LEU:HD13	1.74	0.68
1:G:237:THR:HG23	1:G:238:PRO:HG2	1.76	0.68
2:H:65:PHE:HB2	2:H:100:LEU:HB3	1.74	0.68
2:D:310:ARG:HD2	2:D:344:PHE:O	1.93	0.68
2:D:728:VAL:O	2:D:728:VAL:HG22	1.93	0.68
2:F:728:VAL:O	2:F:728:VAL:HG22	1.91	0.68
2:H:276:TYR:OH	2:H:359:HIS:HD2	1.76	0.68
2:H:457:ILE:O	2:H:458:SER:CB	2.42	0.68
1:A:103:CYS:HB3	1:A:136:CYS:SG	2.33	0.68
2:F:422:GLN:HG2	2:F:427:PHE:CD2	2.28	0.68
2:F:446:ARG:NH1	2:F:630:GLU:OE2	2.25	0.68
1:E:302:GLY:CA	1:E:381:ARG:HH11	2.05	0.68
2:F:324:LEU:HD23	2:F:324:LEU:C	2.19	0.68
2:H:528:ALA:HB1	8:H:4000:141:C7	2.23	0.68
2:H:656:ASN:ND2	2:H:659:LEU:HD12	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:LEU:HD11	2:D:364:MET:CE	2.23	0.68
1:E:299:ILE:HG13	1:E:318:LEU:HD23	1.75	0.68
2:F:730:GLU:C	2:F:732:PRO:HD2	2.18	0.68
2:H:171:GLN:HG3	2:H:678:GLU:OE1	1.94	0.68
2:D:61:VAL:HG12	2:D:62:ILE:N	2.09	0.68
2:F:310:ARG:HD2	2:F:344:PHE:O	1.93	0.68
1:G:283:GLY:O	1:G:284:ASN:C	2.34	0.68
1:G:415:LEU:HB2	1:G:416:PRO:HD3	1.75	0.68
2:B:448:ILE:HG13	2:B:630:GLU:HB2	1.75	0.67
2:B:461:LEU:HD12	2:B:463:HIS:CE1	2.29	0.67
2:B:563:ALA:O	2:B:566:VAL:HG23	1.94	0.67
2:F:195:SER:O	2:F:231:LYS:HD3	1.94	0.67
1:A:361:ILE:HD12	1:A:429:ARG:NH2	2.09	0.67
1:A:408:GLU:CD	2:B:442:ARG:HH22	2.02	0.67
1:A:297:ALA:HA	1:A:367:CYS:SG	2.34	0.67
1:E:399:ALA:C	1:E:401:LEU:N	2.48	0.67
2:F:179:GLN:HB3	2:F:238:LEU:HD13	1.75	0.67
1:G:237:THR:OG1	1:G:238:PRO:HD2	1.94	0.67
2:D:678:GLU:HB3	2:D:696:TYR:CZ	2.29	0.67
1:E:352:LYS:HE3	1:E:362:SER:OG	1.93	0.67
1:G:24:LEU:HD21	1:G:37:GLU:HB2	1.77	0.67
1:E:273:GLU:OE1	1:E:276:ARG:NH1	2.27	0.67
2:D:471:VAL:HG12	2:D:472:GLN:N	2.10	0.67
4:A:3005:FAD:N1	4:A:3005:FAD:H2'	2.10	0.67
2:B:538:MET:HG3	2:B:602:TYR:CE1	2.29	0.67
1:E:283:GLY:O	1:E:284:ASN:C	2.36	0.67
1:E:298:LEU:O	1:E:299:ILE:C	2.34	0.67
1:G:337:GLU:HG3	1:G:337:GLU:O	1.94	0.67
2:H:347:PRO:HG3	2:H:734:LEU:HD11	1.75	0.67
2:H:496:MET:HA	2:H:496:MET:CE	2.14	0.67
2:B:776:ARG:O	2:B:777:ALA:HB3	1.95	0.67
1:G:59:ALA:C	1:G:60:VAL:HG13	2.19	0.67
1:A:445:ARG:HG3	1:A:455:VAL:HG11	1.76	0.67
2:H:644:ARG:HB2	2:H:707:ILE:HB	1.77	0.67
2:D:678:GLU:OE1	2:D:696:TYR:OH	2.13	0.66
1:G:387:MET:HE1	1:G:436:MET:HA	1.76	0.66
2:H:38:GLY:C	2:H:39:LEU:HD23	2.20	0.66
2:H:668:TYR:O	2:H:669:VAL:C	2.35	0.66
2:B:422:GLN:HG2	2:B:427:PHE:CD2	2.30	0.66
2:D:660:ASP:O	2:D:664:ILE:HG13	1.95	0.66
2:H:633:ILE:HD13	2:H:746:ALA:CB	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:3003:MTE:S2'	7:H:3004:MOS:S	2.92	0.66
2:F:325:ARG:C	2:F:326:ILE:HG13	2.20	0.66
1:G:95:MET:SD	1:G:114:MET:HE1	2.35	0.66
2:B:61:VAL:CG1	2:B:62:ILE:N	2.55	0.66
2:B:324:LEU:HD23	2:B:324:LEU:C	2.20	0.66
1:E:68:PRO:HG2	1:E:224:PHE:CE1	2.31	0.66
2:F:23:LEU:HD13	2:F:194:CYS:HA	1.76	0.66
2:F:281:ASP:OD1	2:F:283:SER:OG	2.12	0.66
1:A:53:ASP:C	1:A:53:ASP:OD1	2.37	0.66
2:B:730:GLU:C	2:B:732:PRO:HD2	2.20	0.66
1:E:237:THR:HG23	1:E:238:PRO:HD2	1.75	0.66
1:C:390:VAL:CG2	1:C:391:PRO:HD2	2.25	0.66
2:F:70:LEU:HD12	2:F:74:ASN:HB2	1.76	0.66
2:F:650:ASP:OD2	2:F:726:LYS:NZ	2.29	0.66
2:H:558:ARG:CD	2:H:559:GLU:OE2	2.43	0.66
2:B:305:LEU:HD23	2:B:305:LEU:C	2.21	0.66
2:B:446:ARG:HG2	2:B:632:VAL:CG1	2.25	0.66
1:E:302:GLY:HA2	1:E:381:ARG:NH1	2.11	0.66
2:F:221:MET:HE1	2:F:223:ARG:C	2.21	0.66
1:G:337:GLU:O	1:G:338:SER:HB3	1.95	0.66
2:H:296:ARG:NH1	2:H:296:ARG:CG	2.51	0.66
2:D:446:ARG:NH1	2:D:630:GLU:OE2	2.28	0.66
4:E:3005:FAD:H2'	4:E:3005:FAD:N1	2.11	0.66
7:F:3004:MOS:S	8:F:4000:141:N8	2.69	0.66
2:H:107:ARG:O	2:H:108:ALA:C	2.39	0.66
2:D:671:GLY:O	2:D:674:TRP:HB3	1.96	0.66
1:E:106:CYS:SG	1:E:134:CYS:HB2	2.35	0.66
2:H:173:HIS:HA	2:H:341:PHE:CE1	2.31	0.65
2:B:310:ARG:HD2	2:B:344:PHE:O	1.96	0.65
1:C:316:MET:HB2	1:C:317:PRO:CD	2.25	0.65
1:E:237:THR:HG23	1:E:238:PRO:CG	2.27	0.65
2:H:360:LEU:HD11	2:H:364:MET:HE2	1.78	0.65
2:H:558:ARG:HD3	2:H:559:GLU:OE2	1.96	0.65
1:A:237:THR:CG2	1:A:239:ASP:H	2.08	0.65
2:D:144:VAL:CG1	2:D:312:MET:HE1	2.26	0.65
1:G:59:ALA:C	1:G:60:VAL:CG1	2.68	0.65
1:G:325:TYR:CE1	1:G:326:ARG:HG2	2.32	0.65
1:E:76:ARG:NH1	1:E:161:ASP:OD2	2.24	0.65
1:E:228:CYS:O	1:E:229:LYS:C	2.37	0.65
2:F:40:SER:HB2	2:F:91:VAL:HG11	1.78	0.65
2:F:346:GLY:N	2:F:347:PRO:CD	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:179:GLN:HB3	2:H:238:LEU:HD13	1.79	0.65
2:F:367:ASP:OD1	2:F:368:PRO:HD2	1.96	0.65
2:F:360:LEU:HG	2:F:364:MET:HE3	1.79	0.65
2:F:644:ARG:HB2	2:F:707:ILE:HB	1.78	0.65
2:H:53:GLU:N	2:H:54:PRO:CD	2.59	0.65
2:B:218:ARG:HH22	2:D:218:ARG:HH22	1.44	0.65
2:D:168:ILE:HD13	2:D:351:LEU:HD23	1.78	0.65
2:F:568:PHE:CD2	2:F:573:VAL:HG22	2.31	0.65
1:G:37:GLU:CD	2:H:256:ARG:NH2	2.55	0.65
1:G:141:PRO:HG2	1:G:142:ILE:N	2.12	0.65
4:G:3005:FAD:N1	4:G:3005:FAD:H2'	2.12	0.65
2:H:372:ARG:O	2:H:373:ALA:C	2.39	0.65
1:A:316:MET:HB2	1:A:317:PRO:CD	2.27	0.65
2:H:120:TYR:O	2:H:122:PRO:HD3	1.97	0.65
2:H:144:VAL:HG11	2:H:312:MET:HE1	1.79	0.65
1:A:425:LEU:HD21	2:F:577:GLY:O	1.96	0.65
2:B:737:ILE:O	2:B:738:SER:C	2.38	0.65
2:B:262:ASP:O	2:B:266:THR:HG23	1.96	0.64
1:E:205:GLY:N	4:E:3005:FAD:O2A	2.30	0.64
1:G:164:PHE:O	1:G:166:LEU:HG	1.97	0.64
1:G:299:ILE:HG13	1:G:318:LEU:HD23	1.78	0.64
1:C:102:GLN:HB3	2:D:489:GLY:O	1.97	0.64
7:D:3004:MOS:MO	7:D:3004:MOS:O2	1.68	0.64
2:F:296:ARG:HG3	2:F:296:ARG:HH11	1.60	0.64
1:G:390:VAL:CG2	1:G:391:PRO:CD	2.72	0.64
2:H:198:HIS:CG	2:H:526:ALA:CB	2.79	0.64
2:H:221:MET:HG3	2:H:221:MET:O	1.96	0.64
1:A:349:ARG:HD3	1:A:449:GLU:OE2	1.97	0.64
2:H:329:HIS:HB3	2:H:331:LEU:HD21	1.78	0.64
1:A:28:ARG:NH2	2:B:25:ASP:OD1	2.25	0.64
1:A:231:LEU:CD2	1:A:231:LEU:O	2.46	0.64
7:F:3004:MOS:O2	7:F:3004:MOS:MO	1.69	0.64
2:H:538:MET:HG3	2:H:602:TYR:CD1	2.33	0.64
2:H:737:ILE:O	2:H:738:SER:C	2.37	0.64
2:B:344:PHE:CZ	8:B:4000:141:C6	2.81	0.64
2:F:222:ARG:HB2	2:F:515:ALA:HB2	1.80	0.64
2:H:481:LEU:HD12	2:H:482:ASN:N	2.12	0.64
2:F:166:PHE:CZ	2:F:355:ARG:HG3	2.32	0.64
2:H:700:ALA:O	2:H:701:PHE:C	2.40	0.64
1:C:390:VAL:HG23	1:C:391:PRO:HD2	1.80	0.64
1:E:181:PHE:C	1:E:182:LEU:HD12	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:THR:HG23	1:E:238:PRO:HG2	1.80	0.64
1:E:243:ILE:HD12	1:E:341:LEU:HD11	1.79	0.64
1:C:349:ARG:CD	1:C:449:GLU:OE2	2.45	0.63
2:D:558:ARG:HD3	2:D:559:GLU:OE2	1.98	0.63
2:F:513:ILE:HG23	2:F:513:ILE:O	1.98	0.63
1:G:92:GLN:HG2	2:H:16:VAL:HG13	1.79	0.63
1:G:237:THR:HG23	1:G:238:PRO:N	2.11	0.63
1:A:252:LEU:HD22	1:A:281:ILE:HD13	1.79	0.63
1:C:408:GLU:OE1	2:D:442:ARG:NH2	2.24	0.63
2:D:197:GLN:NE2	2:D:488:MET:HE1	2.13	0.63
1:E:53:ASP:C	1:E:53:ASP:OD1	2.41	0.63
1:E:387:MET:HE1	1:E:436:MET:HA	1.80	0.63
2:F:407:GLN:OE1	2:F:618:PRO:HD2	1.98	0.63
2:F:496:MET:HA	2:F:496:MET:HE2	1.79	0.63
2:H:417:LEU:HG	2:H:648:LEU:CD2	2.27	0.63
6:H:3003:MTE:S1'	7:H:3004:MOS:O2	2.56	0.63
2:B:40:SER:HB2	2:B:98:ILE:HD11	1.79	0.63
2:B:647:ILE:HD13	2:B:735:LEU:HD13	1.79	0.63
2:D:66:THR:HG22	2:D:68:ALA:H	1.63	0.63
2:D:674:TRP:CE3	2:D:675:LEU:HD21	2.34	0.63
1:E:377:ILE:HG13	1:E:404:GLN:O	1.98	0.63
1:E:447:VAL:O	1:E:448:ARG:C	2.37	0.63
1:G:203:ALA:HB3	4:G:3005:FAD:O1P	1.98	0.63
1:G:316:MET:HB2	1:G:317:PRO:HD2	1.81	0.63
2:H:93:PHE:CE2	2:H:299:TRP:NE1	2.67	0.63
2:B:717:ASN:OD1	2:B:719:GLU:N	2.31	0.63
2:D:38:GLY:C	2:D:39:LEU:HD23	2.24	0.63
2:F:497:VAL:O	2:F:500:ALA:HB3	1.98	0.63
2:F:736:GLY:O	2:F:737:ILE:C	2.40	0.63
1:G:231:LEU:O	1:G:231:LEU:HD23	1.99	0.63
2:H:143:PRO:HB3	2:H:329:HIS:ND1	2.13	0.63
1:A:206:THR:HG21	1:A:275:VAL:HG13	1.79	0.63
2:F:593:ARG:NH1	2:H:604:THR:O	2.27	0.63
2:F:595:SER:HB2	2:H:601:PHE:CD1	2.33	0.63
2:H:731:PRO:N	2:H:732:PRO:CD	2.57	0.63
1:A:337:GLU:O	1:A:338:SER:HB3	1.96	0.63
1:A:366:GLY:HA3	1:A:442:MET:SD	2.39	0.63
2:B:166:PHE:CZ	2:B:355:ARG:HG3	2.34	0.63
2:H:733:PHE:HD2	2:H:734:LEU:HD12	1.64	0.63
7:H:3004:MOS:S	7:H:3004:MOS:MO	2.09	0.63
2:B:218:ARG:HH22	2:D:218:ARG:NH2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:MET:SD	1:C:114:MET:HE1	2.39	0.63
1:G:103:CYS:HB3	1:G:136:CYS:SG	2.39	0.63
2:B:776:ARG:O	2:B:777:ALA:CB	2.47	0.63
1:C:37:GLU:OE1	2:D:256:ARG:NH2	2.31	0.63
2:D:674:TRP:CD2	2:D:675:LEU:HD21	2.34	0.63
2:D:731:PRO:N	2:D:732:PRO:CD	2.60	0.63
1:E:390:VAL:CG2	1:E:391:PRO:HD2	2.28	0.63
2:F:61:VAL:HG12	2:F:62:ILE:N	2.10	0.63
2:H:130:ASP:O	2:H:131:GLN:C	2.41	0.63
2:H:262:ASP:O	2:H:266:THR:HG23	1.99	0.63
2:H:507:ASP:OD1	2:H:508:PRO:N	2.32	0.63
1:C:216:LEU:HD12	2:D:114:ARG:NH1	2.14	0.63
2:H:247:ARG:HH11	2:H:247:ARG:CG	2.11	0.63
1:A:399:ALA:C	1:A:401:LEU:N	2.56	0.62
2:B:571:GLY:C	2:B:572:GLN:HG2	2.22	0.62
2:D:645:THR:HG21	2:D:668:TYR:CZ	2.34	0.62
1:E:297:ALA:O	1:E:298:LEU:C	2.41	0.62
2:F:305:LEU:HB3	2:F:306:PRO:CD	2.28	0.62
1:G:237:THR:HG23	1:G:239:ASP:H	1.63	0.62
1:G:325:TYR:O	1:G:326:ARG:CB	2.35	0.62
2:D:324:LEU:HD23	2:D:324:LEU:C	2.24	0.62
1:E:36:LYS:HD3	1:E:105:PHE:CE1	2.35	0.62
1:E:297:ALA:O	1:E:300:ALA:N	2.31	0.62
2:F:214:PHE:CD1	2:F:214:PHE:N	2.64	0.62
1:G:322:PHE:HB3	1:G:390:VAL:HG21	1.80	0.62
2:H:563:ALA:O	2:H:566:VAL:HG23	1.98	0.62
2:H:730:GLU:O	2:H:731:PRO:C	2.41	0.62
2:F:218:ARG:NH2	2:F:517:ASP:OD1	2.32	0.62
2:F:446:ARG:HG2	2:F:632:VAL:HG13	1.81	0.62
1:G:85:ASP:OD2	1:G:87:ARG:HD3	1.99	0.62
2:F:443:THR:C	2:F:444:LEU:HD23	2.25	0.62
1:A:434:TYR:O	1:A:435:ARG:C	2.40	0.62
1:C:322:PHE:HB3	1:C:390:VAL:HG23	1.80	0.62
1:E:151:GLY:O	1:E:152:GLU:HG2	2.00	0.62
2:F:664:ILE:O	2:F:665:GLU:C	2.41	0.62
7:H:3004:MOS:O2	7:H:3004:MOS:MO	1.69	0.62
2:D:312:MET:HE2	2:D:330:ARG:NH1	2.07	0.62
2:D:683:ASP:C	2:D:683:ASP:OD1	2.40	0.62
2:F:461:LEU:HD12	2:F:463:HIS:CE1	2.34	0.62
2:H:476:ASP:OD2	2:H:478:SER:OG	2.13	0.62
2:D:61:VAL:CG1	2:D:62:ILE:N	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:ARG:O	2:D:108:ALA:C	2.42	0.62
2:F:459:PHE:N	2:F:465:ASN:OD1	2.33	0.62
1:G:237:THR:CG2	1:G:238:PRO:HD2	2.30	0.62
1:E:241:TYR:O	1:E:340:THR:HG23	1.99	0.62
1:G:61:ASN:ND2	1:G:61:ASN:H	1.98	0.62
1:G:237:THR:CB	1:G:238:PRO:HD2	2.30	0.62
1:A:228:CYS:O	1:A:229:LYS:C	2.43	0.62
2:B:61:VAL:HG12	2:B:62:ILE:N	2.12	0.61
2:B:457:ILE:O	2:B:458:SER:CB	2.48	0.61
1:C:92:GLN:HG2	2:D:16:VAL:HG13	1.82	0.61
1:E:104:GLY:HA3	2:F:22:TYR:OH	2.00	0.61
1:G:237:THR:HG22	1:G:239:ASP:H	1.63	0.61
2:B:22:TYR:CD1	2:B:22:TYR:N	2.68	0.61
2:D:53:GLU:HA	2:D:53:GLU:OE1	1.98	0.61
1:A:237:THR:OG1	1:A:238:PRO:HD2	1.99	0.61
1:A:316:MET:HB2	1:A:317:PRO:HD2	1.81	0.61
2:B:407:GLN:CD	2:B:617:ARG:HG2	2.26	0.61
1:C:301:MET:CE	1:C:341:LEU:HD13	2.30	0.61
2:D:305:LEU:HB3	2:D:306:PRO:HD3	1.81	0.61
2:B:512:ARG:HD2	2:D:216:ASP:OD1	2.00	0.61
2:D:339:THR:HG23	2:D:340:ALA:H	1.61	0.61
1:G:237:THR:CG2	1:G:238:PRO:CD	2.77	0.61
1:C:85:ASP:OD1	1:C:87:ARG:NH1	2.34	0.61
2:F:197:GLN:NE2	2:F:488:MET:HE1	2.15	0.61
2:B:443:THR:O	2:B:444:LEU:HD23	2.01	0.61
2:F:24:ASP:OD2	2:F:254:LYS:NZ	2.31	0.61
2:F:443:THR:O	2:F:444:LEU:HD23	2.00	0.61
1:G:110:PHE:HB3	1:G:114:MET:HE2	1.83	0.61
1:G:359:GLN:HG3	1:G:359:GLN:O	2.00	0.61
2:H:633:ILE:HD13	2:H:746:ALA:HB1	1.81	0.61
1:A:231:LEU:O	1:A:231:LEU:HD23	1.99	0.61
2:D:70:LEU:HD12	2:D:74:ASN:HB2	1.83	0.61
1:E:78:ILE:HG23	1:E:79:GLU:N	2.15	0.61
2:F:560:GLY:O	2:F:561:CYS:HB3	1.99	0.61
2:H:762:THR:O	2:H:766:VAL:HG23	2.00	0.61
2:B:528:ALA:O	2:B:531:SER:OG	2.16	0.61
2:F:360:LEU:CG	2:F:364:MET:HE3	2.31	0.61
2:F:595:SER:HB2	2:H:601:PHE:CG	2.36	0.61
1:G:423:THR:O	1:G:423:THR:HG22	2.01	0.61
1:A:237:THR:HG23	1:A:239:ASP:H	1.66	0.61
1:G:139:TYR:C	1:G:141:PRO:HD2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:533:ALA:O	2:H:534:ASP:C	2.44	0.61
1:E:18:ASP:OD2	1:E:19:PRO:HD2	2.01	0.60
1:G:83:ALA:HB2	1:G:157:TRP:CE3	2.36	0.60
2:H:46:ALA:HB2	2:H:123:ARG:HH21	1.65	0.60
2:H:721:THR:O	2:H:722:ILE:C	2.44	0.60
2:H:763:PRO:O	2:H:764:GLU:C	2.43	0.60
2:B:171:GLN:HG3	2:B:678:GLU:OE1	2.00	0.60
1:G:81:ILE:HG22	1:G:81:ILE:O	2.00	0.60
2:B:691:HIS:O	2:B:691:HIS:CG	2.52	0.60
2:D:440:THR:HG22	2:D:440:THR:O	2.02	0.60
2:D:731:PRO:HD2	2:D:732:PRO:HD2	1.83	0.60
1:E:67:LEU:O	1:E:68:PRO:C	2.40	0.60
2:F:329:HIS:HB3	2:F:331:LEU:HD21	1.82	0.60
2:H:730:GLU:N	2:H:731:PRO:CD	2.65	0.60
2:H:741:LEU:N	2:H:741:LEU:CD1	2.55	0.60
1:C:314:ARG:HH22	1:C:329:ASP:CG	2.10	0.60
1:A:237:THR:HG23	1:A:238:PRO:CG	2.31	0.60
2:B:58:SER:OG	2:B:59:PRO:HD2	2.00	0.60
2:F:237:HIS:ND1	2:F:237:HIS:N	2.47	0.60
1:G:271:ALA:HA	1:G:359:GLN:HE22	1.66	0.60
2:B:93:PHE:CE2	2:B:299:TRP:NE1	2.70	0.60
2:B:631:VAL:HG21	2:B:743:LEU:HD13	1.83	0.60
2:F:61:VAL:CG1	2:F:62:ILE:N	2.62	0.60
2:F:269:ARG:NH2	2:F:341:PHE:CD2	2.69	0.60
1:A:143:LEU:HD22	1:A:147:GLU:CD	2.26	0.60
2:B:528:ALA:O	2:B:529:ALA:HB3	2.02	0.60
1:C:369:ASN:O	1:C:370:LEU:HD23	2.01	0.60
2:F:591:MET:HE1	2:H:463:HIS:CE1	2.37	0.60
1:A:370:LEU:CD2	1:A:380:ALA:HA	2.32	0.60
2:B:490:GLN:O	2:B:490:GLN:HG2	2.02	0.60
2:B:730:GLU:O	2:B:731:PRO:C	2.43	0.60
1:C:59:ALA:C	1:C:60:VAL:HG13	2.25	0.60
1:C:165:THR:O	1:C:166:LEU:HD23	2.00	0.60
1:E:67:LEU:O	1:E:69:GLN:N	2.34	0.60
1:E:218:ASP:C	1:E:218:ASP:OD1	2.44	0.60
2:H:251:ARG:O	2:H:252:PRO:C	2.43	0.60
2:H:479:VAL:HG12	2:H:480:ALA:N	2.16	0.60
2:H:661:ILE:HD11	2:H:712:LEU:HG	1.82	0.60
1:C:28:ARG:O	1:C:31:GLY:N	2.28	0.60
1:G:349:ARG:CD	1:G:449:GLU:OE2	2.50	0.60
2:H:440:THR:O	2:H:440:THR:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:517:ASP:OD2	2:H:517:ASP:C	2.45	0.60
1:A:22:SER:OG	1:A:25:GLU:HG2	2.02	0.60
1:A:444:LEU:O	1:A:448:ARG:HG3	2.02	0.60
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.35	0.60
1:G:240:GLY:HA2	1:G:343:LYS:HG2	1.83	0.60
2:H:221:MET:HE1	2:H:223:ARG:C	2.26	0.60
2:H:730:GLU:C	2:H:732:PRO:HD2	2.26	0.60
1:A:418:LEU:HB3	1:A:436:MET:HE1	1.84	0.59
2:B:66:THR:HG22	2:B:68:ALA:N	2.13	0.59
2:F:594:ILE:O	2:F:596:LEU:HG	2.02	0.59
2:F:647:ILE:HG22	2:F:648:LEU:N	2.17	0.59
1:G:252:LEU:HD22	1:G:281:ILE:HD13	1.84	0.59
2:H:251:ARG:HB2	2:H:252:PRO:CD	2.32	0.59
1:A:337:GLU:O	1:A:337:GLU:HG3	2.02	0.59
1:A:351:TYR:CE2	1:A:445:ARG:HD3	2.36	0.59
2:B:412:CYS:HA	2:B:624:TYR:CZ	2.38	0.59
2:D:731:PRO:HB2	2:D:732:PRO:CD	2.31	0.59
2:F:721:THR:O	2:F:722:ILE:C	2.43	0.59
2:H:258:ASP:O	2:H:259:ARG:C	2.41	0.59
1:E:144:ARG:O	1:E:145:ALA:C	2.42	0.59
2:B:507:ASP:OD1	2:B:508:PRO:HD2	2.01	0.59
2:D:678:GLU:HB3	2:D:696:TYR:OH	2.02	0.59
2:H:529:ALA:O	2:H:530:SER:C	2.46	0.59
2:H:731:PRO:HD2	2:H:732:PRO:HD2	1.82	0.59
1:A:165:THR:O	1:A:165:THR:HG23	2.01	0.59
2:B:106:HIS:O	2:B:107:ARG:C	2.42	0.59
2:F:533:ALA:O	2:F:534:ASP:C	2.44	0.59
2:F:637:THR:OG1	2:F:639:GLU:HG3	2.03	0.59
2:F:744:HIS:C	2:F:744:HIS:CD2	2.81	0.59
2:H:731:PRO:CB	2:H:732:PRO:CD	2.79	0.59
2:H:263:MET:CE	2:H:692:ALA:HA	2.33	0.59
1:C:399:ALA:C	1:C:401:LEU:H	2.11	0.59
2:D:58:SER:OG	2:D:59:PRO:CD	2.49	0.59
1:E:432:ALA:O	1:E:433:ALA:C	2.43	0.59
2:F:123:ARG:HB3	2:F:124:PRO:HD2	1.85	0.59
2:F:606:LYS:NZ	2:F:719:GLU:OE1	2.33	0.59
1:G:192:TRP:O	1:G:196:HIS:HD2	1.85	0.59
2:H:66:THR:HG22	2:H:68:ALA:N	2.09	0.59
2:H:372:ARG:HG3	2:H:372:ARG:HH11	1.67	0.59
2:H:656:ASN:CG	2:H:659:LEU:HD12	2.27	0.59
1:A:387:MET:HE3	1:A:424:PRO:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:THR:HG23	1:C:238:PRO:N	2.17	0.59
2:D:367:ASP:OD1	2:D:368:PRO:HD2	2.02	0.59
1:E:216:LEU:HD12	2:F:114:ARG:NH1	2.18	0.59
2:H:450:LEU:HG	2:H:451:SER:N	2.14	0.59
2:B:65:PHE:HB2	2:B:100:LEU:HB3	1.85	0.59
2:B:683:ASP:C	2:B:683:ASP:OD1	2.45	0.59
2:D:179:GLN:HB3	2:D:238:LEU:CD1	2.32	0.59
2:F:275:ARG:HB3	2:F:292:VAL:HB	1.85	0.59
2:H:251:ARG:HB2	2:H:252:PRO:HD2	1.85	0.59
1:A:78:ILE:HG23	1:A:79:GLU:N	2.16	0.59
1:C:228:CYS:O	1:C:229:LYS:C	2.45	0.59
2:D:221:MET:HE1	2:D:223:ARG:C	2.28	0.59
2:D:263:MET:CE	2:D:692:ALA:HA	2.32	0.59
2:D:320:PHE:CD2	2:D:401:GLN:NE2	2.71	0.59
2:D:736:GLY:O	2:D:737:ILE:C	2.46	0.59
1:E:138:GLY:O	1:E:139:TYR:HB2	2.02	0.59
2:F:683:ASP:C	2:F:683:ASP:OD1	2.45	0.59
1:C:53:ASP:OD2	1:C:58:ARG:NH2	2.36	0.58
2:D:221:MET:HG3	2:D:221:MET:O	2.01	0.58
1:E:373:LYS:O	1:E:374:GLY:O	2.21	0.58
2:F:462:THR:O	2:F:465:ASN:ND2	2.35	0.58
2:H:128:THR:O	2:H:129:LEU:C	2.46	0.58
2:H:372:ARG:O	2:H:375:ASN:N	2.31	0.58
1:A:267:LEU:O	1:A:268:ARG:C	2.46	0.58
2:B:232:GLU:OE2	8:B:4000:141:H1	2.03	0.58
2:B:443:THR:C	2:B:444:LEU:HD23	2.28	0.58
1:E:58:ARG:HD3	1:E:277:GLN:OE1	2.02	0.58
1:E:318:LEU:O	1:E:319:GLU:C	2.45	0.58
2:F:496:MET:HE2	2:F:496:MET:CA	2.32	0.58
2:F:573:VAL:CG2	2:F:585:ILE:HG13	2.30	0.58
2:F:629:THR:OG1	2:F:645:THR:HG23	2.03	0.58
1:G:281:ILE:O	1:G:282:GLY:C	2.45	0.58
2:B:305:LEU:HB3	2:B:306:PRO:HD3	1.83	0.58
2:B:481:LEU:HD12	2:B:482:ASN:N	2.19	0.58
1:G:34:GLY:O	1:G:36:LYS:HE3	2.04	0.58
1:G:50:MET:HE1	1:G:116:ALA:HA	1.80	0.58
1:G:210:LEU:HD23	1:G:210:LEU:H	1.62	0.58
1:A:324:GLU:O	1:A:325:TYR:C	2.45	0.58
2:B:296:ARG:HG3	2:B:296:ARG:HH11	1.66	0.58
2:D:730:GLU:N	2:D:731:PRO:CD	2.66	0.58
1:E:1:MET:CE	1:E:180:ALA:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:221:MET:HG3	2:F:221:MET:O	2.01	0.58
2:F:691:HIS:CD2	2:F:691:HIS:O	2.57	0.58
2:H:46:ALA:HB2	2:H:123:ARG:NH2	2.18	0.58
2:H:166:PHE:CZ	2:H:355:ARG:HG3	2.39	0.58
2:H:310:ARG:HD2	2:H:344:PHE:O	2.03	0.58
2:H:740:PHE:O	2:H:741:LEU:C	2.44	0.58
2:D:45:ALA:HA	2:D:123:ARG:HG3	1.86	0.58
2:D:166:PHE:CZ	2:D:355:ARG:HG3	2.39	0.58
2:D:661:ILE:HD11	2:D:712:LEU:HG	1.84	0.58
1:G:98:HIS:O	1:G:99:HIS:HB2	2.01	0.58
2:B:730:GLU:N	2:B:731:PRO:HD2	2.18	0.58
2:D:269:ARG:NH2	2:D:341:PHE:CD2	2.71	0.58
1:E:58:ARG:CG	1:E:277:GLN:OE1	2.51	0.58
1:E:354:SER:HB2	1:E:360:ASP:OD2	2.03	0.58
2:F:432:ALA:O	2:F:433:GLU:C	2.46	0.58
1:G:260:HIS:O	1:G:261:PRO:C	2.47	0.58
2:D:398:LYS:O	2:D:399:LYS:HD2	2.04	0.58
2:F:174:PHE:CZ	2:F:693:PRO:HG3	2.38	0.58
2:F:507:ASP:OD1	2:F:508:PRO:CD	2.51	0.58
2:H:269:ARG:NH2	2:H:341:PHE:CD2	2.72	0.58
1:A:455:VAL:HG22	2:B:443:THR:HG21	1.85	0.58
2:D:471:VAL:CG1	2:D:472:GLN:N	2.64	0.58
1:E:322:PHE:HB3	1:E:390:VAL:HG23	1.84	0.58
2:F:360:LEU:HD11	2:F:364:MET:CE	2.33	0.58
1:G:138:GLY:HA2	2:H:669:VAL:HG21	1.85	0.58
1:G:218:ASP:C	1:G:218:ASP:OD1	2.46	0.58
1:G:243:ILE:CD1	1:G:341:LEU:HD11	2.33	0.58
1:C:216:LEU:HD12	2:D:114:ARG:HH11	1.69	0.58
1:C:390:VAL:CG2	1:C:391:PRO:CD	2.81	0.58
2:D:451:SER:HB3	2:D:738:SER:HB3	1.85	0.58
2:D:496:MET:HE2	2:D:496:MET:N	2.18	0.58
1:G:22:SER:OG	1:G:25:GLU:HG2	2.03	0.58
2:H:432:ALA:O	2:H:433:GLU:C	2.43	0.58
2:D:341:PHE:O	2:D:342:ARG:C	2.47	0.58
2:D:496:MET:CE	2:D:496:MET:N	2.66	0.58
2:H:648:LEU:HD12	2:H:711:ALA:O	2.03	0.58
2:B:197:GLN:HG2	2:B:224:MET:HE1	1.85	0.57
2:B:276:TYR:OH	2:B:359:HIS:HD2	1.86	0.57
2:D:238:LEU:HD11	2:D:257:TYR:CE1	2.39	0.57
1:E:266:LEU:C	1:E:268:ARG:N	2.62	0.57
1:E:395:ALA:O	1:E:396:ALA:C	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:730:GLU:O	2:F:731:PRO:C	2.47	0.57
2:F:731:PRO:N	2:F:732:PRO:HD2	2.19	0.57
1:G:351:TYR:CZ	1:G:445:ARG:HG2	2.38	0.57
2:B:120:TYR:O	2:B:122:PRO:HD3	2.05	0.57
2:B:227:GLY:O	2:B:230:GLY:N	2.34	0.57
2:D:650:ASP:OD2	2:D:726:LYS:NZ	2.29	0.57
2:F:341:PHE:O	2:F:342:ARG:C	2.47	0.57
1:G:41:GLU:HG3	1:G:214:LYS:CE	2.33	0.57
1:G:61:ASN:H	1:G:61:ASN:HD22	1.49	0.57
1:G:106:CYS:SG	1:G:134:CYS:HB2	2.44	0.57
1:A:436:MET:O	1:A:438:ALA:N	2.37	0.57
2:B:528:ALA:HB1	8:B:4000:141:C7	2.34	0.57
2:B:632:VAL:HG22	2:B:643:LEU:HD11	1.86	0.57
1:C:369:ASN:C	1:C:370:LEU:HD23	2.30	0.57
1:C:446:TYR:CE2	1:C:450:LEU:HD12	2.39	0.57
2:H:446:ARG:HG2	2:H:632:VAL:HG13	1.82	0.57
2:H:746:ALA:O	2:H:747:CYS:C	2.47	0.57
1:C:138:GLY:O	1:C:139:TYR:HB2	2.04	0.57
2:D:324:LEU:HD21	2:D:326:ILE:HD11	1.86	0.57
1:G:95:MET:CG	1:G:114:MET:HE1	2.35	0.57
1:G:231:LEU:O	1:G:231:LEU:CD2	2.52	0.57
2:H:341:PHE:O	2:H:342:ARG:C	2.46	0.57
2:H:446:ARG:NH1	2:H:630:GLU:OE2	2.37	0.57
1:A:237:THR:HG23	1:A:238:PRO:N	2.17	0.57
1:A:237:THR:CG2	1:A:238:PRO:HD2	2.35	0.57
2:D:372:ARG:O	2:D:373:ALA:C	2.45	0.57
1:G:318:LEU:O	1:G:320:ASP:N	2.37	0.57
1:G:322:PHE:HB3	1:G:390:VAL:HG23	1.85	0.57
1:G:438:ALA:O	1:G:441:ALA:N	2.38	0.57
2:H:645:THR:HG21	2:H:668:TYR:CZ	2.39	0.57
2:B:496:MET:HE2	2:B:496:MET:N	2.20	0.57
2:B:668:TYR:O	2:B:669:VAL:C	2.44	0.57
1:C:215:ALA:O	1:C:216:LEU:HB2	2.05	0.57
1:E:369:ASN:C	1:E:369:ASN:OD1	2.45	0.57
2:F:105:SER:O	2:F:106:HIS:C	2.46	0.57
1:G:69:GLN:NE2	1:G:203:ALA:O	2.37	0.57
1:G:243:ILE:HD12	1:G:341:LEU:HD11	1.86	0.57
1:G:447:VAL:O	1:G:448:ARG:C	2.48	0.57
2:H:305:LEU:HD23	2:H:305:LEU:O	2.04	0.57
2:H:348:GLN:O	2:H:349:GLY:C	2.46	0.57
2:H:380:PRO:O	2:H:381:GLU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:757:LEU:HD12	2:H:758:GLN:H	1.69	0.57
1:A:45:GLY:O	1:A:48:THR:OG1	2.19	0.57
1:A:203:ALA:HB3	4:A:3005:FAD:O1P	2.05	0.57
2:B:339:THR:HG23	2:B:340:ALA:H	1.63	0.57
1:C:129:LEU:O	1:C:130:ALA:C	2.47	0.57
1:E:321:PHE:CG	1:E:321:PHE:O	2.58	0.57
2:F:700:ALA:O	2:F:701:PHE:C	2.48	0.57
1:C:393:ARG:HD2	1:C:398:GLU:OE1	2.05	0.57
1:E:111:ILE:O	1:E:112:VAL:C	2.47	0.57
2:F:671:GLY:O	2:F:674:TRP:HB3	2.04	0.57
1:G:393:ARG:HB3	1:G:398:GLU:OE1	2.05	0.57
1:E:83:ALA:HB2	1:E:157:TRP:CZ3	2.40	0.57
2:F:513:ILE:O	2:F:513:ILE:CG2	2.53	0.57
1:G:436:MET:C	1:G:438:ALA:N	2.62	0.57
1:A:408:GLU:OE1	2:B:442:ARG:NH2	2.27	0.56
1:G:373:LYS:O	1:G:374:GLY:C	2.48	0.56
1:G:436:MET:O	1:G:438:ALA:N	2.38	0.56
2:H:602:TYR:C	2:H:602:TYR:CD2	2.83	0.56
2:H:741:LEU:N	2:H:741:LEU:HD13	2.20	0.56
2:H:776:ARG:O	2:H:777:ALA:CB	2.53	0.56
1:E:250:ALA:O	1:E:253:ARG:N	2.38	0.56
2:F:746:ALA:O	2:F:747:CYS:C	2.47	0.56
1:G:83:ALA:HB2	1:G:157:TRP:CD2	2.40	0.56
1:A:314:ARG:O	1:A:315:ARG:HB2	2.05	0.56
1:A:368:LEU:HB2	1:A:446:TYR:CD1	2.39	0.56
1:A:442:MET:O	1:A:445:ARG:HB3	2.06	0.56
1:A:446:TYR:CE2	1:A:450:LEU:CD1	2.88	0.56
2:B:247:ARG:HG2	2:B:247:ARG:HH11	1.70	0.56
6:D:3003:MTE:S1'	7:D:3004:MOS:S	3.04	0.56
1:E:110:PHE:O	1:E:111:ILE:C	2.48	0.56
1:E:296:PRO:O	1:E:297:ALA:C	2.47	0.56
2:F:776:ARG:O	2:F:777:ALA:HB3	2.06	0.56
1:G:120:ARG:O	1:G:121:ASP:C	2.47	0.56
1:G:350:CYS:HG	1:G:367:CYS:HG	1.53	0.56
2:H:79:ALA:HB1	2:H:80:PRO:CD	2.32	0.56
2:H:309:ASP:O	2:H:313:LEU:HB2	2.05	0.56
1:A:26:LEU:HD13	1:A:67:LEU:CD1	2.34	0.56
2:B:360:LEU:HG	2:B:364:MET:CE	2.35	0.56
1:C:164:PHE:O	1:C:166:LEU:HG	2.05	0.56
2:D:346:GLY:N	2:D:347:PRO:CD	2.68	0.56
2:D:645:THR:HG21	2:D:668:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:360:LEU:CD1	2:F:364:MET:HE3	2.35	0.56
2:F:648:LEU:HA	2:F:711:ALA:O	2.06	0.56
2:H:672:ALA:O	2:H:675:LEU:N	2.35	0.56
1:E:191:ASP:O	1:E:194:LEU:HB3	2.05	0.56
2:F:347:PRO:O	2:F:348:GLN:C	2.48	0.56
2:H:93:PHE:CE1	2:H:96:GLN:N	2.74	0.56
2:H:276:TYR:OH	2:H:359:HIS:CD2	2.57	0.56
2:B:224:MET:HE3	2:B:488:MET:HB3	1.88	0.56
2:D:305:LEU:HD21	2:D:611:ARG:NE	2.21	0.56
1:E:68:PRO:HG2	1:E:224:PHE:HE1	1.67	0.56
2:F:278:ILE:HD11	2:F:286:LEU:HD22	1.87	0.56
1:G:299:ILE:O	1:G:302:GLY:N	2.33	0.56
2:H:733:PHE:C	2:H:733:PHE:CD2	2.83	0.56
1:A:361:ILE:HD12	1:A:429:ARG:HH22	1.71	0.56
2:B:730:GLU:H	2:B:731:PRO:HD2	1.70	0.56
1:E:237:THR:HG22	1:E:239:ASP:N	2.19	0.56
2:F:144:VAL:CG1	2:F:312:MET:HE1	2.36	0.56
2:F:238:LEU:HD11	2:F:257:TYR:CE1	2.41	0.56
1:G:291:ILE:O	1:G:292:GLY:C	2.44	0.56
1:G:370:LEU:CD2	1:G:380:ALA:HA	2.36	0.56
2:H:760:PRO:O	2:H:762:THR:N	2.38	0.56
1:A:237:THR:CB	1:A:238:PRO:HD2	2.35	0.56
1:C:427:ASP:OD1	1:C:435:ARG:NH2	2.39	0.56
1:E:61:ASN:H	1:E:61:ASN:ND2	2.03	0.56
1:G:50:MET:CE	1:G:116:ALA:CA	2.65	0.56
1:G:91:VAL:CG1	1:G:111:ILE:HD12	2.36	0.56
2:D:198:HIS:ND1	2:D:526:ALA:HB2	2.21	0.56
1:E:12:ARG:HH11	1:E:12:ARG:HG3	1.70	0.56
1:E:249:ILE:O	1:E:250:ALA:C	2.47	0.56
2:F:66:THR:HB	2:F:69:ASP:OD2	2.06	0.56
2:F:720:GLU:CG	2:F:724:ARG:NH2	2.64	0.56
1:G:316:MET:HE1	1:G:329:ASP:OD2	2.06	0.56
1:A:75:LEU:HD12	1:A:76:ARG:H	1.71	0.56
1:A:243:ILE:O	1:A:338:SER:HB2	2.06	0.56
1:A:316:MET:HE1	1:A:329:ASP:OD2	2.06	0.56
1:A:426:SER:O	1:A:427:ASP:HB3	2.06	0.56
2:B:660:ASP:O	2:B:661:ILE:C	2.48	0.56
1:C:37:GLU:CD	2:D:256:ARG:NH2	2.64	0.56
1:C:60:VAL:HG21	1:C:65:MET:CE	2.36	0.56
2:D:93:PHE:CE2	2:D:96:GLN:HB2	2.41	0.56
1:E:1:MET:HE1	1:E:180:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:79:ALA:HB1	2:F:80:PRO:CD	2.34	0.56
2:H:66:THR:HB	2:H:69:ASP:OD2	2.06	0.56
2:H:324:LEU:C	2:H:324:LEU:HD23	2.31	0.56
2:H:595:SER:C	2:H:596:LEU:HD23	2.31	0.56
1:C:78:ILE:HG23	1:C:79:GLU:N	2.20	0.55
2:D:635:ARG:NH1	2:D:774:GLU:OE2	2.32	0.55
1:E:237:THR:HG23	1:E:238:PRO:N	2.19	0.55
2:F:130:ASP:O	2:F:131:GLN:C	2.44	0.55
2:F:736:GLY:O	2:F:739:ALA:N	2.39	0.55
2:F:776:ARG:O	2:F:777:ALA:CB	2.55	0.55
2:B:247:ARG:HG2	2:B:247:ARG:NH1	2.21	0.55
1:C:316:MET:HE1	1:C:329:ASP:OD2	2.06	0.55
2:D:674:TRP:CD2	2:D:675:LEU:CD2	2.89	0.55
1:E:301:MET:HB3	1:E:348:LEU:HD22	1.88	0.55
1:E:436:MET:O	1:E:437:ASN:C	2.48	0.55
2:F:343:GLY:O	2:F:344:PHE:C	2.47	0.55
2:F:704:ARG:HG3	2:F:704:ARG:O	2.04	0.55
2:H:316:ASP:N	2:H:316:ASP:OD1	2.39	0.55
1:A:314:ARG:HH22	1:A:329:ASP:CG	2.14	0.55
1:A:423:THR:O	1:A:423:THR:HG22	2.06	0.55
2:B:271:ASP:OD2	2:B:296:ARG:NH1	2.38	0.55
2:B:479:VAL:HG12	2:B:480:ALA:N	2.19	0.55
2:B:618:PRO:HG2	2:B:619:PHE:N	2.20	0.55
1:E:439:ALA:O	1:E:440:GLN:C	2.43	0.55
2:H:728:VAL:O	2:H:732:PRO:HG3	2.06	0.55
1:A:39:CYS:O	1:A:40:ASN:CB	2.53	0.55
1:A:319:GLU:N	1:A:319:GLU:OE2	2.39	0.55
2:B:105:SER:O	2:B:106:HIS:C	2.49	0.55
2:B:437:TRP:CZ3	2:B:446:ARG:HG3	2.42	0.55
1:C:374:GLY:C	1:C:376:LYS:H	2.15	0.55
2:H:196:SER:HG	2:H:198:HIS:H	1.51	0.55
2:H:359:HIS:O	2:H:360:LEU:C	2.47	0.55
2:B:344:PHE:CE1	8:B:4000:141:C6	2.90	0.55
2:B:513:ILE:HG13	2:B:514:THR:H	1.69	0.55
2:B:556:ALA:O	2:B:557:ALA:C	2.48	0.55
1:E:266:LEU:C	1:E:268:ARG:H	2.14	0.55
1:G:67:LEU:O	1:G:69:GLN:N	2.40	0.55
1:G:140:ALA:N	1:G:141:PRO:HD2	2.21	0.55
1:G:301:MET:HG3	1:G:301:MET:O	2.05	0.55
4:G:3005:FAD:N1	4:G:3005:FAD:C2'	2.65	0.55
2:H:106:HIS:O	2:H:107:ARG:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:THR:HG23	1:A:238:PRO:HG2	1.88	0.55
2:D:201:GLU:O	2:D:202:ILE:C	2.45	0.55
2:D:360:LEU:HD11	2:D:364:MET:HE2	1.87	0.55
1:E:37:GLU:OE1	2:F:256:ARG:NH2	2.39	0.55
1:G:144:ARG:O	1:G:145:ALA:C	2.46	0.55
1:G:382:ILE:O	1:G:382:ILE:HG22	2.06	0.55
2:H:143:PRO:HB3	2:H:329:HIS:CE1	2.42	0.55
2:B:742:ALA:O	2:B:743:LEU:C	2.49	0.55
1:C:24:LEU:HD21	1:C:37:GLU:HB2	1.88	0.55
2:D:286:LEU:HG	2:D:375:ASN:OD1	2.06	0.55
2:D:723:PHE:O	2:D:724:ARG:HB2	2.07	0.55
1:E:390:VAL:CG2	1:E:391:PRO:CD	2.84	0.55
2:F:499:VAL:O	2:F:503:VAL:HG23	2.07	0.55
1:G:369:ASN:O	1:G:370:LEU:HD23	2.07	0.55
2:H:767:LEU:HD12	2:H:767:LEU:O	2.06	0.55
1:C:356:ARG:CZ	2:D:697:LYS:NZ	2.70	0.55
2:D:721:THR:O	2:D:722:ILE:C	2.49	0.55
2:F:289:ALA:O	2:F:324:LEU:HA	2.06	0.55
2:H:179:GLN:HB3	2:H:238:LEU:CD1	2.36	0.55
2:H:558:ARG:HD2	2:H:559:GLU:OE2	2.07	0.55
2:H:674:TRP:CD2	2:H:675:LEU:HD21	2.41	0.55
1:A:388:ALA:C	1:A:390:VAL:H	2.14	0.55
1:A:414:ALA:O	1:A:415:LEU:C	2.48	0.55
2:B:278:ILE:HD11	2:B:286:LEU:HD22	1.89	0.55
1:E:237:THR:HG23	1:E:239:ASP:H	1.69	0.55
4:E:3005:FAD:H2B	4:E:3005:FAD:O5B	2.07	0.55
2:F:321:VAL:HG12	2:F:323:ALA:O	2.07	0.55
1:G:237:THR:CG2	1:G:238:PRO:N	2.70	0.55
2:H:367:ASP:CG	2:H:431:ARG:HH12	2.12	0.55
1:A:18:ASP:OD2	1:A:19:PRO:CD	2.52	0.55
2:B:16:VAL:O	2:B:16:VAL:HG13	2.06	0.55
2:D:412:CYS:HA	2:D:624:TYR:CZ	2.42	0.55
2:D:672:ALA:O	2:D:673:GLY:C	2.50	0.55
2:F:201:GLU:O	2:F:202:ILE:C	2.50	0.55
1:G:44:CYS:N	3:G:3002:FES:S1	2.78	0.55
2:H:683:ASP:C	2:H:683:ASP:OD1	2.48	0.55
2:D:164:GLY:HA3	2:D:276:TYR:CZ	2.42	0.54
1:E:351:TYR:CE1	1:E:445:ARG:HG2	2.43	0.54
2:F:571:GLY:C	2:F:572:GLN:HG2	2.31	0.54
2:H:120:TYR:C	2:H:122:PRO:HD3	2.31	0.54
1:C:50:MET:HE3	1:C:116:ALA:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:THR:HB	1:E:108:PRO:HD3	1.89	0.54
1:E:293:ASP:O	1:E:296:PRO:HD2	2.06	0.54
1:E:348:LEU:HD12	1:E:349:ARG:N	2.23	0.54
1:E:368:LEU:N	1:E:368:LEU:CD1	2.59	0.54
1:A:301:MET:HB3	1:A:348:LEU:HD22	1.90	0.54
1:A:368:LEU:CB	1:A:446:TYR:CD1	2.90	0.54
2:D:152:GLU:O	2:D:153:THR:C	2.48	0.54
1:E:115:ALA:O	1:E:116:ALA:C	2.50	0.54
2:F:634:ASP:C	2:F:634:ASP:OD1	2.44	0.54
1:G:136:CYS:HB2	3:G:3001:FES:S1	2.46	0.54
2:H:407:GLN:OE1	2:H:618:PRO:HD2	2.07	0.54
1:A:260:HIS:O	1:A:261:PRO:C	2.50	0.54
1:C:283:GLY:O	1:C:284:ASN:C	2.49	0.54
1:E:7:LEU:HD21	1:E:32:LEU:HD11	1.88	0.54
2:B:61:VAL:HA	2:B:103:ALA:CB	2.37	0.54
1:E:369:ASN:O	1:E:370:LEU:HD23	2.07	0.54
1:G:281:ILE:HG23	1:G:282:GLY:N	2.22	0.54
2:H:39:LEU:HB3	2:H:95:GLY:O	2.07	0.54
2:H:536:ASN:O	2:H:537:GLY:C	2.50	0.54
2:H:650:ASP:OD2	2:H:726:LYS:NZ	2.30	0.54
1:A:144:ARG:O	1:A:145:ALA:C	2.48	0.54
2:B:251:ARG:O	2:B:252:PRO:C	2.50	0.54
2:B:367:ASP:CG	2:B:431:ARG:HH12	2.16	0.54
1:G:151:GLY:O	1:G:152:GLU:HG2	2.07	0.54
2:H:528:ALA:O	2:H:529:ALA:HB3	2.06	0.54
1:A:216:LEU:HD12	2:B:114:ARG:NH1	2.22	0.54
1:A:408:GLU:CD	2:B:442:ARG:NH2	2.65	0.54
2:B:517:ASP:OD2	2:B:519:SER:N	2.35	0.54
1:C:25:GLU:O	1:C:26:LEU:C	2.48	0.54
2:D:150:ASP:OD2	2:D:153:THR:OG1	2.25	0.54
2:F:661:ILE:CD1	2:F:712:LEU:HG	2.37	0.54
2:H:492:LEU:O	2:H:493:HIS:C	2.51	0.54
2:H:496:MET:CA	2:H:496:MET:CE	2.82	0.54
2:H:621:TYR:CE1	2:H:726:LYS:CG	2.85	0.54
1:A:261:PRO:O	1:A:262:ALA:C	2.48	0.54
2:B:221:MET:HE1	2:B:223:ARG:C	2.33	0.54
2:D:691:HIS:CD2	2:D:691:HIS:O	2.61	0.54
1:E:434:TYR:O	1:E:435:ARG:C	2.49	0.54
2:F:466:GLN:NE2	2:H:593:ARG:HG2	2.22	0.54
1:G:81:ILE:O	1:G:81:ILE:CG2	2.55	0.54
1:G:237:THR:HG22	1:G:239:ASP:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:MET:HB2	1:G:317:PRO:CD	2.37	0.54
1:G:318:LEU:O	1:G:319:GLU:C	2.51	0.54
1:A:139:TYR:C	1:A:141:PRO:HD2	2.32	0.54
2:D:171:GLN:HG3	2:D:678:GLU:OE1	2.08	0.54
2:D:720:GLU:CG	2:D:724:ARG:HH21	2.20	0.54
2:F:655:LEU:HD21	2:F:722:ILE:HG23	1.90	0.54
1:A:129:LEU:O	1:A:130:ALA:C	2.46	0.54
2:B:341:PHE:O	2:B:342:ARG:C	2.49	0.54
1:E:139:TYR:O	1:E:140:ALA:C	2.51	0.54
1:A:75:LEU:HD12	1:A:76:ARG:N	2.23	0.53
1:A:78:ILE:HD13	1:A:108:PRO:HA	1.90	0.53
1:C:139:TYR:O	1:C:140:ALA:C	2.50	0.53
1:C:374:GLY:O	1:C:376:LYS:N	2.41	0.53
2:F:238:LEU:HD11	2:F:257:TYR:CZ	2.43	0.53
2:H:330:ARG:NH2	2:H:611:ARG:NH2	2.56	0.53
2:H:730:GLU:H	2:H:731:PRO:CD	2.21	0.53
1:C:53:ASP:C	1:C:53:ASP:OD1	2.51	0.53
1:E:301:MET:CE	1:E:341:LEU:CB	2.79	0.53
2:F:171:GLN:HG2	2:F:341:PHE:CE1	2.43	0.53
2:F:344:PHE:CD2	8:F:4000:141:C2	2.92	0.53
2:F:411:ASP:OD1	2:F:411:ASP:N	2.39	0.53
2:F:627:ALA:HB2	2:F:735:LEU:HD22	1.89	0.53
2:H:61:VAL:HA	2:H:103:ALA:CB	2.38	0.53
2:H:346:GLY:N	2:H:347:PRO:CD	2.70	0.53
2:D:247:ARG:HH11	2:D:247:ARG:CG	2.18	0.53
1:E:118:HIS:HE1	1:E:154:PRO:HA	1.74	0.53
2:F:218:ARG:HE	2:F:220:GLU:CD	2.14	0.53
2:F:412:CYS:HA	2:F:624:TYR:CZ	2.42	0.53
2:H:456:GLY:O	2:H:457:ILE:HD13	2.07	0.53
2:H:617:ARG:HD3	2:H:619:PHE:O	2.08	0.53
1:A:297:ALA:CA	1:A:367:CYS:SG	2.96	0.53
6:B:3003:MTE:S1'	7:B:3004:MOS:S	3.07	0.53
1:E:390:VAL:HG23	1:E:391:PRO:CD	2.35	0.53
2:F:152:GLU:O	2:F:153:THR:C	2.51	0.53
2:F:496:MET:HE2	2:F:496:MET:N	2.23	0.53
1:G:296:PRO:O	1:G:297:ALA:C	2.46	0.53
2:H:744:HIS:C	2:H:744:HIS:CD2	2.86	0.53
1:A:360:ASP:OD1	2:B:697:LYS:HE3	2.08	0.53
2:B:351:LEU:HD13	2:B:737:ILE:HG12	1.89	0.53
2:B:481:LEU:HD12	2:B:482:ASN:H	1.74	0.53
2:B:595:SER:HB2	2:D:601:PHE:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:ASP:HB2	2:B:713:TRP:CD1	2.43	0.53
2:F:419:THR:O	2:F:420:ARG:C	2.51	0.53
1:G:428:MET:SD	1:G:429:ARG:N	2.81	0.53
2:H:12:ALA:O	2:H:13:ARG:C	2.49	0.53
2:H:536:ASN:O	2:H:540:VAL:HG23	2.09	0.53
1:A:436:MET:O	1:A:437:ASN:C	2.49	0.53
2:D:110:ARG:O	2:D:111:ILE:C	2.52	0.53
2:F:34:HIS:C	2:F:35:LEU:HD23	2.33	0.53
2:F:96:GLN:HG3	2:F:97:PRO:HD2	1.89	0.53
1:G:202:ILE:HD12	1:G:222:VAL:HG13	1.91	0.53
2:H:278:ILE:HD11	2:H:286:LEU:HD22	1.91	0.53
1:A:102:GLN:NE2	1:A:137:THR:HA	2.24	0.53
2:D:347:PRO:O	2:D:348:GLN:C	2.46	0.53
1:E:61:ASN:H	1:E:61:ASN:HD22	1.57	0.53
1:G:353:LEU:O	1:G:363:ALA:N	2.30	0.53
2:B:492:LEU:O	2:B:493:HIS:C	2.50	0.53
1:E:92:GLN:NE2	2:F:17:THR:HG22	2.24	0.53
2:F:164:GLY:HA3	2:F:276:TYR:CZ	2.44	0.53
2:H:494:ALA:O	2:H:495:LYS:C	2.49	0.53
1:A:271:ALA:HB2	4:A:3005:FAD:N5	2.24	0.53
1:C:423:THR:HG22	1:C:423:THR:O	2.09	0.53
1:E:237:THR:CG2	1:E:238:PRO:N	2.72	0.53
2:F:35:LEU:HD23	2:F:35:LEU:N	2.24	0.53
2:H:422:GLN:HG2	2:H:427:PHE:CD2	2.43	0.53
2:B:359:HIS:O	2:B:360:LEU:C	2.49	0.53
1:C:36:LYS:HD3	1:C:105:PHE:CE1	2.43	0.53
1:E:92:GLN:HE22	2:F:17:THR:HG22	1.74	0.53
1:E:324:GLU:O	1:E:325:TYR:C	2.52	0.53
2:F:198:HIS:ND1	2:F:526:ALA:HB2	2.24	0.53
2:F:448:ILE:HG23	2:F:448:ILE:O	2.09	0.53
2:F:704:ARG:HG2	2:F:704:ARG:HH11	1.74	0.53
1:G:295:PRO:HB2	1:G:296:PRO:HD3	1.89	0.53
2:H:731:PRO:O	2:H:732:PRO:C	2.51	0.53
1:C:124:ASP:O	1:C:128:LEU:HD22	2.08	0.52
2:D:457:ILE:O	2:D:458:SER:HB2	2.09	0.52
2:D:746:ALA:O	2:D:747:CYS:C	2.48	0.52
2:F:276:TYR:OH	2:F:359:HIS:HD2	1.92	0.52
1:G:37:GLU:CD	2:H:256:ARG:HH22	2.15	0.52
1:G:191:ASP:O	1:G:194:LEU:HB3	2.10	0.52
2:H:573:VAL:HG11	2:H:585:ILE:HG13	1.91	0.52
2:H:631:VAL:HG21	2:H:743:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:CZ	2:B:697:LYS:NZ	2.73	0.52
2:B:661:ILE:O	2:B:665:GLU:HG3	2.09	0.52
1:C:237:THR:CG2	1:C:239:ASP:H	2.22	0.52
1:E:120:ARG:O	1:E:121:ASP:C	2.53	0.52
1:G:67:LEU:O	1:G:68:PRO:C	2.50	0.52
2:B:251:ARG:HB2	2:B:252:PRO:HD2	1.91	0.52
1:C:324:GLU:O	1:C:325:TYR:C	2.51	0.52
2:F:618:PRO:HG2	2:F:619:PHE:CD1	2.45	0.52
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.91	0.52
2:B:380:PRO:O	2:B:381:GLU:HB2	2.09	0.52
2:B:696:TYR:C	2:B:697:LYS:HD2	2.34	0.52
1:C:192:TRP:O	1:C:196:HIS:HD2	1.92	0.52
2:D:66:THR:O	2:D:67:ALA:C	2.49	0.52
1:G:399:ALA:C	1:G:401:LEU:H	2.17	0.52
2:H:556:ALA:O	2:H:557:ALA:C	2.53	0.52
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.39	0.52
1:G:368:LEU:N	1:G:368:LEU:CD1	2.60	0.52
2:H:166:PHE:HB3	2:H:355:ARG:NH2	2.24	0.52
2:H:411:ASP:OD1	2:H:411:ASP:N	2.42	0.52
1:A:415:LEU:O	1:A:416:PRO:C	2.49	0.52
1:A:440:GLN:O	1:A:441:ALA:C	2.52	0.52
2:B:339:THR:CG2	2:B:340:ALA:N	2.37	0.52
2:D:130:ASP:O	2:D:131:GLN:C	2.47	0.52
2:F:568:PHE:CE2	2:F:573:VAL:HG22	2.45	0.52
1:G:409:ASP:OD2	1:G:409:ASP:N	2.42	0.52
2:H:196:SER:OG	2:H:198:HIS:N	2.27	0.52
2:H:214:PHE:N	2:H:214:PHE:CD1	2.71	0.52
2:H:634:ASP:OD2	2:H:637:THR:OG1	2.17	0.52
2:B:601:PHE:CG	2:D:595:SER:HB2	2.44	0.52
2:D:69:ASP:O	2:D:70:LEU:C	2.51	0.52
1:E:411:ILE:O	1:E:412:ALA:C	2.51	0.52
2:F:210:LEU:HD12	2:F:212:LEU:HD12	1.92	0.52
1:G:282:GLY:O	1:G:285:ILE:HB	2.10	0.52
2:D:74:ASN:OD1	2:D:85:VAL:N	2.38	0.52
1:E:22:SER:HG	1:E:25:GLU:HG2	1.74	0.52
2:F:566:VAL:HG13	2:F:575:ALA:HB2	1.91	0.52
2:F:721:THR:O	2:F:724:ARG:N	2.39	0.52
2:H:16:VAL:HG13	2:H:16:VAL:O	2.03	0.52
2:H:347:PRO:HG3	2:H:734:LEU:CD1	2.39	0.52
2:B:28:CYS:HB2	2:B:29:PRO:HD2	1.91	0.52
2:B:45:ALA:HA	2:B:123:ARG:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ILE:O	2:B:98:ILE:CG2	2.58	0.52
2:B:214:PHE:N	2:B:214:PHE:CD1	2.74	0.52
2:B:367:ASP:OD1	2:B:368:PRO:CD	2.58	0.52
1:E:78:ILE:CG2	1:E:79:GLU:N	2.72	0.52
2:F:453:VAL:HG12	2:F:454:LYS:N	2.16	0.52
2:F:617:ARG:HD3	2:F:619:PHE:O	2.09	0.52
1:A:132:ASN:OD1	1:A:274:GLN:NE2	2.35	0.52
1:A:428:MET:HE2	2:B:695:THR:HG21	1.90	0.52
2:D:263:MET:HE3	2:D:692:ALA:HA	1.91	0.52
2:F:328:SER:OG	2:F:330:ARG:NH1	2.39	0.52
1:G:141:PRO:HA	1:G:144:ARG:HH11	1.75	0.52
2:H:355:ARG:O	2:H:356:ALA:C	2.48	0.52
2:H:513:ILE:HG13	2:H:514:THR:N	2.25	0.52
2:D:351:LEU:HD13	2:D:737:ILE:HG12	1.92	0.51
1:E:165:THR:HG23	1:E:165:THR:O	2.10	0.51
1:E:382:ILE:O	1:E:393:ARG:HA	2.10	0.51
2:F:360:LEU:HD11	2:F:364:MET:HE3	1.91	0.51
1:G:141:PRO:CG	1:G:142:ILE:N	2.73	0.51
2:H:92:HIS:O	2:H:93:PHE:HB3	2.10	0.51
2:H:418:VAL:O	2:H:419:THR:C	2.52	0.51
2:H:771:ARG:O	2:H:772:ARG:C	2.51	0.51
1:A:202:ILE:HD12	1:A:222:VAL:HG13	1.93	0.51
2:B:334:ASN:C	2:B:335:THR:HG23	2.35	0.51
1:C:237:THR:CG2	1:C:238:PRO:N	2.72	0.51
1:E:68:PRO:CB	1:E:224:PHE:CE1	2.92	0.51
1:E:423:THR:HG22	1:E:423:THR:O	2.10	0.51
2:F:453:VAL:CG1	2:F:454:LYS:N	2.69	0.51
2:F:621:TYR:CE1	2:F:726:LYS:CG	2.83	0.51
2:H:691:HIS:O	2:H:692:ALA:CB	2.54	0.51
1:C:237:THR:CG2	1:C:238:PRO:HD2	2.35	0.51
2:D:185:PRO:O	2:D:185:PRO:HG2	2.10	0.51
2:D:398:LYS:C	2:D:399:LYS:HD2	2.35	0.51
2:D:737:ILE:O	2:D:738:SER:C	2.49	0.51
2:F:482:ASN:ND2	2:F:514:THR:OG1	2.32	0.51
1:G:118:HIS:O	1:G:120:ARG:N	2.44	0.51
2:H:280:ALA:C	2:H:287:LEU:CD1	2.83	0.51
2:B:218:ARG:NH2	2:D:218:ARG:HH22	2.08	0.51
2:B:237:HIS:ND1	2:B:237:HIS:N	2.58	0.51
1:E:381:ARG:NH2	1:E:393:ARG:HH21	1.98	0.51
2:F:296:ARG:HH11	2:F:296:ARG:CG	2.18	0.51
2:F:305:LEU:HD21	2:F:611:ARG:NE	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:448:ILE:HG13	2:F:630:GLU:HB2	1.91	0.51
1:A:25:GLU:O	1:A:26:LEU:C	2.53	0.51
1:C:106:CYS:SG	1:C:134:CYS:HB2	2.51	0.51
1:C:399:ALA:C	1:C:401:LEU:N	2.66	0.51
2:D:360:LEU:CD1	2:D:364:MET:CE	2.89	0.51
1:G:359:GLN:HA	1:G:359:GLN:HE21	1.75	0.51
2:H:305:LEU:HB3	2:H:306:PRO:HD3	1.91	0.51
2:B:652:GLY:N	2:B:726:LYS:HB2	2.26	0.51
1:C:331:ARG:HG3	1:C:331:ARG:HH11	1.76	0.51
2:D:528:ALA:O	2:D:529:ALA:CB	2.41	0.51
2:D:648:LEU:HA	2:D:711:ALA:O	2.11	0.51
2:D:776:ARG:O	2:D:777:ALA:HB3	2.10	0.51
1:E:201:LEU:O	4:E:3005:FAD:O2B	2.27	0.51
1:E:348:LEU:HD12	1:E:349:ARG:H	1.75	0.51
2:F:631:VAL:HG12	2:F:642:ILE:HA	1.92	0.51
1:G:436:MET:C	1:G:438:ALA:H	2.16	0.51
2:H:547:LEU:O	2:H:550:ARG:N	2.43	0.51
1:A:370:LEU:HD23	1:A:380:ALA:HA	1.93	0.51
1:A:371:THR:C	1:A:372:LEU:HD23	2.35	0.51
1:A:447:VAL:O	1:A:448:ARG:C	2.50	0.51
2:B:52:LEU:O	2:B:55:VAL:N	2.43	0.51
2:B:93:PHE:CE2	2:B:299:TRP:CE2	2.99	0.51
1:E:6:LEU:HA	1:E:10:GLU:O	2.10	0.51
1:E:279:ALA:HB1	4:E:3005:FAD:H4'	1.92	0.51
1:G:141:PRO:HG2	1:G:142:ILE:H	1.75	0.51
1:G:368:LEU:HB2	1:G:446:TYR:CD1	2.45	0.51
2:H:449:ALA:CB	2:H:741:LEU:HB3	2.41	0.51
1:A:271:ALA:CA	1:A:359:GLN:NE2	2.74	0.51
1:A:373:LYS:O	1:A:374:GLY:O	2.29	0.51
2:B:760:PRO:O	2:B:760:PRO:HG2	2.11	0.51
1:C:322:PHE:HB3	1:C:390:VAL:CG2	2.40	0.51
2:D:398:LYS:N	2:D:398:LYS:HE3	2.25	0.51
2:D:552:ALA:O	2:D:553:GLY:C	2.54	0.51
2:F:417:LEU:O	2:F:418:VAL:C	2.53	0.51
1:G:267:LEU:O	1:G:268:ARG:C	2.50	0.51
2:H:760:PRO:O	2:H:760:PRO:HG2	2.11	0.51
1:A:16:ILE:HD13	1:A:68:PRO:HG3	1.92	0.51
1:A:85:ASP:OD2	1:A:87:ARG:HD3	2.11	0.51
2:D:320:PHE:CG	2:D:401:GLN:NE2	2.78	0.51
1:E:83:ALA:HB2	1:E:157:TRP:CZ2	2.46	0.51
2:F:354:GLU:OE1	2:F:372:ARG:NE	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:656:ASN:O	2:F:657:PRO:C	2.52	0.51
2:F:767:LEU:O	2:F:768:ALA:C	2.52	0.51
1:A:194:LEU:HD12	1:A:194:LEU:O	2.11	0.51
1:A:415:LEU:HB2	1:A:416:PRO:HD3	1.93	0.51
2:B:171:GLN:O	2:B:268:LYS:HB3	2.11	0.51
2:D:218:ARG:NE	2:D:220:GLU:OE2	2.44	0.51
2:D:343:GLY:O	2:D:344:PHE:C	2.53	0.51
2:D:532:GLY:N	6:D:3003:MTE:O1P	2.30	0.51
2:D:533:ALA:O	2:D:534:ASP:C	2.53	0.51
1:E:237:THR:CG2	1:E:238:PRO:CD	2.86	0.51
1:E:370:LEU:HD22	1:E:380:ALA:CB	2.41	0.51
1:E:390:VAL:HG22	1:E:391:PRO:N	2.26	0.51
2:F:319:TYR:OH	2:F:354:GLU:OE2	2.29	0.51
1:G:370:LEU:HD21	1:G:380:ALA:HB1	1.92	0.51
1:A:102:GLN:HB3	2:B:489:GLY:O	2.11	0.50
1:A:140:ALA:N	1:A:141:PRO:HD2	2.27	0.50
2:D:554:PHE:HB2	2:D:594:ILE:HD12	1.93	0.50
2:F:33:LEU:HD21	2:F:251:ARG:NH1	2.25	0.50
2:F:471:VAL:HG12	2:F:472:GLN:N	2.26	0.50
2:F:649:HIS:HB3	2:F:664:ILE:HD13	1.93	0.50
2:H:7:LEU:HB3	2:H:8:PRO:HD2	1.94	0.50
2:H:198:HIS:CD2	2:H:526:ALA:HA	2.46	0.50
2:H:360:LEU:HG	2:H:364:MET:HE3	1.93	0.50
2:H:690:THR:HA	2:H:695:THR:OG1	2.11	0.50
1:A:191:ASP:O	1:A:194:LEU:HB3	2.11	0.50
2:B:621:TYR:HE1	2:B:726:LYS:HG2	1.74	0.50
1:E:316:MET:HB2	1:E:317:PRO:CD	2.38	0.50
2:H:28:CYS:HB2	2:H:29:PRO:HD2	1.93	0.50
1:A:89:HIS:ND1	1:A:90:PRO:HD2	2.27	0.50
2:B:398:LYS:N	2:B:398:LYS:HE3	2.27	0.50
2:D:459:PHE:N	2:D:465:ASN:OD1	2.44	0.50
1:E:37:GLU:OE2	2:F:256:ARG:NH2	2.44	0.50
1:E:58:ARG:CD	1:E:277:GLN:OE1	2.60	0.50
2:F:278:ILE:HG12	2:F:279:GLY:N	2.27	0.50
2:F:704:ARG:HH11	2:F:704:ARG:CG	2.24	0.50
1:G:298:LEU:O	1:G:299:ILE:C	2.53	0.50
2:H:95:GLY:O	2:H:96:GLN:C	2.54	0.50
2:H:633:ILE:CD1	2:H:746:ALA:HB1	2.42	0.50
1:A:210:LEU:HD23	1:A:210:LEU:N	2.25	0.50
2:B:166:PHE:CE1	2:B:355:ARG:HG3	2.47	0.50
2:B:329:HIS:HB3	2:B:331:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:674:TRP:CD2	2:B:675:LEU:HD21	2.45	0.50
1:G:18:ASP:OD2	1:G:20:THR:N	2.32	0.50
2:B:372:ARG:O	2:B:373:ALA:C	2.51	0.50
1:C:349:ARG:HG2	1:C:351:TYR:OH	2.11	0.50
1:C:390:VAL:HG22	1:C:391:PRO:HD2	1.93	0.50
2:D:731:PRO:CB	2:D:732:PRO:CD	2.85	0.50
2:F:730:GLU:N	2:F:731:PRO:CD	2.74	0.50
1:G:314:ARG:O	1:G:315:ARG:HB2	2.10	0.50
2:H:448:ILE:HG23	2:H:448:ILE:O	2.11	0.50
2:H:586:VAL:HG13	2:H:596:LEU:HD13	1.94	0.50
2:H:722:ILE:HG13	2:H:723:PHE:CD1	2.46	0.50
1:A:105:PHE:CD1	2:B:177:GLU:HB2	2.46	0.50
2:B:38:GLY:C	2:B:39:LEU:HD23	2.37	0.50
2:B:123:ARG:HB3	2:B:124:PRO:HD2	1.93	0.50
2:B:356:ALA:O	2:B:357:ILE:C	2.53	0.50
2:B:582:PHE:O	2:B:586:VAL:HG23	2.11	0.50
2:B:731:PRO:CB	2:B:732:PRO:CD	2.81	0.50
1:C:305:LEU:HD21	1:C:307:LEU:HD21	1.94	0.50
2:D:450:LEU:HG	2:D:451:SER:N	2.24	0.50
1:E:231:LEU:O	1:E:231:LEU:HD23	2.11	0.50
2:F:221:MET:CE	2:F:223:ARG:C	2.84	0.50
2:F:569:ASP:O	2:F:570:ALA:HB3	2.10	0.50
1:G:129:LEU:O	1:G:130:ALA:C	2.54	0.50
2:H:547:LEU:O	2:H:548:ARG:C	2.55	0.50
1:C:439:ALA:O	1:C:440:GLN:C	2.50	0.50
2:D:478:SER:C	2:D:479:VAL:HG23	2.36	0.50
1:E:5:PHE:CG	1:E:70:ILE:HD12	2.47	0.50
1:E:100:GLY:HA2	1:E:141:PRO:HB2	1.94	0.50
2:F:160:HIS:CB	2:F:364:MET:HE2	2.41	0.50
2:F:210:LEU:HD12	2:F:212:LEU:CD1	2.41	0.50
2:F:528:ALA:O	2:F:529:ALA:HB3	2.12	0.50
2:F:536:ASN:O	2:F:537:GLY:C	2.55	0.50
1:G:134:CYS:SG	1:G:136:CYS:HB2	2.52	0.50
2:H:93:PHE:CD2	2:H:299:TRP:NE1	2.79	0.50
2:H:496:MET:HE2	2:H:496:MET:N	2.26	0.50
1:A:294:GLY:N	1:A:295:PRO:CD	2.74	0.50
2:B:70:LEU:HD12	2:B:74:ASN:HB2	1.92	0.50
2:D:28:CYS:HB2	2:D:29:PRO:CD	2.42	0.50
1:E:103:CYS:HA	2:F:489:GLY:CA	2.42	0.50
1:E:111:ILE:HD11	2:F:16:VAL:HG22	1.93	0.50
1:E:118:HIS:CE1	1:E:154:PRO:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:ASP:C	1:G:53:ASP:OD1	2.55	0.50
1:G:266:LEU:O	1:G:267:LEU:C	2.51	0.50
1:G:344:SER:OG	1:G:346:PRO:HD3	2.11	0.50
1:A:207:ASP:OD2	4:A:3005:FAD:H3'	2.12	0.50
1:C:89:HIS:O	1:C:90:PRO:C	2.53	0.50
2:D:195:SER:O	2:D:231:LYS:HD3	2.11	0.50
2:F:310:ARG:HD2	2:F:344:PHE:HB3	1.94	0.50
1:G:111:ILE:HD13	1:G:114:MET:HE3	1.94	0.50
1:G:261:PRO:O	1:G:262:ALA:C	2.52	0.50
2:H:674:TRP:C	2:H:675:LEU:HD23	2.36	0.50
1:A:37:GLU:OE1	2:B:256:ARG:NH2	2.45	0.49
2:B:146:TRP:CH2	2:B:312:MET:HE3	2.47	0.49
2:B:164:GLY:HA3	2:B:276:TYR:CZ	2.45	0.49
1:E:110:PHE:O	1:E:114:MET:N	2.35	0.49
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.12	0.49
6:F:3003:MTE:S2'	7:F:3004:MOS:S	3.10	0.49
1:G:25:GLU:O	1:G:26:LEU:C	2.53	0.49
2:H:461:LEU:HD12	2:H:463:HIS:CE1	2.47	0.49
1:A:181:PHE:CD2	1:A:183:PRO:HD3	2.46	0.49
4:A:3005:FAD:N1	4:A:3005:FAD:C2'	2.74	0.49
2:B:674:TRP:CZ3	2:B:675:LEU:HD21	2.48	0.49
1:C:359:GLN:O	1:C:359:GLN:CG	2.58	0.49
2:D:131:GLN:O	2:D:134:ALA:HB3	2.12	0.49
2:D:229:GLY:HA2	7:D:3004:MOS:S	2.53	0.49
1:E:205:GLY:N	4:E:3005:FAD:O2P	2.44	0.49
2:F:319:TYR:N	2:F:319:TYR:CD1	2.80	0.49
2:F:547:LEU:O	2:F:548:ARG:C	2.53	0.49
2:F:698:ILE:HB	2:F:699:PRO:CD	2.41	0.49
1:G:66:MET:HE2	1:G:209:SER:HB3	1.94	0.49
1:G:165:THR:O	1:G:166:LEU:HD23	2.12	0.49
1:G:264:ALA:O	1:G:265:GLY:C	2.55	0.49
2:H:507:ASP:OD1	2:H:507:ASP:C	2.54	0.49
2:H:633:ILE:HD13	2:H:746:ALA:HB3	1.94	0.49
1:A:237:THR:CG2	1:A:238:PRO:CD	2.85	0.49
1:C:165:THR:O	1:C:165:THR:HG23	2.12	0.49
1:C:205:GLY:O	1:C:209:SER:OG	2.30	0.49
1:C:337:GLU:O	1:C:338:SER:HB3	2.12	0.49
2:D:281:ASP:OD1	2:D:283:SER:OG	2.20	0.49
2:D:720:GLU:HG2	2:D:724:ARG:NH2	2.27	0.49
2:D:731:PRO:CD	2:D:732:PRO:CD	2.90	0.49
2:F:258:ASP:O	2:F:259:ARG:C	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:MET:HG3	1:G:111:ILE:HD11	1.94	0.49
1:G:118:HIS:O	1:G:121:ASP:N	2.35	0.49
1:G:299:ILE:O	1:G:300:ALA:C	2.52	0.49
2:B:296:ARG:HH11	2:B:296:ARG:CG	2.25	0.49
2:B:492:LEU:HD12	2:B:492:LEU:O	2.12	0.49
2:D:214:PHE:N	2:D:214:PHE:CD1	2.75	0.49
2:D:238:LEU:HD23	2:D:255:MET:HG2	1.95	0.49
1:E:151:GLY:C	1:E:152:GLU:HG2	2.37	0.49
2:F:574:GLN:HG3	2:F:579:SER:HB2	1.94	0.49
2:F:647:ILE:HD13	2:F:735:LEU:HD13	1.94	0.49
1:A:78:ILE:CG2	1:A:79:GLU:N	2.76	0.49
1:A:125:TYR:O	1:A:126:ASP:C	2.55	0.49
2:B:507:ASP:OD1	2:B:508:PRO:CD	2.61	0.49
2:B:566:VAL:HG13	2:B:575:ALA:HB2	1.95	0.49
2:B:671:GLY:O	2:B:674:TRP:HB3	2.12	0.49
2:B:736:GLY:O	2:B:737:ILE:C	2.55	0.49
1:C:237:THR:HG23	1:C:238:PRO:CG	2.40	0.49
1:E:12:ARG:HH11	1:E:12:ARG:CG	2.23	0.49
2:F:478:SER:C	2:F:479:VAL:CG2	2.85	0.49
1:G:52:ARG:NH1	1:G:57:SER:HB3	2.27	0.49
1:G:61:ASN:ND2	1:G:61:ASN:N	2.60	0.49
2:B:233:SER:C	2:B:235:GLY:H	2.20	0.49
2:B:258:ASP:O	2:B:259:ARG:C	2.53	0.49
2:B:331:LEU:N	2:B:331:LEU:HD23	2.25	0.49
2:D:700:ALA:O	2:D:701:PHE:C	2.55	0.49
1:E:102:GLN:NE2	1:E:137:THR:HA	2.27	0.49
2:F:197:GLN:HG2	2:F:488:MET:HE2	1.95	0.49
2:F:288:GLY:HA2	2:F:323:ALA:O	2.13	0.49
1:G:356:ARG:NH2	1:G:359:GLN:O	2.45	0.49
2:H:466:GLN:HA	2:H:602:TYR:O	2.13	0.49
1:A:18:ASP:OD2	1:A:18:ASP:C	2.55	0.49
1:A:165:THR:O	1:A:165:THR:CG2	2.61	0.49
1:A:271:ALA:HA	1:A:359:GLN:HE21	1.75	0.49
2:B:674:TRP:CD2	2:B:675:LEU:CD2	2.96	0.49
2:D:258:ASP:O	2:D:259:ARG:C	2.52	0.49
1:E:198:GLU:HA	1:E:198:GLU:OE2	2.13	0.49
1:E:429:ARG:O	1:E:430:ALA:HB2	2.12	0.49
2:F:407:GLN:OE1	2:F:617:ARG:HG2	2.13	0.49
1:G:370:LEU:HD21	1:G:380:ALA:CB	2.42	0.49
2:H:79:ALA:O	2:H:80:PRO:C	2.56	0.49
2:H:110:ARG:O	2:H:111:ILE:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:419:THR:O	2:H:420:ARG:C	2.53	0.49
1:A:415:LEU:O	1:A:417:LEU:N	2.45	0.49
1:C:139:TYR:C	1:C:141:PRO:HD2	2.38	0.49
1:C:368:LEU:HB2	1:C:446:TYR:CD1	2.47	0.49
2:D:720:GLU:CG	2:D:724:ARG:NH2	2.76	0.49
2:F:512:ARG:NH1	2:H:216:ASP:OD2	2.45	0.49
2:F:556:ALA:HB1	2:F:561:CYS:O	2.12	0.49
2:F:588:ALA:O	2:F:589:ALA:C	2.56	0.49
2:F:740:PHE:O	2:F:741:LEU:C	2.52	0.49
1:G:50:MET:CE	1:G:116:ALA:CB	2.84	0.49
2:H:158:ALA:O	2:H:159:ALA:C	2.52	0.49
2:H:263:MET:HE3	2:H:692:ALA:CA	2.39	0.49
1:A:41:GLU:HG2	1:A:210:LEU:HD13	1.95	0.49
2:B:79:ALA:HB1	2:B:80:PRO:CD	2.43	0.49
2:B:650:ASP:HA	2:B:713:TRP:HB3	1.94	0.49
1:C:50:MET:HE3	1:C:116:ALA:CA	2.38	0.49
1:E:394:ALA:O	1:E:397:PHE:N	2.41	0.49
1:G:75:LEU:HD12	1:G:76:ARG:N	2.27	0.49
1:G:105:PHE:HD2	2:H:176:LEU:HB3	1.77	0.49
1:G:117:ALA:O	1:G:118:HIS:C	2.54	0.49
1:G:418:LEU:HD23	1:G:418:LEU:HA	1.63	0.49
2:B:53:GLU:N	2:B:54:PRO:CD	2.76	0.49
2:B:700:ALA:O	2:B:701:PHE:C	2.55	0.49
1:C:390:VAL:HG23	1:C:391:PRO:CD	2.42	0.49
2:D:335:THR:O	2:D:336:GLN:C	2.55	0.49
2:D:370:GLU:O	2:D:371:LEU:C	2.54	0.49
1:E:37:GLU:CD	2:F:256:ARG:HH21	2.21	0.49
1:G:358:ASP:O	1:G:359:GLN:C	2.55	0.49
1:G:370:LEU:CD2	1:G:380:ALA:CB	2.91	0.49
1:G:429:ARG:O	1:G:430:ALA:HB2	2.13	0.49
2:H:35:LEU:HA	2:H:101:VAL:O	2.13	0.49
2:H:93:PHE:CD2	2:H:299:TRP:CD1	3.01	0.49
2:H:112:ALA:C	2:H:114:ARG:N	2.68	0.49
2:H:238:LEU:HD11	2:H:257:TYR:CE1	2.47	0.49
2:H:335:THR:O	2:H:336:GLN:C	2.55	0.49
1:A:165:THR:O	1:A:166:LEU:HD23	2.12	0.48
1:A:252:LEU:HD23	1:A:281:ILE:CD1	2.43	0.48
2:D:65:PHE:O	2:D:99:PHE:HB2	2.12	0.48
4:E:3005:FAD:O5B	4:E:3005:FAD:C2B	2.58	0.48
2:F:198:HIS:CG	2:F:526:ALA:HB2	2.48	0.48
2:F:232:GLU:OE2	8:F:4000:141:H1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:LEU:HD12	1:G:194:LEU:O	2.11	0.48
2:H:339:THR:HG23	2:H:340:ALA:H	1.73	0.48
2:H:635:ARG:CD	2:H:750:CYS:SG	2.98	0.48
1:A:353:LEU:HD21	1:A:434:TYR:OH	2.13	0.48
1:A:359:GLN:HE21	1:A:359:GLN:HA	1.78	0.48
1:A:430:ALA:HB1	1:A:434:TYR:HD2	1.78	0.48
2:B:407:GLN:OE1	2:B:617:ARG:HG2	2.12	0.48
1:E:98:HIS:O	1:E:99:HIS:HB2	2.13	0.48
2:F:452:PRO:O	2:F:452:PRO:HG2	2.13	0.48
7:F:3004:MOS:S	8:F:4000:141:C7	3.01	0.48
1:G:228:CYS:O	1:G:229:LYS:C	2.55	0.48
1:G:271:ALA:CA	1:G:359:GLN:HE22	2.26	0.48
2:H:112:ALA:O	2:H:113:ALA:C	2.52	0.48
2:D:227:GLY:N	6:D:3003:MTE:O4	2.37	0.48
2:D:661:ILE:CD1	2:D:712:LEU:HG	2.44	0.48
7:D:3004:MOS:S	8:D:4000:141:N8	2.86	0.48
1:E:231:LEU:O	1:E:231:LEU:CD2	2.61	0.48
2:F:756:ASP:O	2:F:758:GLN:NE2	2.39	0.48
2:H:319:TYR:N	2:H:319:TYR:CD1	2.81	0.48
2:H:370:GLU:O	2:H:371:LEU:C	2.53	0.48
1:A:59:ALA:C	1:A:60:VAL:CG1	2.86	0.48
2:B:150:ASP:OD1	2:B:150:ASP:O	2.30	0.48
2:B:346:GLY:N	2:B:347:PRO:CD	2.77	0.48
2:D:263:MET:HE1	2:D:692:ALA:HA	1.95	0.48
2:D:528:ALA:HB1	8:D:4000:141:H1	1.93	0.48
2:D:581:ARG:O	2:D:582:PHE:C	2.56	0.48
2:D:653:ALA:O	2:D:654:SER:C	2.54	0.48
1:G:319:GLU:N	1:G:319:GLU:OE2	2.46	0.48
1:G:412:ALA:O	1:G:415:LEU:HG	2.13	0.48
2:H:205:LYS:HB3	2:H:240:ILE:HD11	1.95	0.48
2:H:307:VAL:O	2:H:310:ARG:N	2.45	0.48
2:B:751:GLY:HA3	2:B:773:ALA:O	2.14	0.48
2:D:197:GLN:HG3	2:D:231:LYS:HB2	1.96	0.48
2:D:328:SER:OG	2:D:330:ARG:NH1	2.42	0.48
2:D:432:ALA:O	2:D:433:GLU:C	2.55	0.48
2:D:722:ILE:HG23	2:D:722:ILE:O	2.12	0.48
1:E:300:ALA:C	1:E:302:GLY:H	2.21	0.48
1:E:301:MET:HE3	1:E:341:LEU:CB	2.22	0.48
1:G:78:ILE:HG21	1:G:108:PRO:HB3	1.94	0.48
2:H:443:THR:O	2:H:444:LEU:HD23	2.13	0.48
1:A:252:LEU:CD2	1:A:281:ILE:CD1	2.88	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ASP:OD2	2:D:512:ARG:NH1	2.46	0.48
2:D:237:HIS:ND1	2:D:237:HIS:N	2.55	0.48
2:D:731:PRO:HB2	2:D:732:PRO:HD3	1.95	0.48
2:D:742:ALA:O	2:D:743:LEU:C	2.55	0.48
1:E:61:ASN:ND2	1:E:61:ASN:N	2.61	0.48
1:E:364:VAL:CG2	1:E:435:ARG:HG2	2.44	0.48
2:F:214:PHE:N	2:F:214:PHE:HD1	2.08	0.48
2:H:107:ARG:O	2:H:110:ARG:N	2.47	0.48
2:H:330:ARG:NH2	2:H:611:ARG:HH21	2.10	0.48
2:H:481:LEU:HD12	2:H:482:ASN:H	1.77	0.48
2:H:487:GLU:OE2	2:H:489:GLY:CA	2.61	0.48
2:H:641:ARG:HH21	2:H:706:ARG:NE	2.12	0.48
1:A:52:ARG:HG2	1:A:53:ASP:N	2.28	0.48
1:A:218:ASP:C	1:A:218:ASP:OD1	2.56	0.48
2:B:65:PHE:O	2:B:99:PHE:HB2	2.13	0.48
2:B:130:ASP:O	2:B:131:GLN:C	2.54	0.48
2:D:457:ILE:O	2:D:458:SER:CB	2.62	0.48
2:D:755:PRO:O	2:D:772:ARG:HD2	2.14	0.48
1:E:408:GLU:OE1	2:F:442:ARG:NH2	2.31	0.48
2:F:38:GLY:C	2:F:39:LEU:HD23	2.38	0.48
2:F:348:GLN:O	2:F:349:GLY:C	2.51	0.48
2:H:722:ILE:HG13	2:H:723:PHE:HD1	1.77	0.48
1:A:105:PHE:CE1	2:B:177:GLU:HB2	2.48	0.48
1:C:291:ILE:O	1:C:292:GLY:C	2.52	0.48
2:D:39:LEU:HD23	2:D:39:LEU:N	2.29	0.48
2:D:65:PHE:HB2	2:D:100:LEU:HB3	1.95	0.48
1:E:68:PRO:HB2	1:E:224:PHE:CE1	2.48	0.48
1:E:107:THR:HG21	2:F:16:VAL:HA	1.96	0.48
1:E:139:TYR:C	1:E:141:PRO:HD2	2.38	0.48
1:E:192:TRP:O	1:E:196:HIS:CD2	2.59	0.48
1:E:295:PRO:HB2	1:E:296:PRO:HD3	1.95	0.48
1:C:50:MET:CE	1:C:116:ALA:HA	2.40	0.48
1:C:399:ALA:O	1:C:401:LEU:N	2.47	0.48
2:D:265:ILE:O	2:D:265:ILE:HG22	2.11	0.48
1:E:286:ALA:O	1:E:287:ASN:C	2.51	0.48
1:E:331:ARG:O	1:E:334:GLU:HB2	2.14	0.48
1:G:34:GLY:C	1:G:36:LYS:HE3	2.39	0.48
1:G:324:GLU:O	1:G:325:TYR:C	2.56	0.48
1:A:59:ALA:C	1:A:60:VAL:HG13	2.38	0.48
1:A:237:THR:CG2	1:A:238:PRO:N	2.77	0.48
2:B:198:HIS:CG	2:B:526:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ASP:OD1	2:D:512:ARG:HD2	2.14	0.48
2:B:432:ALA:O	2:B:433:GLU:C	2.55	0.48
2:B:747:CYS:O	2:B:748:ALA:C	2.56	0.48
2:B:771:ARG:O	2:B:772:ARG:C	2.56	0.48
2:D:66:THR:HB	2:D:69:ASP:OD2	2.13	0.48
2:D:464:LEU:HA	2:D:464:LEU:HD23	1.64	0.48
1:E:353:LEU:HD12	1:E:353:LEU:HA	1.53	0.48
2:F:166:PHE:CE1	2:F:355:ARG:HG3	2.49	0.48
2:F:551:LEU:O	2:F:552:ALA:C	2.56	0.48
1:G:78:ILE:HD13	1:G:108:PRO:HA	1.95	0.48
1:G:151:GLY:C	1:G:152:GLU:HG2	2.38	0.48
2:B:166:PHE:HB3	2:B:355:ARG:NH2	2.28	0.47
2:B:274:ILE:HG12	2:B:293:HIS:HD2	1.78	0.47
1:C:59:ALA:C	1:C:60:VAL:CG1	2.86	0.47
2:D:560:GLY:O	2:D:561:CYS:CB	2.44	0.47
2:D:644:ARG:HB2	2:D:707:ILE:HB	1.96	0.47
1:E:314:ARG:NH1	1:E:334:GLU:OE2	2.47	0.47
1:E:314:ARG:O	1:E:315:ARG:HB2	2.12	0.47
1:G:331:ARG:HH11	1:G:331:ARG:HG3	1.78	0.47
1:A:141:PRO:HG2	1:A:142:ILE:N	2.29	0.47
2:B:556:ALA:HB1	2:B:561:CYS:O	2.14	0.47
1:E:45:GLY:O	1:E:48:THR:OG1	2.27	0.47
1:E:301:MET:CE	1:E:341:LEU:HD22	2.34	0.47
1:E:317:PRO:O	1:E:318:LEU:C	2.57	0.47
2:F:437:TRP:CZ3	2:F:446:ARG:HG3	2.50	0.47
2:F:448:ILE:O	2:F:448:ILE:CG2	2.60	0.47
1:G:205:GLY:O	1:G:209:SER:OG	2.31	0.47
1:G:317:PRO:O	1:G:320:ASP:HB2	2.14	0.47
2:H:360:LEU:CD1	2:H:364:MET:HE2	2.43	0.47
2:H:560:GLY:O	2:H:561:CYS:CB	2.45	0.47
1:A:436:MET:C	1:A:438:ALA:N	2.72	0.47
1:C:102:GLN:NE2	1:C:137:THR:HA	2.28	0.47
1:C:193:TYR:O	1:C:196:HIS:N	2.47	0.47
1:C:238:PRO:HG2	1:C:239:ASP:CG	2.39	0.47
2:D:741:LEU:HD12	2:D:741:LEU:HA	1.60	0.47
1:E:6:LEU:HD11	1:E:9:GLY:C	2.39	0.47
2:F:179:GLN:HB3	2:F:238:LEU:CD1	2.41	0.47
1:G:297:ALA:HA	1:G:367:CYS:SG	2.55	0.47
2:H:58:SER:OG	2:H:59:PRO:CD	2.61	0.47
2:H:701:PHE:HE2	2:H:704:ARG:NH1	2.13	0.47
2:B:344:PHE:CD1	8:B:4000:141:C5	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:ALA:O	2:B:495:LYS:C	2.55	0.47
2:B:533:ALA:O	2:B:534:ASP:C	2.54	0.47
2:B:744:HIS:HE1	2:B:754:TRP:CZ3	2.33	0.47
1:C:191:ASP:O	1:C:194:LEU:HB3	2.14	0.47
1:C:252:LEU:O	1:C:252:LEU:HD12	2.14	0.47
2:F:77:SER:HB2	2:F:83:GLU:HB3	1.96	0.47
2:F:372:ARG:O	2:F:373:ALA:C	2.56	0.47
1:G:78:ILE:HG23	1:G:79:GLU:N	2.30	0.47
1:G:290:PRO:O	1:G:386:GLY:N	2.36	0.47
1:G:302:GLY:HA2	1:G:381:ARG:NH1	2.29	0.47
2:H:197:GLN:HG2	2:H:224:MET:HE1	1.95	0.47
2:H:330:ARG:HH21	2:H:611:ARG:NH2	2.13	0.47
2:H:398:LYS:O	2:H:399:LYS:O	2.32	0.47
2:H:450:LEU:HD12	2:H:628:ILE:HG13	1.96	0.47
2:H:487:GLU:OE2	2:H:489:GLY:N	2.46	0.47
2:H:730:GLU:O	2:H:733:PHE:N	2.42	0.47
1:A:358:ASP:O	1:A:359:GLN:C	2.57	0.47
2:B:218:ARG:NH2	2:B:517:ASP:OD1	2.48	0.47
1:C:295:PRO:O	1:C:296:PRO:C	2.52	0.47
1:C:432:ALA:O	1:C:433:ALA:C	2.51	0.47
2:D:166:PHE:CE1	2:D:355:ARG:HG3	2.49	0.47
2:D:673:GLY:O	2:D:678:GLU:HG3	2.15	0.47
2:F:174:PHE:CE1	2:F:693:PRO:HG3	2.49	0.47
2:B:361:ALA:O	2:B:362:ARG:C	2.58	0.47
2:D:648:LEU:HD12	2:D:711:ALA:O	2.15	0.47
2:D:701:PHE:O	2:D:704:ARG:HG2	2.15	0.47
1:E:92:GLN:HB3	2:F:16:VAL:CG1	2.45	0.47
2:F:278:ILE:CG1	2:F:279:GLY:N	2.77	0.47
2:H:261:ASP:O	2:H:262:ASP:C	2.58	0.47
2:H:303:LEU:C	2:H:306:PRO:HD2	2.38	0.47
2:H:367:ASP:C	2:H:367:ASP:OD1	2.57	0.47
1:A:388:ALA:C	1:A:390:VAL:N	2.71	0.47
2:B:31:ASN:HB2	2:B:251:ARG:HH11	1.79	0.47
2:B:179:GLN:HB3	2:B:238:LEU:HD13	1.95	0.47
2:B:627:ALA:HB2	2:B:735:LEU:HD22	1.96	0.47
1:C:281:ILE:O	1:C:281:ILE:HG13	2.15	0.47
2:D:609:TRP:HA	2:D:616:GLY:HA3	1.95	0.47
2:D:649:HIS:HB3	2:D:664:ILE:HD13	1.96	0.47
1:E:237:THR:CG2	1:E:238:PRO:HD2	2.41	0.47
1:E:237:THR:CB	1:E:238:PRO:HD2	2.45	0.47
1:E:241:TYR:N	1:E:341:LEU:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:GLY:CA	1:E:442:MET:SD	3.00	0.47
1:E:415:LEU:N	1:E:416:PRO:CD	2.78	0.47
1:E:440:GLN:O	1:E:441:ALA:C	2.57	0.47
2:F:28:CYS:HB2	2:F:29:PRO:CD	2.44	0.47
2:F:74:ASN:OD1	2:F:85:VAL:N	2.44	0.47
2:F:224:MET:HE3	2:F:488:MET:HB3	1.95	0.47
2:F:414:LEU:HG	2:F:624:TYR:CD2	2.50	0.47
1:G:39:CYS:SG	1:G:40:ASN:N	2.87	0.47
1:G:89:HIS:ND1	1:G:91:VAL:HB	2.29	0.47
1:G:353:LEU:HD21	1:G:434:TYR:CZ	2.49	0.47
2:H:347:PRO:O	2:H:348:GLN:C	2.57	0.47
2:H:448:ILE:O	2:H:448:ILE:CG2	2.61	0.47
2:H:674:TRP:O	2:H:675:LEU:HD23	2.14	0.47
1:A:143:LEU:HD22	1:A:147:GLU:OE2	2.15	0.47
2:B:153:THR:O	2:B:154:ALA:C	2.57	0.47
2:B:238:LEU:HD11	2:B:257:TYR:CE1	2.50	0.47
2:D:233:SER:C	2:D:235:GLY:H	2.22	0.47
2:D:609:TRP:HB2	2:D:616:GLY:HA3	1.95	0.47
1:E:394:ALA:O	1:E:395:ALA:C	2.58	0.47
2:F:342:ARG:CZ	2:F:667:ALA:HB2	2.45	0.47
2:F:367:ASP:OD1	2:F:368:PRO:CD	2.63	0.47
2:F:680:LEU:C	2:F:681:VAL:HG23	2.39	0.47
2:F:706:ARG:HD3	2:F:706:ARG:HA	1.65	0.47
1:G:115:ALA:O	1:G:117:ALA:N	2.46	0.47
1:G:301:MET:CE	1:G:341:LEU:HD22	2.37	0.47
2:H:137:SER:OG	2:H:332:ARG:HB3	2.15	0.47
2:H:144:VAL:CG1	2:H:312:MET:HE1	2.42	0.47
2:H:198:HIS:CD2	2:H:526:ALA:CA	2.97	0.47
2:H:227:GLY:N	6:H:3003:MTE:O4	2.43	0.47
2:H:311:ALA:O	2:H:312:MET:C	2.54	0.47
2:H:731:PRO:HB2	2:H:732:PRO:HD3	1.95	0.47
1:A:91:VAL:HG12	1:A:111:ILE:HD13	1.96	0.47
1:A:281:ILE:O	1:A:282:GLY:C	2.57	0.47
1:A:351:TYR:OH	1:A:449:GLU:OE1	2.29	0.47
1:A:361:ILE:HG21	1:A:429:ARG:CZ	2.45	0.47
2:B:647:ILE:HG22	2:B:648:LEU:N	2.30	0.47
2:B:683:ASP:HB3	2:B:689:MET:SD	2.55	0.47
2:B:746:ALA:O	2:B:747:CYS:C	2.53	0.47
1:C:256:ALA:HB1	1:C:260:HIS:HB2	1.97	0.47
1:C:273:GLU:OE1	1:C:276:ARG:NH1	2.47	0.47
2:D:456:GLY:O	2:D:457:ILE:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:559:GLU:O	2:D:560:GLY:O	2.33	0.47
1:E:401:LEU:HA	1:E:401:LEU:HD12	1.50	0.47
2:F:367:ASP:CG	2:F:431:ARG:HH12	2.18	0.47
1:G:81:ILE:HA	1:G:81:ILE:HD13	1.44	0.47
1:G:361:ILE:HG21	1:G:429:ARG:CZ	2.45	0.47
1:A:273:GLU:OE1	1:A:276:ARG:NH1	2.48	0.47
1:A:348:LEU:CD1	1:A:349:ARG:H	2.02	0.47
1:A:351:TYR:HB2	1:A:442:MET:HE2	1.92	0.47
1:A:368:LEU:HB3	1:A:446:TYR:CE1	2.50	0.47
1:A:441:ALA:HB1	2:B:636:LEU:HB3	1.97	0.47
2:B:446:ARG:NH1	2:B:630:GLU:OE2	2.42	0.47
2:B:552:ALA:O	2:B:553:GLY:C	2.54	0.47
2:B:720:GLU:HG3	2:B:724:ARG:NH2	2.29	0.47
2:B:731:PRO:N	2:B:732:PRO:HD2	2.30	0.47
1:E:224:PHE:C	1:E:225:LEU:HD23	2.39	0.47
4:E:3005:FAD:N1	4:E:3005:FAD:C2'	2.78	0.47
2:F:303:LEU:O	2:F:304:SER:C	2.58	0.47
2:F:464:LEU:HD23	2:F:464:LEU:HA	1.69	0.47
2:F:661:ILE:HD13	2:F:712:LEU:HG	1.97	0.47
2:F:736:GLY:C	2:F:738:SER:N	2.70	0.47
1:G:121:ASP:OD1	1:G:123:LYS:HE2	2.15	0.47
2:H:34:HIS:C	2:H:35:LEU:HD23	2.41	0.47
2:H:164:GLY:HA3	2:H:276:TYR:CZ	2.50	0.47
2:H:316:ASP:O	2:H:317:GLY:C	2.56	0.47
1:A:266:LEU:O	1:A:267:LEU:C	2.59	0.46
2:B:344:PHE:CE1	8:B:4000:141:C5	2.98	0.46
1:E:314:ARG:NH2	1:E:329:ASP:CG	2.70	0.46
1:G:89:HIS:O	1:G:90:PRO:C	2.57	0.46
1:G:281:ILE:CG2	1:G:282:GLY:N	2.78	0.46
1:G:453:GLU:OE1	2:H:442:ARG:NH1	2.48	0.46
2:H:717:ASN:OD1	2:H:719:GLU:N	2.48	0.46
1:A:67:LEU:CB	1:A:68:PRO:HD3	2.45	0.46
1:A:382:ILE:O	1:A:393:ARG:HA	2.14	0.46
2:B:367:ASP:OD1	2:B:367:ASP:C	2.58	0.46
1:C:272:SER:O	1:C:273:GLU:C	2.58	0.46
1:C:373:LYS:HB2	1:C:378:GLU:HG2	1.97	0.46
2:D:494:ALA:O	2:D:495:LYS:C	2.57	0.46
1:E:241:TYR:O	1:E:340:THR:CG2	2.63	0.46
1:E:241:TYR:O	1:E:340:THR:HA	2.15	0.46
2:F:321:VAL:CG1	2:F:323:ALA:O	2.63	0.46
2:F:348:GLN:OE1	2:F:348:GLN:N	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:GLY:O	1:G:107:THR:HB	2.15	0.46
1:G:131:GLY:HA3	1:G:274:GLN:OE1	2.15	0.46
1:G:275:VAL:HG21	4:G:3005:FAD:HM72	1.97	0.46
2:H:66:THR:O	2:H:67:ALA:C	2.54	0.46
2:H:667:ALA:O	2:H:668:TYR:C	2.57	0.46
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.59	0.46
1:C:390:VAL:HG22	1:C:391:PRO:N	2.31	0.46
2:D:538:MET:O	2:D:539:ALA:C	2.58	0.46
1:E:45:GLY:O	1:E:47:CYS:N	2.48	0.46
2:F:133:LEU:HA	2:F:133:LEU:HD12	1.27	0.46
2:F:610:ASP:C	2:F:610:ASP:OD2	2.58	0.46
2:F:691:HIS:O	2:F:691:HIS:CG	2.66	0.46
1:G:293:ASP:OD1	1:G:362:SER:OG	2.31	0.46
1:G:345:ALA:C	1:G:347:GLY:N	2.72	0.46
4:G:3005:FAD:HM72	4:G:3005:FAD:HM83	1.80	0.46
2:H:628:ILE:O	2:H:628:ILE:HG22	2.16	0.46
1:A:284:ASN:OD1	1:A:295:PRO:HD3	2.16	0.46
1:A:322:PHE:HB3	1:A:390:VAL:HG22	1.97	0.46
2:B:133:LEU:HA	2:B:133:LEU:HD12	1.32	0.46
1:C:434:TYR:O	1:C:435:ARG:C	2.55	0.46
2:D:312:MET:CE	2:D:330:ARG:HH12	2.13	0.46
1:E:12:ARG:CG	1:E:12:ARG:NH1	2.76	0.46
2:F:101:VAL:HG12	2:F:102:ALA:N	2.30	0.46
2:F:457:ILE:O	2:F:458:SER:CB	2.64	0.46
1:G:322:PHE:CB	1:G:390:VAL:CG2	2.86	0.46
2:H:75:ASP:C	2:H:75:ASP:OD1	2.57	0.46
1:A:117:ALA:O	1:A:118:HIS:C	2.56	0.46
1:A:327:LYS:N	1:A:328:GLN:NE2	2.64	0.46
1:A:390:VAL:HG13	1:A:391:PRO:C	2.41	0.46
2:B:60:GLY:O	2:B:103:ALA:HB1	2.16	0.46
2:B:227:GLY:O	2:B:228:PHE:C	2.59	0.46
2:B:493:HIS:ND1	2:B:513:ILE:HD13	2.31	0.46
1:C:350:CYS:HG	1:C:367:CYS:HG	1.64	0.46
1:C:390:VAL:HG22	1:C:391:PRO:CD	2.44	0.46
2:D:101:VAL:HG12	2:D:102:ALA:N	2.30	0.46
2:D:367:ASP:OD1	2:D:367:ASP:C	2.58	0.46
2:F:197:GLN:HG2	2:F:488:MET:CE	2.46	0.46
2:H:152:GLU:O	2:H:153:THR:C	2.58	0.46
2:H:627:ALA:HB2	2:H:735:LEU:HD22	1.97	0.46
1:A:67:LEU:O	1:A:68:PRO:C	2.58	0.46
1:A:349:ARG:CD	1:A:449:GLU:OE2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASN:HB2	2:B:251:ARG:NH1	2.31	0.46
2:B:66:THR:HB	2:B:69:ASP:OD2	2.16	0.46
2:B:110:ARG:O	2:B:111:ILE:C	2.57	0.46
2:B:199:PRO:HB3	2:B:219:VAL:CG1	2.46	0.46
1:C:21:GLN:HG2	1:C:22:SER:N	2.29	0.46
1:C:41:GLU:HG3	1:C:214:LYS:CE	2.38	0.46
1:C:83:ALA:HB1	1:C:84:PRO:CD	2.45	0.46
1:C:181:PHE:CD2	1:C:183:PRO:HD3	2.51	0.46
1:C:231:LEU:O	1:C:231:LEU:HD22	2.15	0.46
2:D:310:ARG:HD2	2:D:344:PHE:HB3	1.97	0.46
2:D:325:ARG:C	2:D:326:ILE:CG1	2.86	0.46
2:D:507:ASP:OD1	2:D:508:PRO:N	2.47	0.46
2:D:730:GLU:O	2:D:731:PRO:C	2.57	0.46
1:E:252:LEU:HD22	1:E:281:ILE:HD13	1.98	0.46
1:G:33:THR:O	1:G:36:LYS:NZ	2.44	0.46
1:G:369:ASN:HB3	1:G:381:ARG:HB2	1.96	0.46
2:H:61:VAL:HA	2:H:103:ALA:HB2	1.97	0.46
1:A:153:PRO:HA	1:A:154:PRO:HD3	1.81	0.46
1:A:231:LEU:O	1:A:231:LEU:HD22	2.15	0.46
1:A:425:LEU:O	1:A:432:ALA:HB2	2.16	0.46
2:B:645:THR:HG21	2:B:668:TYR:CZ	2.50	0.46
1:C:388:ALA:C	1:C:390:VAL:H	2.21	0.46
2:D:53:GLU:N	2:D:54:PRO:CD	2.78	0.46
2:D:584:GLU:O	2:D:585:ILE:C	2.54	0.46
1:E:103:CYS:HA	2:F:489:GLY:HA3	1.98	0.46
2:F:380:PRO:O	2:F:381:GLU:HB2	2.16	0.46
2:F:414:LEU:HG	2:F:624:TYR:HD2	1.81	0.46
2:F:425:ALA:O	2:F:426:ASN:CB	2.64	0.46
2:F:759:ALA:HA	2:F:760:PRO:C	2.41	0.46
2:H:302:ASP:OD1	2:H:303:LEU:N	2.48	0.46
1:A:387:MET:HE1	1:A:436:MET:HA	1.98	0.46
2:B:263:MET:HE3	2:B:692:ALA:HA	1.98	0.46
2:B:697:LYS:HD2	2:B:697:LYS:N	2.31	0.46
1:C:446:TYR:CE2	1:C:450:LEU:CD1	2.98	0.46
2:D:312:MET:O	2:D:313:LEU:C	2.57	0.46
2:D:425:ALA:O	2:D:426:ASN:CB	2.63	0.46
1:E:37:GLU:CD	2:F:256:ARG:HH22	2.23	0.46
1:E:408:GLU:CD	2:F:442:ARG:HH22	2.19	0.46
2:F:563:ALA:C	2:F:565:ASP:H	2.23	0.46
2:H:173:HIS:HA	2:H:341:PHE:CZ	2.51	0.46
2:H:734:LEU:CD1	2:H:734:LEU:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:753:HIS:O	2:H:755:PRO:HD3	2.16	0.46
1:A:26:LEU:O	1:A:27:LEU:C	2.56	0.46
1:A:206:THR:OG1	4:A:3005:FAD:O3'	2.27	0.46
1:A:368:LEU:HB3	1:A:446:TYR:CD1	2.51	0.46
2:B:582:PHE:O	2:B:583:ALA:C	2.58	0.46
1:C:45:GLY:O	1:C:48:THR:OG1	2.24	0.46
2:D:23:LEU:HD13	2:D:194:CYS:HA	1.98	0.46
2:D:123:ARG:HB3	2:D:124:PRO:HD2	1.98	0.46
2:D:461:LEU:HD12	2:D:463:HIS:CE1	2.50	0.46
2:D:691:HIS:O	2:D:692:ALA:HB2	2.14	0.46
1:E:350:CYS:C	1:E:351:TYR:CD2	2.94	0.46
2:F:222:ARG:HB2	2:F:515:ALA:CB	2.46	0.46
2:F:638:GLY:O	2:F:639:GLU:C	2.57	0.46
1:G:374:GLY:C	1:G:376:LYS:H	2.24	0.46
1:G:450:LEU:HA	1:G:450:LEU:HD23	1.54	0.46
2:H:93:PHE:CD1	2:H:93:PHE:C	2.92	0.46
2:H:305:LEU:C	2:H:305:LEU:CD2	2.78	0.46
2:H:367:ASP:OD1	2:H:368:PRO:HD2	2.15	0.46
2:H:531:SER:O	2:H:532:GLY:C	2.58	0.46
2:D:776:ARG:O	2:D:777:ALA:CB	2.63	0.46
1:E:364:VAL:HG22	1:E:435:ARG:HG2	1.98	0.46
2:F:301:ALA:O	2:F:302:ASP:C	2.58	0.46
2:F:554:PHE:O	2:F:555:VAL:C	2.53	0.46
1:G:249:ILE:O	1:G:250:ALA:C	2.59	0.46
2:H:568:PHE:CD2	2:H:573:VAL:HG22	2.50	0.46
1:A:428:MET:HG2	1:A:429:ARG:N	2.30	0.45
2:B:488:MET:HG3	6:B:3003:MTE:C4	2.46	0.45
2:B:659:LEU:HD23	2:B:659:LEU:HA	1.73	0.45
1:C:446:TYR:O	1:C:447:VAL:C	2.53	0.45
2:D:609:TRP:CB	2:D:616:GLY:HA3	2.46	0.45
4:E:3005:FAD:H2B	4:E:3005:FAD:H8A	1.54	0.45
2:F:65:PHE:O	2:F:99:PHE:HB2	2.16	0.45
2:F:109:ALA:O	2:F:110:ARG:C	2.57	0.45
2:F:260:ASP:OD1	2:F:691:HIS:CD2	2.70	0.45
2:F:325:ARG:C	2:F:326:ILE:CG1	2.89	0.45
2:F:339:THR:HG23	2:F:340:ALA:O	2.16	0.45
2:F:767:LEU:HA	2:F:767:LEU:HD12	1.60	0.45
2:H:537:GLY:O	2:H:538:MET:C	2.59	0.45
2:H:639:GLU:O	2:H:640:ASN:HB3	2.15	0.45
2:H:641:ARG:NH2	2:H:706:ARG:NE	2.64	0.45
1:A:41:GLU:HG3	1:A:214:LYS:CE	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:THR:OG1	1:A:379:THR:HB	2.16	0.45
2:B:93:PHE:CD2	2:B:299:TRP:NE1	2.84	0.45
2:D:321:VAL:HG12	2:D:323:ALA:O	2.16	0.45
2:D:411:ASP:N	2:D:411:ASP:OD1	2.48	0.45
2:F:644:ARG:HG3	2:F:707:ILE:HG22	1.97	0.45
2:F:722:ILE:HD12	2:F:722:ILE:HA	1.65	0.45
1:A:49:VAL:HA	1:A:112:VAL:HG11	1.99	0.45
2:B:344:PHE:CE2	8:B:4000:141:N1	2.84	0.45
2:D:23:LEU:O	2:D:23:LEU:HG	2.17	0.45
2:D:218:ARG:NH2	2:D:517:ASP:OD1	2.49	0.45
2:D:496:MET:N	2:D:496:MET:HE3	2.31	0.45
2:D:751:GLY:HA3	2:D:773:ALA:O	2.16	0.45
1:E:67:LEU:HA	1:E:67:LEU:HD23	1.52	0.45
2:F:299:TRP:CD1	2:F:299:TRP:H	2.33	0.45
2:F:547:LEU:C	2:F:549:GLY:N	2.73	0.45
2:F:551:LEU:HD23	2:F:551:LEU:HA	1.69	0.45
2:H:551:LEU:HD23	2:H:551:LEU:HA	1.49	0.45
1:A:271:ALA:HA	1:A:359:GLN:HE22	1.81	0.45
1:C:27:LEU:HD23	1:C:27:LEU:HA	1.80	0.45
1:E:68:PRO:CG	1:E:224:PHE:CE1	2.98	0.45
1:E:83:ALA:HB2	1:E:157:TRP:CH2	2.51	0.45
1:E:269:ARG:NH2	1:E:357:PHE:HA	2.32	0.45
2:F:137:SER:OG	2:F:332:ARG:HB3	2.16	0.45
2:F:184:LEU:O	2:F:185:PRO:C	2.55	0.45
2:F:517:ASP:OD2	2:F:517:ASP:C	2.60	0.45
1:G:103:CYS:CB	1:G:136:CYS:SG	3.02	0.45
1:G:104:GLY:HA3	2:H:22:TYR:OH	2.17	0.45
2:H:155:LEU:O	2:H:156:ALA:C	2.59	0.45
2:H:239:ALA:O	2:H:240:ILE:C	2.55	0.45
2:H:263:MET:CE	2:H:692:ALA:CA	2.94	0.45
1:A:237:THR:HG22	1:A:239:ASP:H	1.80	0.45
1:A:299:ILE:O	1:A:300:ALA:C	2.58	0.45
2:B:93:PHE:CD2	2:B:299:TRP:CD1	3.05	0.45
2:B:558:ARG:HD2	2:B:559:GLU:OE2	2.15	0.45
1:E:53:ASP:HB3	1:E:73:LYS:HD3	1.97	0.45
1:E:308:ARG:HD3	1:E:337:GLU:OE1	2.16	0.45
1:E:337:GLU:O	1:E:337:GLU:HG3	2.17	0.45
2:F:143:PRO:HB3	2:F:329:HIS:ND1	2.32	0.45
2:F:440:THR:O	2:F:440:THR:HG22	2.16	0.45
1:G:12:ARG:HH11	1:G:12:ARG:CG	2.29	0.45
1:G:202:ILE:HG12	1:G:208:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:ALA:O	1:G:396:ALA:C	2.58	0.45
2:H:297:CYS:HB3	2:H:304:SER:OG	2.16	0.45
2:H:306:PRO:HB2	2:H:344:PHE:CE2	2.52	0.45
2:H:532:GLY:N	6:H:3003:MTE:O1P	2.48	0.45
2:H:656:ASN:HA	2:H:657:PRO:HD3	1.86	0.45
1:A:220:PRO:O	1:A:221:GLU:O	2.35	0.45
1:A:260:HIS:O	1:A:263:LEU:N	2.50	0.45
2:B:361:ALA:HB2	2:B:371:LEU:HD23	1.99	0.45
2:B:683:ASP:OD1	2:B:685:CYS:N	2.50	0.45
2:B:743:LEU:HD12	2:B:743:LEU:HA	1.61	0.45
2:D:288:GLY:HA2	2:D:323:ALA:O	2.16	0.45
2:D:476:ASP:OD2	2:D:478:SER:OG	2.34	0.45
2:D:696:TYR:C	2:D:697:LYS:HD2	2.41	0.45
1:E:124:ASP:O	1:E:128:LEU:HD22	2.16	0.45
1:E:290:PRO:O	1:E:386:GLY:N	2.50	0.45
2:F:66:THR:CG2	2:F:67:ALA:N	2.74	0.45
2:F:246:ALA:O	2:F:247:ARG:C	2.56	0.45
2:F:731:PRO:N	2:F:732:PRO:CD	2.80	0.45
1:G:122:ARG:NH2	1:G:124:ASP:OD2	2.49	0.45
2:H:232:GLU:OE2	8:H:4000:141:H1	2.16	0.45
1:A:318:LEU:O	1:A:319:GLU:C	2.57	0.45
2:B:730:GLU:O	2:B:733:PHE:N	2.44	0.45
2:F:221:MET:HE1	2:F:224:MET:N	2.31	0.45
1:G:129:LEU:HA	1:G:129:LEU:HD23	1.49	0.45
1:G:318:LEU:C	1:G:320:ASP:N	2.75	0.45
2:H:227:GLY:O	2:H:230:GLY:N	2.46	0.45
2:H:344:PHE:CE1	8:H:4000:141:C6	3.00	0.45
1:A:37:GLU:CD	2:B:256:ARG:NH2	2.75	0.45
1:A:40:ASN:N	3:A:3002:FES:S2	2.75	0.45
2:B:551:LEU:HA	2:B:551:LEU:HD23	1.55	0.45
2:D:350:ALA:O	2:D:351:LEU:C	2.55	0.45
2:D:659:LEU:HD23	2:D:659:LEU:HA	1.59	0.45
1:E:273:GLU:O	1:E:274:GLN:C	2.57	0.45
2:H:173:HIS:N	2:H:341:PHE:HE1	2.14	0.45
2:H:453:VAL:CG1	2:H:454:LYS:N	2.72	0.45
2:H:657:PRO:O	2:H:658:ALA:C	2.56	0.45
2:B:596:LEU:HA	2:B:596:LEU:HD23	1.72	0.45
1:C:353:LEU:HD12	2:D:639:GLU:CD	2.42	0.45
2:D:79:ALA:HB1	2:D:80:PRO:CD	2.47	0.45
2:D:210:LEU:HD12	2:D:212:LEU:HD12	1.97	0.45
6:D:3003:MTE:S1'	7:D:3004:MOS:O2	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:112:ALA:O	2:F:113:ALA:C	2.57	0.45
2:F:602:TYR:C	2:F:602:TYR:CD2	2.94	0.45
2:F:691:HIS:O	2:F:692:ALA:HB2	2.15	0.45
2:H:93:PHE:CZ	2:H:96:GLN:N	2.85	0.45
2:H:701:PHE:C	2:H:701:PHE:CD2	2.93	0.45
2:B:354:GLU:O	2:B:357:ILE:HG22	2.17	0.45
2:D:535:MET:O	2:D:536:ASN:C	2.58	0.45
1:E:45:GLY:C	1:E:47:CYS:H	2.25	0.45
1:E:103:CYS:HB3	1:E:136:CYS:SG	2.56	0.45
1:E:194:LEU:O	1:E:194:LEU:HD12	2.17	0.45
2:F:93:PHE:CE2	2:F:299:TRP:NE1	2.85	0.45
2:F:172:GLU:CD	2:F:172:GLU:C	2.85	0.45
2:F:532:GLY:N	6:F:3003:MTE:O1P	2.31	0.45
2:F:660:ASP:O	2:F:661:ILE:C	2.59	0.45
1:G:279:ALA:HB1	4:G:3005:FAD:H4'	1.97	0.45
1:G:345:ALA:O	1:G:346:PRO:C	2.58	0.45
1:G:393:ARG:NH1	1:G:398:GLU:OE2	2.50	0.45
2:H:52:LEU:O	2:H:53:GLU:C	2.58	0.45
2:H:672:ALA:C	2:H:674:TRP:N	2.74	0.45
1:A:271:ALA:C	1:A:359:GLN:NE2	2.75	0.44
1:A:371:THR:O	1:A:372:LEU:HD23	2.16	0.44
2:B:139:PHE:O	2:B:140:GLU:HB2	2.16	0.44
2:B:146:TRP:CZ2	2:B:312:MET:HE3	2.51	0.44
2:B:184:LEU:HA	2:B:185:PRO:HD2	1.81	0.44
2:B:233:SER:C	2:B:235:GLY:N	2.73	0.44
2:B:309:ASP:O	2:B:313:LEU:HB2	2.17	0.44
2:B:496:MET:CA	2:B:496:MET:CE	2.92	0.44
2:B:721:THR:O	2:B:722:ILE:C	2.59	0.44
1:C:104:GLY:HA3	2:D:22:TYR:OH	2.17	0.44
1:C:276:ARG:HH11	1:C:276:ARG:HD2	1.50	0.44
2:D:53:GLU:HB3	2:D:54:PRO:HD3	1.99	0.44
2:D:276:TYR:OH	2:D:359:HIS:CD2	2.70	0.44
1:E:40:ASN:HD22	1:E:40:ASN:HA	1.56	0.44
1:E:398:GLU:O	1:E:401:LEU:HB2	2.17	0.44
2:F:500:ALA:O	2:F:501:ALA:C	2.57	0.44
2:H:123:ARG:CB	2:H:124:PRO:HD2	2.38	0.44
2:H:174:PHE:CZ	2:H:693:PRO:HG3	2.52	0.44
2:H:203:GLN:O	2:H:204:HIS:C	2.59	0.44
2:H:671:GLY:O	2:H:672:ALA:C	2.59	0.44
1:A:145:ALA:O	1:A:146:ALA:C	2.58	0.44
1:A:231:LEU:HD22	1:A:246:GLY:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HH11	1:A:276:ARG:HD2	1.63	0.44
1:A:297:ALA:O	1:A:298:LEU:C	2.59	0.44
2:B:444:LEU:HD23	2:B:444:LEU:HA	1.63	0.44
1:C:83:ALA:HB2	1:C:157:TRP:CD2	2.52	0.44
2:D:132:ALA:O	2:D:133:LEU:C	2.61	0.44
2:D:273:ARG:HH11	2:D:273:ARG:HD2	1.44	0.44
2:D:321:VAL:CG1	2:D:323:ALA:O	2.65	0.44
2:D:367:ASP:O	2:D:368:PRO:C	2.59	0.44
1:G:253:ARG:NH2	1:G:268:ARG:HG3	2.32	0.44
1:G:388:ALA:C	1:G:390:VAL:H	2.24	0.44
2:H:66:THR:CG2	2:H:67:ALA:N	2.79	0.44
2:H:133:LEU:HD12	2:H:133:LEU:HA	1.26	0.44
2:H:538:MET:O	2:H:539:ALA:C	2.59	0.44
2:B:12:ALA:O	2:B:13:ARG:C	2.60	0.44
2:B:334:ASN:O	2:B:335:THR:CG2	2.65	0.44
2:D:651:ALA:C	2:D:726:LYS:HB2	2.42	0.44
1:E:67:LEU:C	1:E:69:GLN:N	2.71	0.44
1:E:252:LEU:CD2	1:E:281:ILE:HD13	2.47	0.44
1:E:434:TYR:CD1	2:F:764:GLU:HG3	2.52	0.44
2:F:398:LYS:C	2:F:399:LYS:HD2	2.43	0.44
2:F:444:LEU:HD23	2:F:444:LEU:HA	1.33	0.44
2:F:547:LEU:O	2:F:550:ARG:N	2.50	0.44
1:G:271:ALA:CA	1:G:359:GLN:NE2	2.77	0.44
1:G:399:ALA:O	1:G:401:LEU:N	2.51	0.44
2:H:241:ALA:O	2:H:242:CYS:C	2.57	0.44
2:H:556:ALA:O	2:H:560:GLY:N	2.50	0.44
2:B:216:ASP:C	2:B:217:VAL:HG23	2.42	0.44
2:B:316:ASP:N	2:B:316:ASP:OD1	2.43	0.44
2:B:517:ASP:O	2:B:519:SER:N	2.51	0.44
1:C:271:ALA:HB2	4:C:3005:FAD:N5	2.33	0.44
2:D:354:GLU:OE1	2:D:372:ARG:NE	2.47	0.44
1:E:42:GLY:C	3:E:3002:FES:S1	3.01	0.44
1:E:44:CYS:N	3:E:3002:FES:S1	2.89	0.44
1:E:45:GLY:C	1:E:47:CYS:N	2.75	0.44
1:E:294:GLY:O	1:E:295:PRO:C	2.58	0.44
2:F:227:GLY:N	6:F:3003:MTE:O4	2.49	0.44
2:F:367:ASP:OD1	2:F:367:ASP:C	2.58	0.44
2:F:421:LEU:HG	2:F:628:ILE:HD12	1.98	0.44
2:F:461:LEU:O	2:F:462:THR:C	2.59	0.44
2:F:590:TYR:CE1	2:H:466:GLN:NE2	2.86	0.44
2:F:671:GLY:HA2	2:F:733:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:771:ARG:O	2:F:772:ARG:C	2.53	0.44
2:H:96:GLN:HG3	2:H:97:PRO:HD2	1.97	0.44
2:H:273:ARG:HH11	2:H:273:ARG:HD2	1.63	0.44
1:A:436:MET:HE2	1:A:440:GLN:NE2	2.33	0.44
2:B:236:ASN:N	2:B:236:ASN:ND2	2.65	0.44
2:B:449:ALA:CB	2:B:741:LEU:HB3	2.47	0.44
2:B:602:TYR:CD2	2:B:602:TYR:C	2.94	0.44
2:D:263:MET:HE1	2:D:692:ALA:CA	2.47	0.44
2:D:691:HIS:O	2:D:691:HIS:CG	2.70	0.44
1:E:364:VAL:O	1:E:442:MET:HE1	2.17	0.44
2:F:654:SER:OG	2:F:656:ASN:N	2.50	0.44
1:G:301:MET:O	1:G:301:MET:CG	2.65	0.44
1:G:455:VAL:O	1:G:455:VAL:HG13	2.16	0.44
2:H:407:GLN:CD	2:H:617:ARG:HG2	2.41	0.44
1:A:1:MET:HE1	1:A:182:LEU:HD13	1.99	0.44
1:A:327:LYS:H	1:A:328:GLN:NE2	2.14	0.44
2:B:75:ASP:HA	2:B:83:GLU:O	2.17	0.44
2:B:407:GLN:OE1	2:B:618:PRO:HD2	2.17	0.44
2:B:456:GLY:O	2:B:457:ILE:HD13	2.16	0.44
2:B:586:VAL:HG23	2:B:586:VAL:H	1.59	0.44
2:B:586:VAL:O	2:B:587:ALA:C	2.61	0.44
1:E:222:VAL:CG1	1:E:223:ALA:N	2.79	0.44
2:F:91:VAL:HG11	2:F:98:ILE:HD11	1.98	0.44
2:F:110:ARG:O	2:F:111:ILE:C	2.56	0.44
2:F:160:HIS:HB3	2:F:364:MET:HE2	1.99	0.44
1:G:331:ARG:O	1:G:334:GLU:CB	2.66	0.44
1:G:345:ALA:O	1:G:347:GLY:N	2.51	0.44
2:H:228:PHE:O	2:H:341:PHE:HA	2.17	0.44
2:B:128:THR:O	2:B:129:LEU:C	2.61	0.44
2:B:201:GLU:O	2:B:202:ILE:C	2.59	0.44
2:B:238:LEU:HD11	2:B:257:TYR:CZ	2.53	0.44
2:B:612:LEU:HD23	2:B:612:LEU:HA	1.81	0.44
1:C:194:LEU:HD12	1:C:194:LEU:O	2.18	0.44
1:C:298:LEU:O	1:C:299:ILE:C	2.60	0.44
2:D:93:PHE:CE2	2:D:299:TRP:NE1	2.86	0.44
2:D:276:TYR:OH	2:D:359:HIS:HD2	2.01	0.44
2:D:414:LEU:HG	2:D:624:TYR:CD2	2.53	0.44
2:D:641:ARG:HH11	2:D:641:ARG:HD3	1.63	0.44
1:E:331:ARG:O	1:E:332:PRO:C	2.61	0.44
2:F:398:LYS:O	2:F:399:LYS:HD2	2.17	0.44
2:F:407:GLN:CD	2:F:617:ARG:HG2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:GLN:HA	2:H:97:PRO:HD3	1.66	0.44
2:H:112:ALA:O	2:H:114:ARG:N	2.51	0.44
1:A:181:PHE:CE2	1:A:183:PRO:HD3	2.53	0.44
1:A:266:LEU:O	1:A:268:ARG:N	2.51	0.44
2:B:108:ALA:O	2:B:109:ALA:C	2.60	0.44
2:B:517:ASP:O	2:B:518:THR:C	2.59	0.44
1:E:436:MET:O	1:E:438:ALA:N	2.51	0.44
2:F:498:GLN:C	2:F:500:ALA:N	2.73	0.44
1:G:143:LEU:O	1:G:144:ARG:C	2.60	0.44
1:G:216:LEU:HA	1:G:216:LEU:HD23	1.74	0.44
1:G:266:LEU:O	1:G:268:ARG:N	2.51	0.44
1:G:407:ARG:HB3	1:G:409:ASP:OD2	2.18	0.44
2:H:443:THR:C	2:H:444:LEU:HD23	2.42	0.44
2:H:491:GLY:O	2:H:495:LYS:HG3	2.17	0.44
2:H:550:ARG:O	2:H:551:LEU:C	2.58	0.44
2:H:556:ALA:HB1	2:H:561:CYS:O	2.17	0.44
1:A:368:LEU:N	1:A:368:LEU:CD1	2.71	0.44
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.40	0.44
2:B:303:LEU:O	2:B:304:SER:C	2.60	0.44
2:B:674:TRP:CE3	2:B:675:LEU:CD2	2.98	0.44
1:C:252:LEU:CD2	1:C:281:ILE:HD13	2.48	0.44
2:D:66:THR:HG22	2:D:68:ALA:N	2.31	0.44
2:D:105:SER:O	2:D:106:HIS:C	2.57	0.44
2:D:221:MET:HE3	2:D:223:ARG:N	2.32	0.44
2:D:602:TYR:CD2	2:D:602:TYR:C	2.95	0.44
2:D:771:ARG:O	2:D:772:ARG:C	2.59	0.44
1:E:321:PHE:O	1:E:321:PHE:CD1	2.71	0.44
2:F:7:LEU:HA	2:F:7:LEU:HD23	1.77	0.44
2:F:79:ALA:HB1	2:F:80:PRO:HD2	2.00	0.44
2:F:302:ASP:OD1	2:F:303:LEU:N	2.49	0.44
2:F:494:ALA:O	2:F:495:LYS:C	2.61	0.44
2:F:647:ILE:CG2	2:F:648:LEU:N	2.80	0.44
6:F:3003:MTE:H1S	7:F:3004:MOS:MO	1.54	0.44
1:G:124:ASP:C	1:G:128:LEU:HD22	2.43	0.44
1:G:153:PRO:HA	1:G:154:PRO:HD2	1.67	0.44
2:H:221:MET:HE1	2:H:224:MET:N	2.32	0.44
2:H:367:ASP:O	2:H:368:PRO:C	2.61	0.44
1:A:353:LEU:HD12	2:B:639:GLU:CD	2.43	0.43
2:B:64:VAL:HG12	2:B:65:PHE:N	2.33	0.43
2:B:112:ALA:O	2:B:113:ALA:C	2.58	0.43
2:B:532:GLY:HA3	6:B:3003:MTE:O3P	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:462:THR:O	2:D:465:ASN:ND2	2.45	0.43
1:E:44:CYS:SG	3:E:3002:FES:S2	3.16	0.43
1:E:436:MET:O	1:E:439:ALA:N	2.50	0.43
2:F:731:PRO:O	2:F:732:PRO:C	2.60	0.43
2:H:60:GLY:O	2:H:103:ALA:CB	2.60	0.43
2:H:319:TYR:HE2	2:H:372:ARG:HB3	1.83	0.43
1:A:36:LYS:HD3	1:A:36:LYS:HA	1.61	0.43
1:A:348:LEU:CD1	1:A:349:ARG:N	2.56	0.43
1:A:369:ASN:HB3	1:A:381:ARG:HB2	2.00	0.43
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.19	0.43
2:B:763:PRO:O	2:B:764:GLU:C	2.61	0.43
2:D:174:PHE:CZ	2:D:693:PRO:HG3	2.53	0.43
2:D:251:ARG:CB	2:D:252:PRO:CD	2.96	0.43
2:D:300:SER:O	2:D:301:ALA:C	2.60	0.43
2:D:490:GLN:HA	2:D:663:GLN:NE2	2.32	0.43
2:D:736:GLY:O	2:D:739:ALA:N	2.50	0.43
1:E:139:TYR:O	1:E:142:ILE:N	2.46	0.43
1:E:152:GLU:HA	1:E:153:PRO:HD3	1.81	0.43
1:E:249:ILE:HG23	1:E:267:LEU:HD22	1.99	0.43
1:E:330:ARG:HH11	1:E:330:ARG:HD3	1.61	0.43
1:E:390:VAL:HG22	1:E:391:PRO:O	2.17	0.43
2:F:263:MET:HE3	2:F:692:ALA:HA	2.01	0.43
2:F:575:ALA:O	2:F:576:SER:C	2.60	0.43
2:F:585:ILE:HD12	2:F:585:ILE:HG23	1.57	0.43
1:G:89:HIS:C	1:G:91:VAL:N	2.72	0.43
1:G:206:THR:HG1	4:G:3005:FAD:C3'	2.28	0.43
1:G:305:LEU:HD11	1:G:336:VAL:HG13	1.99	0.43
1:G:388:ALA:C	1:G:390:VAL:N	2.72	0.43
2:H:591:MET:HE3	2:H:591:MET:HB3	1.81	0.43
2:H:730:GLU:N	2:H:731:PRO:HD2	2.32	0.43
2:H:766:VAL:O	2:H:770:VAL:HG23	2.18	0.43
1:A:296:PRO:O	1:A:297:ALA:C	2.58	0.43
2:B:66:THR:O	2:B:67:ALA:C	2.61	0.43
2:B:638:GLY:O	2:B:639:GLU:C	2.56	0.43
2:D:168:ILE:CD1	2:D:351:LEU:HD23	2.48	0.43
2:D:265:ILE:O	2:D:265:ILE:CG2	2.63	0.43
1:E:92:GLN:O	1:E:93:GLN:C	2.61	0.43
2:F:316:ASP:O	2:F:317:GLY:C	2.61	0.43
2:F:764:GLU:O	2:F:765:ALA:C	2.59	0.43
2:H:55:VAL:O	2:H:56:ARG:C	2.58	0.43
2:H:135:ALA:O	2:H:136:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:240:ILE:O	2:H:241:ALA:C	2.61	0.43
2:H:457:ILE:HD13	2:H:457:ILE:HA	1.65	0.43
2:H:545:GLU:O	2:H:546:THR:C	2.60	0.43
2:B:214:PHE:N	2:B:214:PHE:HD1	2.15	0.43
2:B:499:VAL:O	2:B:503:VAL:HG23	2.19	0.43
2:B:731:PRO:CB	2:B:732:PRO:HD3	2.35	0.43
2:D:238:LEU:HD11	2:D:257:TYR:CZ	2.53	0.43
2:D:413:VAL:O	2:D:414:LEU:C	2.60	0.43
2:D:609:TRP:CD2	2:D:618:PRO:HB3	2.54	0.43
1:E:261:PRO:O	1:E:262:ALA:C	2.58	0.43
2:F:111:ILE:O	2:F:112:ALA:C	2.56	0.43
2:F:123:ARG:HB3	2:F:124:PRO:CD	2.48	0.43
2:F:273:ARG:HH11	2:F:273:ARG:HD2	1.53	0.43
2:F:657:PRO:O	2:F:661:ILE:CG1	2.47	0.43
1:G:206:THR:HG21	1:G:275:VAL:HG13	2.01	0.43
2:H:528:ALA:HA	6:H:3003:MTE:S2'	2.59	0.43
2:H:645:THR:CG2	2:H:668:TYR:CZ	3.01	0.43
2:H:675:LEU:C	2:H:676:THR:HG23	2.43	0.43
1:A:374:GLY:C	1:A:376:LYS:H	2.27	0.43
2:B:360:LEU:HD11	2:B:364:MET:HE2	2.00	0.43
1:C:231:LEU:O	1:C:231:LEU:CD2	2.66	0.43
1:C:295:PRO:HB2	1:C:296:PRO:HD3	1.99	0.43
1:E:303:ALA:CB	1:E:341:LEU:HD23	2.48	0.43
1:E:454:ALA:O	1:E:455:VAL:HG23	2.18	0.43
2:F:266:THR:O	2:F:268:LYS:HE2	2.19	0.43
2:F:283:SER:C	2:F:366:ARG:HH22	2.26	0.43
2:F:636:LEU:HD23	2:F:636:LEU:HA	1.55	0.43
1:G:61:ASN:ND2	1:G:274:GLN:HB3	2.33	0.43
1:G:64:LEU:HA	1:G:64:LEU:HD23	1.47	0.43
1:G:301:MET:HB3	1:G:348:LEU:HD22	1.99	0.43
2:H:93:PHE:CE2	2:H:299:TRP:CE2	3.07	0.43
2:H:93:PHE:CE2	2:H:96:GLN:HB2	2.53	0.43
2:H:254:LYS:HG2	2:H:255:MET:N	2.34	0.43
2:H:660:ASP:O	2:H:661:ILE:C	2.59	0.43
2:B:302:ASP:CG	2:B:303:LEU:N	2.76	0.43
1:C:93:GLN:O	1:C:94:ALA:C	2.59	0.43
1:C:126:ASP:OD1	2:D:704:ARG:NH1	2.48	0.43
1:C:374:GLY:C	1:C:376:LYS:N	2.77	0.43
2:F:224:MET:HE1	2:F:488:MET:HE2	1.99	0.43
2:F:491:GLY:HA3	2:F:659:LEU:HD13	2.01	0.43
2:H:39:LEU:HD23	2:H:39:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:PHE:N	2:H:99:PHE:CD2	2.86	0.43
2:H:237:HIS:ND1	2:H:237:HIS:N	2.65	0.43
1:A:179:PRO:O	1:A:180:ALA:HB2	2.19	0.43
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.78	0.43
2:B:35:LEU:HA	2:B:101:VAL:O	2.19	0.43
2:B:39:LEU:HD23	2:B:39:LEU:N	2.34	0.43
1:C:83:ALA:HB2	1:C:157:TRP:CE3	2.53	0.43
2:D:303:LEU:C	2:D:306:PRO:HD2	2.43	0.43
2:F:221:MET:HE3	2:F:223:ARG:CA	2.49	0.43
1:G:363:ALA:O	1:G:435:ARG:HD3	2.18	0.43
1:G:387:MET:HE3	1:G:424:PRO:HG3	2.00	0.43
2:H:173:HIS:CD2	2:H:341:PHE:CD1	3.06	0.43
2:H:344:PHE:CD1	8:H:4000:141:C5	3.02	0.43
2:H:448:ILE:CG1	2:H:630:GLU:HB2	2.47	0.43
2:H:457:ILE:HG21	2:H:621:TYR:CZ	2.54	0.43
1:A:248:THR:O	1:A:251:ALA:N	2.51	0.43
2:B:48:THR:HG22	2:B:119:THR:OG1	2.17	0.43
2:B:286:LEU:HA	2:B:286:LEU:HD23	1.81	0.43
2:B:737:ILE:O	2:B:740:PHE:N	2.51	0.43
1:C:92:GLN:O	1:C:93:GLN:C	2.61	0.43
2:D:175:TYR:O	2:D:176:LEU:C	2.62	0.43
2:D:222:ARG:O	2:D:222:ARG:HG3	2.16	0.43
1:E:295:PRO:O	1:E:296:PRO:C	2.58	0.43
1:E:448:ARG:O	1:E:449:GLU:C	2.59	0.43
1:E:461:MET:HE3	1:E:461:MET:HB3	1.78	0.43
2:F:55:VAL:O	2:F:56:ARG:C	2.60	0.43
2:F:127:LEU:HA	2:F:127:LEU:HD23	1.71	0.43
2:F:143:PRO:HB3	2:F:329:HIS:CE1	2.53	0.43
2:F:563:ALA:C	2:F:565:ASP:N	2.77	0.43
1:G:18:ASP:OD2	1:G:18:ASP:C	2.61	0.43
1:G:67:LEU:C	1:G:69:GLN:N	2.75	0.43
1:G:139:TYR:O	1:G:142:ILE:N	2.52	0.43
2:H:418:VAL:O	2:H:421:LEU:N	2.51	0.43
1:A:192:TRP:O	1:A:196:HIS:HD2	2.01	0.43
1:A:279:ALA:HB1	4:A:3005:FAD:H4'	2.01	0.43
2:B:324:LEU:HD21	2:B:326:ILE:HD11	2.01	0.43
1:C:388:ALA:C	1:C:390:VAL:N	2.75	0.43
2:D:280:ALA:HB1	2:D:285:LYS:O	2.18	0.43
2:D:430:ARG:NH1	2:D:630:GLU:OE1	2.51	0.43
2:D:660:ASP:O	2:D:661:ILE:C	2.62	0.43
1:E:83:ALA:CB	1:E:157:TRP:CD2	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:GLN:HB3	2:F:16:VAL:HG11	2.00	0.43
1:E:381:ARG:NH2	1:E:393:ARG:NE	2.67	0.43
2:F:150:ASP:C	2:F:150:ASP:OD1	2.60	0.43
2:F:493:HIS:CG	2:F:513:ILE:HG12	2.54	0.43
2:F:495:LYS:C	2:F:496:MET:HE2	2.44	0.43
1:G:6:LEU:HB3	1:G:74:ALA:HA	2.01	0.43
1:G:371:THR:CB	1:G:379:THR:HG1	2.32	0.43
2:H:214:PHE:O	2:H:215:HIS:C	2.58	0.43
2:H:653:ALA:O	2:H:654:SER:C	2.57	0.43
2:H:701:PHE:CE2	2:H:704:ARG:NH1	2.86	0.43
2:H:730:GLU:C	2:H:732:PRO:CD	2.92	0.43
2:H:736:GLY:O	2:H:737:ILE:C	2.61	0.43
1:A:253:ARG:HH11	1:A:253:ARG:HD3	1.72	0.43
2:B:55:VAL:O	2:B:56:ARG:C	2.59	0.43
2:B:233:SER:O	2:B:235:GLY:N	2.52	0.43
2:B:234:GLN:H	2:B:234:GLN:HG2	1.67	0.43
2:B:236:ASN:N	2:B:236:ASN:HD22	2.16	0.43
6:B:3003:MTE:S2'	7:B:3004:MOS:S	3.17	0.43
2:D:278:ILE:HD11	2:D:286:LEU:CD2	2.42	0.43
2:D:575:ALA:O	2:D:576:SER:C	2.61	0.43
2:D:722:ILE:HG13	2:D:723:PHE:CD1	2.54	0.43
1:E:69:GLN:NE2	1:E:203:ALA:O	2.52	0.43
1:E:374:GLY:C	1:E:376:LYS:H	2.27	0.43
2:F:62:ILE:O	2:F:62:ILE:CG2	2.65	0.43
2:F:321:VAL:O	2:F:322:PRO:C	2.61	0.43
1:G:237:THR:CG2	1:G:239:ASP:OD2	2.67	0.43
1:G:266:LEU:C	1:G:268:ARG:N	2.76	0.43
1:G:399:ALA:C	1:G:401:LEU:N	2.77	0.43
1:G:430:ALA:HB1	1:G:434:TYR:HD2	1.84	0.43
2:H:288:GLY:HA2	2:H:323:ALA:O	2.19	0.43
2:H:731:PRO:O	2:H:733:PHE:N	2.52	0.43
2:H:763:PRO:O	2:H:766:VAL:N	2.52	0.43
1:A:256:ALA:O	1:A:257:GLU:C	2.62	0.42
2:B:302:ASP:CG	2:B:303:LEU:H	2.25	0.42
1:C:299:ILE:O	1:C:300:ALA:C	2.57	0.42
1:E:83:ALA:HB1	1:E:84:PRO:HD2	2.01	0.42
2:F:148:ARG:HH11	2:F:148:ARG:HD2	1.65	0.42
2:F:591:MET:HE3	2:F:591:MET:HB3	1.87	0.42
2:F:722:ILE:HG23	2:F:722:ILE:O	2.19	0.42
1:G:12:ARG:CG	1:G:12:ARG:NH1	2.81	0.42
1:G:364:VAL:HG23	1:G:435:ARG:HG2	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:A:182:LEU:HD13	2.49	0.42
2:D:278:ILE:CG1	2:D:279:GLY:N	2.82	0.42
1:E:24:LEU:HA	1:E:24:LEU:HD12	1.86	0.42
1:E:438:ALA:O	1:E:441:ALA:N	2.52	0.42
2:F:233:SER:C	2:F:235:GLY:H	2.27	0.42
2:F:540:VAL:O	2:F:541:LYS:C	2.60	0.42
1:G:81:ILE:HG23	1:G:81:ILE:HD12	1.70	0.42
1:G:193:TYR:O	1:G:196:HIS:N	2.48	0.42
2:H:360:LEU:HG	2:H:364:MET:CE	2.49	0.42
2:H:663:GLN:O	2:H:664:ILE:C	2.60	0.42
2:B:581:ARG:O	2:B:582:PHE:C	2.61	0.42
2:B:741:LEU:HD12	2:B:741:LEU:HA	1.43	0.42
2:D:417:LEU:HG	2:D:648:LEU:HD23	2.00	0.42
1:E:351:TYR:CD2	1:E:351:TYR:N	2.85	0.42
2:F:472:GLN:O	2:F:479:VAL:HG13	2.19	0.42
1:G:49:VAL:HA	1:G:112:VAL:HG11	2.01	0.42
1:G:67:LEU:HA	1:G:67:LEU:HD23	1.36	0.42
1:A:95:MET:CE	1:A:114:MET:HE1	2.48	0.42
4:A:3005:FAD:HM83	4:A:3005:FAD:HM71	1.87	0.42
2:B:531:SER:CB	2:B:535:MET:HE2	2.44	0.42
1:C:237:THR:HG23	1:C:238:PRO:HG2	2.01	0.42
1:C:358:ASP:O	1:C:359:GLN:C	2.61	0.42
2:D:436:ALA:O	2:D:437:TRP:C	2.61	0.42
2:D:540:VAL:O	2:D:541:LYS:C	2.58	0.42
1:E:118:HIS:O	1:E:119:ASP:C	2.59	0.42
1:E:399:ALA:O	1:E:400:ALA:C	2.57	0.42
2:F:166:PHE:CE2	2:F:355:ARG:HG3	2.54	0.42
2:F:197:GLN:HG3	2:F:231:LYS:HB2	2.01	0.42
2:F:286:LEU:HA	2:F:286:LEU:HD23	1.81	0.42
2:B:274:ILE:HG12	2:B:293:HIS:CD2	2.54	0.42
2:B:503:VAL:O	2:B:548:ARG:NH2	2.52	0.42
2:B:546:THR:O	2:B:547:LEU:C	2.61	0.42
2:B:585:ILE:HG23	2:B:585:ILE:HD12	1.64	0.42
2:B:666:GLY:O	2:B:667:ALA:C	2.62	0.42
1:C:83:ALA:HB1	1:C:84:PRO:HD2	2.01	0.42
1:C:198:GLU:OE2	1:C:198:GLU:HA	2.20	0.42
1:C:218:ASP:C	1:C:219:LEU:HD23	2.45	0.42
2:D:158:ALA:O	2:D:159:ALA:C	2.61	0.42
2:D:234:GLN:H	2:D:234:GLN:HG2	1.44	0.42
2:D:289:ALA:O	2:D:324:LEU:HA	2.19	0.42
2:D:581:ARG:O	2:D:584:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:641:ARG:HH21	2:D:706:ARG:CZ	2.33	0.42
1:E:68:PRO:HB2	1:E:224:PHE:CD1	2.55	0.42
1:E:103:CYS:N	3:E:3001:FES:S1	2.90	0.42
2:F:341:PHE:HD2	2:F:342:ARG:N	2.18	0.42
2:F:367:ASP:O	2:F:368:PRO:C	2.62	0.42
1:G:23:LEU:O	1:G:24:LEU:C	2.61	0.42
1:G:124:ASP:O	1:G:128:LEU:N	2.44	0.42
1:G:143:LEU:HD22	1:G:147:GLU:CD	2.44	0.42
1:G:209:SER:O	1:G:212:VAL:N	2.52	0.42
1:G:335:PHE:CD1	1:G:335:PHE:C	2.97	0.42
2:H:160:HIS:CD2	2:H:364:MET:HB3	2.55	0.42
2:H:214:PHE:N	2:H:214:PHE:HD1	2.14	0.42
2:H:473:ILE:HB	2:H:596:LEU:HB3	2.01	0.42
2:H:540:VAL:O	2:H:541:LYS:C	2.61	0.42
1:A:68:PRO:HB2	1:A:224:PHE:CE1	2.55	0.42
1:A:155:ALA:HB1	1:A:157:TRP:CE2	2.55	0.42
1:C:125:TYR:O	1:C:126:ASP:C	2.60	0.42
1:C:426:SER:OG	1:C:432:ALA:N	2.42	0.42
2:D:303:LEU:O	2:D:304:SER:C	2.61	0.42
2:D:609:TRP:CG	2:D:618:PRO:HB3	2.54	0.42
1:E:105:PHE:HD2	2:F:176:LEU:HB3	1.83	0.42
1:E:303:ALA:HB2	1:E:341:LEU:HD23	2.01	0.42
1:G:107:THR:O	1:G:108:PRO:C	2.63	0.42
1:G:417:LEU:HD23	1:G:417:LEU:HA	1.69	0.42
2:H:301:ALA:O	2:H:302:ASP:C	2.61	0.42
2:H:361:ALA:O	2:H:362:ARG:C	2.62	0.42
1:A:39:CYS:SG	1:A:40:ASN:N	2.93	0.42
1:A:164:PHE:CG	1:A:165:THR:N	2.87	0.42
2:B:144:VAL:CG1	2:B:312:MET:HE1	2.49	0.42
2:B:334:ASN:O	2:B:335:THR:HG23	2.18	0.42
1:C:26:LEU:O	1:C:27:LEU:C	2.63	0.42
1:C:64:LEU:HA	1:C:64:LEU:HD23	1.66	0.42
1:C:248:THR:O	1:C:251:ALA:N	2.53	0.42
2:D:367:ASP:CG	2:D:431:ARG:HH12	2.27	0.42
2:D:762:THR:HB	2:D:763:PRO:CD	2.49	0.42
1:E:7:LEU:HD21	1:E:32:LEU:CD1	2.50	0.42
1:E:348:LEU:HD12	1:E:348:LEU:HA	1.26	0.42
2:F:172:GLU:HB3	2:F:696:TYR:CZ	2.54	0.42
2:F:487:GLU:HB2	2:F:493:HIS:CD2	2.55	0.42
1:G:23:LEU:HD12	1:G:23:LEU:HA	1.69	0.42
1:G:92:GLN:O	1:G:93:GLN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:ALA:HB2	1:G:350:CYS:HG	1.84	0.42
1:G:411:ILE:O	1:G:412:ALA:C	2.62	0.42
2:H:91:VAL:H	2:H:91:VAL:HG22	1.57	0.42
2:H:437:TRP:CZ3	2:H:446:ARG:HG3	2.54	0.42
2:H:471:VAL:HG12	2:H:472:GLN:N	2.32	0.42
2:B:239:ALA:O	2:B:240:ILE:C	2.61	0.42
1:C:301:MET:CE	1:C:341:LEU:HD22	2.34	0.42
2:D:174:PHE:HZ	2:D:693:PRO:HG3	1.84	0.42
2:D:443:THR:C	2:D:444:LEU:HD23	2.44	0.42
1:E:122:ARG:HD2	1:E:122:ARG:HA	1.89	0.42
2:F:538:MET:O	2:F:539:ALA:C	2.60	0.42
1:G:83:ALA:HB2	1:G:157:TRP:CZ3	2.55	0.42
1:G:204:GLY:HA3	4:G:3005:FAD:O2P	2.18	0.42
2:H:414:LEU:O	2:H:415:GLY:C	2.62	0.42
2:H:655:LEU:HA	2:H:655:LEU:HD23	1.84	0.42
1:C:78:ILE:CG2	1:C:79:GLU:N	2.82	0.42
2:D:170:GLY:N	2:D:271:ASP:HB3	2.35	0.42
2:D:202:ILE:HD12	2:D:202:ILE:HG23	1.76	0.42
2:D:203:GLN:O	2:D:204:HIS:C	2.61	0.42
2:D:414:LEU:O	2:D:415:GLY:C	2.62	0.42
1:E:272:SER:O	1:E:273:GLU:C	2.62	0.42
1:E:390:VAL:CG2	1:E:391:PRO:N	2.83	0.42
1:E:462:PRO:HG2	2:F:706:ARG:HB2	2.02	0.42
2:F:185:PRO:O	2:F:185:PRO:HG2	2.19	0.42
2:F:660:ASP:O	2:F:664:ILE:HG13	2.20	0.42
2:F:734:LEU:N	2:F:734:LEU:HD12	2.35	0.42
4:G:3005:FAD:H9	4:G:3005:FAD:H1'2	1.84	0.42
2:H:398:LYS:N	2:H:398:LYS:HE3	2.35	0.42
1:A:290:PRO:O	1:A:386:GLY:N	2.53	0.42
1:C:77:THR:O	1:C:78:ILE:C	2.59	0.42
2:D:720:GLU:HG3	2:D:724:ARG:HH21	1.83	0.42
1:E:102:GLN:O	2:F:489:GLY:HA2	2.19	0.42
1:E:444:LEU:O	1:E:445:ARG:C	2.60	0.42
2:F:278:ILE:HD11	2:F:286:LEU:CD2	2.50	0.42
1:G:457:VAL:HG22	2:H:632:VAL:CG2	2.50	0.42
2:H:251:ARG:CB	2:H:252:PRO:CD	2.95	0.42
2:H:307:VAL:O	2:H:308:CYS:C	2.63	0.42
2:H:631:VAL:HG12	2:H:642:ILE:CA	2.25	0.42
2:H:696:TYR:C	2:H:697:LYS:HD2	2.45	0.42
2:B:107:ARG:O	2:B:110:ARG:N	2.52	0.41
2:B:229:GLY:C	2:B:231:LYS:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:ARG:HD2	2:D:603:ALA:HB1	2.02	0.41
1:C:103:CYS:HA	2:D:489:GLY:CA	2.50	0.41
1:C:248:THR:O	1:C:251:ALA:HB3	2.20	0.41
2:D:199:PRO:O	2:D:200:SER:C	2.62	0.41
2:D:417:LEU:O	2:D:418:VAL:C	2.63	0.41
2:D:667:ALA:O	2:D:668:TYR:C	2.63	0.41
2:D:763:PRO:O	2:D:764:GLU:C	2.60	0.41
1:E:276:ARG:HH11	1:E:276:ARG:HD2	1.69	0.41
1:E:370:LEU:CD2	1:E:380:ALA:CB	2.98	0.41
2:F:305:LEU:CB	2:F:306:PRO:HD3	2.31	0.41
2:F:311:ALA:O	2:F:312:MET:C	2.60	0.41
1:A:95:MET:CG	1:A:114:MET:HE1	2.50	0.41
1:A:111:ILE:O	1:A:112:VAL:C	2.60	0.41
2:B:70:LEU:HD23	2:B:70:LEU:HA	1.67	0.41
2:B:251:ARG:CB	2:B:252:PRO:HD2	2.49	0.41
2:B:464:LEU:HA	2:B:464:LEU:HD23	1.80	0.41
2:B:620:LEU:HD12	2:B:620:LEU:HA	1.77	0.41
2:B:651:ALA:C	2:B:726:LYS:HB2	2.44	0.41
2:B:767:LEU:HD12	2:B:767:LEU:HA	1.80	0.41
1:C:144:ARG:O	1:C:145:ALA:C	2.59	0.41
2:D:202:ILE:HD13	2:D:236:ASN:HD22	1.85	0.41
2:D:680:LEU:C	2:D:681:VAL:HG23	2.45	0.41
1:E:369:ASN:C	1:E:370:LEU:HD23	2.46	0.41
1:E:381:ARG:HA	1:E:398:GLU:OE1	2.20	0.41
2:F:63:ALA:C	2:F:64:VAL:HG23	2.44	0.41
2:F:96:GLN:HA	2:F:97:PRO:HD3	1.84	0.41
1:G:133:LEU:HA	1:G:139:TYR:OH	2.20	0.41
1:G:185:THR:O	1:G:186:SER:C	2.61	0.41
2:H:81:SER:HA	2:H:82:PRO:HD3	1.72	0.41
2:H:638:GLY:O	2:H:639:GLU:C	2.63	0.41
1:A:45:GLY:C	1:A:47:CYS:N	2.78	0.41
1:A:259:PRO:O	1:A:260:HIS:CG	2.73	0.41
1:A:364:VAL:HG23	1:A:435:ARG:HG2	2.02	0.41
2:B:35:LEU:HD23	2:B:35:LEU:N	2.32	0.41
2:B:98:ILE:O	2:B:98:ILE:HG22	2.17	0.41
1:C:81:ILE:HD12	1:C:81:ILE:HG23	1.82	0.41
1:C:368:LEU:N	1:C:368:LEU:CD1	2.77	0.41
2:D:324:LEU:C	2:D:324:LEU:CD2	2.93	0.41
2:D:538:MET:HG3	2:D:602:TYR:CD1	2.50	0.41
2:D:650:ASP:OD1	2:D:650:ASP:C	2.63	0.41
1:E:94:ALA:HB1	1:E:145:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ASP:O	1:E:128:LEU:C	2.63	0.41
1:E:370:LEU:CD2	1:E:380:ALA:HA	2.50	0.41
2:F:697:LYS:HA	2:F:697:LYS:HD2	1.93	0.41
2:H:28:CYS:HB2	2:H:29:PRO:CD	2.49	0.41
2:H:66:THR:HG22	2:H:67:ALA:N	2.32	0.41
2:H:138:ARG:HH11	2:H:138:ARG:HD2	1.73	0.41
2:H:184:LEU:HA	2:H:185:PRO:HD2	1.85	0.41
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.57	0.41
1:A:250:ALA:O	1:A:251:ALA:C	2.64	0.41
1:A:364:VAL:CG1	1:A:365:CYS:N	2.81	0.41
2:B:60:GLY:O	2:B:104:THR:N	2.53	0.41
2:B:450:LEU:HD12	2:B:628:ILE:HG13	2.01	0.41
2:B:730:GLU:N	2:B:731:PRO:CD	2.83	0.41
2:D:221:MET:HE1	2:D:224:MET:HG3	2.02	0.41
2:D:360:LEU:CG	2:D:364:MET:CE	2.95	0.41
1:E:125:TYR:O	1:E:126:ASP:C	2.62	0.41
1:E:140:ALA:O	1:E:141:PRO:C	2.60	0.41
1:E:164:PHE:CG	1:E:165:THR:N	2.88	0.41
2:F:722:ILE:O	2:F:722:ILE:CG2	2.69	0.41
1:G:14:VAL:HG12	1:G:15:ARG:N	2.35	0.41
1:G:89:HIS:CE1	1:G:91:VAL:HB	2.55	0.41
1:G:125:TYR:O	1:G:126:ASP:C	2.62	0.41
1:G:164:PHE:CG	1:G:165:THR:N	2.88	0.41
1:G:308:ARG:HG3	1:G:309:ARG:N	2.35	0.41
2:H:654:SER:OG	2:H:656:ASN:N	2.53	0.41
1:A:104:GLY:HA3	2:B:22:TYR:OH	2.20	0.41
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.71	0.41
2:B:34:HIS:O	2:B:35:LEU:HD23	2.20	0.41
2:B:176:LEU:HD13	2:B:176:LEU:HA	1.86	0.41
1:C:153:PRO:HA	1:C:154:PRO:HD3	1.75	0.41
1:C:237:THR:CB	1:C:238:PRO:HD2	2.51	0.41
2:D:437:TRP:CZ3	2:D:446:ARG:HG3	2.56	0.41
1:E:110:PHE:CE2	1:E:132:ASN:HB2	2.55	0.41
1:E:181:PHE:CD2	1:E:192:TRP:CD2	3.09	0.41
1:E:415:LEU:HB3	1:E:440:GLN:HG2	2.03	0.41
2:F:218:ARG:HH22	2:H:218:ARG:HH22	1.67	0.41
2:F:241:ALA:O	2:F:242:CYS:C	2.63	0.41
2:F:457:ILE:O	2:F:458:SER:HB2	2.21	0.41
2:F:536:ASN:O	2:F:539:ALA:N	2.53	0.41
1:G:353:LEU:HA	1:G:353:LEU:HD12	1.77	0.41
2:H:38:GLY:HA3	2:H:99:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:228:PHE:H	6:H:3003:MTE:HN5	1.69	0.41
2:H:446:ARG:HA	2:H:631:VAL:O	2.21	0.41
2:H:582:PHE:O	2:H:583:ALA:C	2.64	0.41
1:A:331:ARG:O	1:A:332:PRO:C	2.63	0.41
2:B:307:VAL:O	2:B:308:CYS:C	2.57	0.41
2:B:414:LEU:HA	2:B:414:LEU:HD23	1.66	0.41
2:B:731:PRO:O	2:B:732:PRO:C	2.62	0.41
1:C:89:HIS:ND1	1:C:90:PRO:HD2	2.36	0.41
2:D:184:LEU:HD23	2:D:252:PRO:HB3	2.03	0.41
1:E:307:LEU:HD23	1:E:307:LEU:HA	1.74	0.41
1:E:345:ALA:N	1:E:346:PRO:HD3	2.35	0.41
2:F:48:THR:O	2:F:48:THR:HG23	2.20	0.41
2:F:413:VAL:O	2:F:413:VAL:HG23	2.21	0.41
2:F:538:MET:O	2:F:541:LYS:HB3	2.21	0.41
2:F:550:ARG:O	2:F:551:LEU:C	2.59	0.41
1:G:133:LEU:HD13	2:H:698:ILE:HD11	2.02	0.41
1:G:219:LEU:HA	1:G:220:PRO:HD3	1.86	0.41
1:G:314:ARG:NH2	1:G:329:ASP:CG	2.76	0.41
2:H:327:GLU:OE2	2:H:329:HIS:NE2	2.52	0.41
2:H:372:ARG:HG3	2:H:372:ARG:NH1	2.35	0.41
2:H:641:ARG:HH21	2:H:706:ARG:CZ	2.33	0.41
2:B:40:SER:HB2	2:B:91:VAL:CG1	2.44	0.41
2:B:251:ARG:CB	2:B:252:PRO:CD	2.99	0.41
2:B:283:SER:C	2:B:366:ARG:HH22	2.29	0.41
2:B:764:GLU:O	2:B:765:ALA:C	2.61	0.41
7:B:3004:MOS:S	8:B:4000:141:N8	2.93	0.41
1:C:314:ARG:NH2	1:C:329:ASP:CG	2.78	0.41
1:C:370:LEU:HD22	1:C:380:ALA:HA	2.01	0.41
2:D:28:CYS:HB2	2:D:29:PRO:HD2	2.01	0.41
2:D:79:ALA:HB1	2:D:80:PRO:HD2	2.03	0.41
2:D:414:LEU:HA	2:D:414:LEU:HD23	1.76	0.41
1:E:5:PHE:CD2	1:E:70:ILE:HD12	2.56	0.41
1:E:283:GLY:C	1:E:285:ILE:N	2.77	0.41
2:F:53:GLU:N	2:F:54:PRO:CD	2.83	0.41
2:F:529:ALA:C	2:F:531:SER:N	2.75	0.41
2:F:740:PHE:O	2:F:743:LEU:N	2.53	0.41
2:H:86:LEU:HD23	2:H:86:LEU:HA	1.80	0.41
2:H:302:ASP:CG	2:H:303:LEU:N	2.78	0.41
2:H:608:SER:O	2:H:609:TRP:HB3	2.19	0.41
2:H:631:VAL:CG1	2:H:642:ILE:HA	2.25	0.41
1:A:47:CYS:O	1:A:49:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:CA	1:A:359:GLN:HE22	2.33	0.41
1:A:356:ARG:NH2	1:A:359:GLN:O	2.52	0.41
1:A:401:LEU:HD11	1:A:411:ILE:HD13	2.02	0.41
1:A:423:THR:HA	1:A:424:PRO:HD3	1.61	0.41
2:B:320:PHE:CG	2:B:401:GLN:NE2	2.89	0.41
2:B:517:ASP:C	2:B:519:SER:N	2.78	0.41
2:B:715:GLN:HA	2:B:716:PRO:HD3	1.82	0.41
2:B:731:PRO:N	2:B:732:PRO:CD	2.83	0.41
1:C:296:PRO:O	1:C:297:ALA:C	2.60	0.41
1:C:301:MET:HB3	1:C:348:LEU:HD22	2.02	0.41
1:C:418:LEU:HB3	1:C:436:MET:HE1	2.03	0.41
1:C:447:VAL:O	1:C:448:ARG:C	2.61	0.41
1:E:322:PHE:CB	1:E:390:VAL:HG23	2.51	0.41
2:F:215:HIS:CG	2:H:478:SER:HB2	2.56	0.41
2:F:216:ASP:CG	2:H:512:ARG:HH11	2.28	0.41
2:F:504:LEU:HD23	2:F:504:LEU:HA	1.92	0.41
2:F:666:GLY:O	2:F:667:ALA:C	2.59	0.41
1:A:95:MET:HG3	1:A:111:ILE:HD11	2.03	0.41
1:A:283:GLY:O	1:A:284:ASN:C	2.61	0.41
1:A:331:ARG:HG2	1:A:334:GLU:OE2	2.21	0.41
2:B:61:VAL:HA	2:B:103:ALA:HB2	2.03	0.41
2:B:302:ASP:OD1	2:B:303:LEU:N	2.50	0.41
2:B:344:PHE:CD2	8:B:4000:141:C2	3.04	0.41
2:B:367:ASP:HA	2:B:368:PRO:HD3	1.96	0.41
1:C:134:CYS:SG	1:C:137:THR:HG23	2.61	0.41
1:C:318:LEU:O	1:C:319:GLU:C	2.61	0.41
1:C:356:ARG:NH1	2:D:697:LYS:HZ3	2.19	0.41
1:C:370:LEU:HD22	1:C:380:ALA:CB	2.51	0.41
1:C:373:LYS:O	1:C:374:GLY:C	2.64	0.41
2:D:197:GLN:HG2	2:D:224:MET:HE1	2.02	0.41
2:D:251:ARG:O	2:D:252:PRO:C	2.60	0.41
1:E:94:ALA:O	1:E:95:MET:C	2.63	0.41
2:F:28:CYS:HB2	2:F:29:PRO:HD2	2.03	0.41
2:F:201:GLU:O	2:F:204:HIS:N	2.54	0.41
2:F:234:GLN:H	2:F:234:GLN:HG2	1.58	0.41
2:F:247:ARG:HH11	2:F:247:ARG:CG	2.20	0.41
2:F:479:VAL:HG12	2:F:480:ALA:N	2.36	0.41
2:F:528:ALA:HA	6:F:3003:MTE:S2'	2.60	0.41
2:F:552:ALA:O	2:F:553:GLY:C	2.64	0.41
2:F:581:ARG:O	2:F:582:PHE:C	2.64	0.41
1:G:93:GLN:O	1:G:97:ASP:N	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:ALA:O	1:G:117:ALA:C	2.58	0.41
1:G:118:HIS:O	1:G:119:ASP:C	2.63	0.41
1:G:359:GLN:O	1:G:359:GLN:CG	2.58	0.41
1:G:416:PRO:O	1:G:417:LEU:C	2.64	0.41
2:H:201:GLU:O	2:H:202:ILE:C	2.61	0.41
2:H:559:GLU:O	2:H:560:GLY:C	2.62	0.41
2:H:734:LEU:HD12	2:H:734:LEU:N	2.34	0.41
1:A:301:MET:HB3	1:A:348:LEU:CD2	2.51	0.41
1:A:301:MET:HE1	1:A:341:LEU:HD13	2.03	0.41
2:B:306:PRO:O	2:B:307:VAL:C	2.62	0.41
2:B:496:MET:O	2:B:497:VAL:C	2.63	0.41
1:C:61:ASN:H	1:C:61:ASN:ND2	2.19	0.41
1:C:219:LEU:HA	1:C:220:PRO:HD3	1.90	0.41
1:E:278:VAL:O	1:E:279:ALA:C	2.61	0.41
4:E:3005:FAD:H9	4:E:3005:FAD:H1'2	1.61	0.41
2:F:306:PRO:O	2:F:307:VAL:C	2.61	0.41
2:F:496:MET:O	2:F:497:VAL:C	2.64	0.41
2:F:512:ARG:HD2	2:H:216:ASP:OD1	2.20	0.41
1:G:16:ILE:HD13	1:G:68:PRO:HG3	2.03	0.41
1:G:68:PRO:HG2	1:G:224:PHE:CE1	2.55	0.41
1:G:91:VAL:CG2	1:G:114:MET:HB3	2.50	0.41
1:G:91:VAL:HG21	1:G:114:MET:HB3	2.03	0.41
1:G:300:ALA:C	1:G:302:GLY:H	2.29	0.41
2:H:40:SER:HB2	2:H:91:VAL:HG11	2.03	0.41
2:H:84:PRO:HB2	2:H:86:LEU:O	2.21	0.41
2:H:150:ASP:OD1	2:H:150:ASP:C	2.64	0.41
2:H:166:PHE:CE1	2:H:355:ARG:HG3	2.56	0.41
2:H:171:GLN:O	2:H:268:LYS:HB3	2.21	0.41
2:H:552:ALA:O	2:H:553:GLY:C	2.64	0.41
2:H:588:ALA:O	2:H:589:ALA:C	2.63	0.41
2:H:602:TYR:CG	2:H:603:ALA:N	2.89	0.41
1:A:140:ALA:HB3	1:A:141:PRO:CD	2.51	0.40
1:A:152:GLU:HA	1:A:153:PRO:HD2	1.67	0.40
1:C:7:LEU:O	1:C:8:ASN:C	2.64	0.40
2:D:151:VAL:O	2:D:152:GLU:C	2.64	0.40
2:D:551:LEU:HA	2:D:551:LEU:HD23	1.73	0.40
2:D:596:LEU:HD23	2:D:596:LEU:HA	1.67	0.40
2:D:647:ILE:HG22	2:D:648:LEU:N	2.35	0.40
1:E:351:TYR:HB2	1:E:442:MET:SD	2.62	0.40
2:F:242:CYS:O	2:F:243:ALA:C	2.63	0.40
2:F:653:ALA:O	2:F:654:SER:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:ASN:HD22	1:G:40:ASN:HA	1.42	0.40
1:G:93:GLN:O	1:G:94:ALA:C	2.64	0.40
1:G:102:GLN:NE2	1:G:137:THR:HA	2.36	0.40
2:H:271:ASP:OD2	2:H:296:ARG:NH1	2.54	0.40
2:H:325:ARG:C	2:H:326:ILE:HG13	2.47	0.40
2:H:417:LEU:O	2:H:418:VAL:C	2.63	0.40
1:A:300:ALA:HB2	1:A:367:CYS:HB3	2.02	0.40
2:B:96:GLN:HA	2:B:97:PRO:HD3	1.78	0.40
2:B:372:ARG:O	2:B:375:ASN:N	2.53	0.40
2:B:591:MET:HB3	2:B:591:MET:HE3	1.65	0.40
1:C:129:LEU:C	1:C:131:GLY:N	2.77	0.40
1:C:444:LEU:HD23	1:C:444:LEU:HA	1.90	0.40
1:E:115:ALA:O	1:E:118:HIS:N	2.53	0.40
1:E:203:ALA:HB3	1:E:204:GLY:H	1.55	0.40
1:E:237:THR:CG2	1:E:239:ASP:OD2	2.69	0.40
1:E:253:ARG:NH2	1:E:268:ARG:HG3	2.36	0.40
1:E:296:PRO:O	1:E:297:ALA:O	2.40	0.40
1:E:358:ASP:OD2	2:F:702:SER:CB	2.65	0.40
2:F:587:ALA:O	2:F:588:ALA:C	2.62	0.40
1:G:91:VAL:HG12	1:G:92:GLN:N	2.35	0.40
1:G:356:ARG:HH21	1:G:359:GLN:HB3	1.86	0.40
2:H:734:LEU:C	2:H:736:GLY:N	2.77	0.40
1:A:16:ILE:CD1	1:A:68:PRO:HG3	2.52	0.40
1:A:53:ASP:OD1	1:A:54:ALA:N	2.54	0.40
1:A:281:ILE:CG2	1:A:282:GLY:N	2.84	0.40
2:B:112:ALA:C	2:B:114:ARG:N	2.77	0.40
1:C:95:MET:HE2	1:C:114:MET:HE1	2.04	0.40
1:C:120:ARG:O	1:C:121:ASP:C	2.64	0.40
1:C:124:ASP:OD1	1:C:128:LEU:HD22	2.21	0.40
2:D:12:ALA:O	2:D:13:ARG:C	2.63	0.40
2:D:720:GLU:HG2	2:D:724:ARG:HH21	1.86	0.40
1:E:216:LEU:HD23	1:E:216:LEU:HA	1.92	0.40
1:E:436:MET:C	1:E:438:ALA:N	2.79	0.40
2:F:238:LEU:HD23	2:F:255:MET:HG2	2.03	0.40
2:H:140:GLU:O	2:H:141:GLY:C	2.64	0.40
2:H:310:ARG:HD2	2:H:344:PHE:HB3	2.02	0.40
2:H:497:VAL:O	2:H:498:GLN:C	2.61	0.40
2:H:770:VAL:O	2:H:773:ALA:HB3	2.21	0.40
1:A:143:LEU:O	1:A:144:ARG:C	2.62	0.40
1:A:308:ARG:HG3	1:A:309:ARG:N	2.37	0.40
1:A:359:GLN:O	1:A:359:GLN:CG	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ILE:HD11	1:A:406:PHE:HD1	1.87	0.40
2:B:520:LYS:NZ	2:D:218:ARG:HH12	2.19	0.40
2:B:720:GLU:HA	2:B:724:ARG:HH21	1.85	0.40
1:C:237:THR:OG1	1:C:238:PRO:HD2	2.22	0.40
2:D:92:HIS:CD2	2:D:92:HIS:N	2.89	0.40
2:D:165:CYS:SG	2:D:166:PHE:N	2.92	0.40
2:D:173:HIS:CD2	2:D:341:PHE:CD1	3.09	0.40
2:D:744:HIS:CD2	2:D:744:HIS:C	2.97	0.40
1:E:129:LEU:HA	1:E:129:LEU:HD23	1.83	0.40
2:F:179:GLN:O	2:F:180:ALA:HB2	2.21	0.40
2:F:371:LEU:HD12	2:F:371:LEU:HA	1.62	0.40
1:G:83:ALA:HA	1:G:84:PRO:HD3	1.96	0.40
1:G:222:VAL:CG1	1:G:223:ALA:N	2.83	0.40
1:G:325:TYR:CZ	1:G:326:ARG:HG2	2.56	0.40
2:H:280:ALA:CA	2:H:287:LEU:HD12	2.50	0.40
1:A:409:ASP:O	1:A:410:THR:C	2.64	0.40
2:B:52:LEU:O	2:B:53:GLU:C	2.64	0.40
2:B:304:SER:O	2:B:305:LEU:C	2.61	0.40
2:B:493:HIS:ND1	2:B:513:ILE:CD1	2.85	0.40
1:C:81:ILE:HD13	1:C:81:ILE:HA	1.94	0.40
2:D:129:LEU:O	2:D:130:ASP:C	2.62	0.40
7:D:3004:MOS:O2	8:D:4000:141:N8	2.55	0.40
1:E:26:LEU:O	1:E:27:LEU:C	2.58	0.40
1:E:77:THR:O	1:E:78:ILE:C	2.64	0.40
1:E:107:THR:O	1:E:108:PRO:C	2.65	0.40
1:E:193:TYR:HE2	1:E:334:GLU:O	2.04	0.40
1:E:266:LEU:HA	1:E:266:LEU:HD12	1.58	0.40
1:E:309:ARG:HH11	1:E:309:ARG:HD2	1.73	0.40
1:E:408:GLU:CD	2:F:442:ARG:NH2	2.79	0.40
2:F:3:VAL:HG21	2:F:723:PHE:CE1	2.56	0.40
2:F:227:GLY:O	2:F:228:PHE:C	2.64	0.40
2:F:342:ARG:NH2	2:F:667:ALA:HB2	2.37	0.40
1:G:56:GLY:HA3	1:G:120:ARG:HH21	1.86	0.40
2:H:246:ALA:O	2:H:247:ARG:C	2.64	0.40
2:H:360:LEU:HA	2:H:360:LEU:HD12	1.79	0.40
2:H:743:LEU:HA	2:H:743:LEU:HD12	1.13	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ARG:CD	1:G:152:GLU:OE2[1_655]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/462 (96%)	385 (86%)	53 (12%)	8 (2%)	6	31
1	C	446/462 (96%)	408 (92%)	31 (7%)	7 (2%)	7	34
1	E	446/462 (96%)	370 (83%)	63 (14%)	13 (3%)	3	20
1	G	446/462 (96%)	375 (84%)	58 (13%)	13 (3%)	3	20
2	B	756/777 (97%)	696 (92%)	47 (6%)	13 (2%)	7	32
2	D	756/777 (97%)	697 (92%)	46 (6%)	13 (2%)	7	32
2	F	756/777 (97%)	688 (91%)	57 (8%)	11 (2%)	8	35
2	H	756/777 (97%)	678 (90%)	67 (9%)	11 (2%)	8	35
All	All	4808/4956 (97%)	4297 (89%)	422 (9%)	89 (2%)	6	30

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ALA
2	B	281	ASP
2	B	399	LYS
2	B	458	SER
2	B	561	CYS
1	C	180	ALA
1	C	315	ARG
1	C	374	GLY
2	D	281	ASP
2	D	399	LYS
2	D	458	SER
1	E	374	GLY

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Mol	Chain	Res	Type
2	F	399	LYS
2	F	458	SER
1	G	119	ASP
1	G	180	ALA
1	G	374	GLY
2	H	399	LYS
2	H	458	SER
2	H	560	GLY
2	H	561	CYS
2	H	761	ALA
1	A	163	ALA
1	A	315	ARG
1	A	374	GLY
2	B	187	GLU
2	B	227	GLY
2	B	342	ARG
2	B	560	GLY
2	B	761	ALA
1	C	163	ALA
1	C	375	SER
2	D	187	GLU
2	D	342	ARG
2	D	560	GLY
1	E	267	LEU
1	E	297	ALA
1	E	395	ALA
1	E	400	ALA
2	F	187	GLU
2	F	227	GLY
2	F	342	ARG
2	F	560	GLY
1	G	163	ALA
1	G	315	ARG
1	G	319	GLU
1	G	400	ALA
2	H	187	GLU
2	H	227	GLY
2	H	342	ARG
2	B	234	GLN
2	D	315	ALA
2	F	561	CYS
1	G	437	ASN

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Mol	Chain	Res	Type
2	H	530	SER
1	A	139	TYR
2	B	692	ALA
2	B	722	ILE
2	D	227	GLY
2	D	234	GLN
2	D	462	THR
2	D	561	CYS
1	E	266	LEU
1	E	315	ARG
1	E	399	ALA
1	E	455	VAL
2	F	611	ARG
1	G	199	ALA
2	H	692	ALA
1	A	221	GLU
1	A	375	SER
1	A	399	ALA
1	C	160	ALA
2	D	72	HIS
2	D	723	PHE
1	E	33	THR
2	F	692	ALA
1	G	375	SER
2	B	731	PRO
1	E	163	ALA
2	F	701	PHE
2	H	141	GLY
1	C	455	VAL
1	G	154	PRO
2	F	722	ILE
1	G	68	PRO
1	G	455	VAL
1	E	68	PRO
1	E	364	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/347 (98%)	284 (84%)	55 (16%)	2	12
1	C	339/347 (98%)	290 (86%)	49 (14%)	3	15
1	E	339/347 (98%)	277 (82%)	62 (18%)	2	9
1	G	339/347 (98%)	276 (81%)	63 (19%)	1	9
2	B	571/584 (98%)	491 (86%)	80 (14%)	3	16
2	D	571/584 (98%)	498 (87%)	73 (13%)	4	19
2	F	571/584 (98%)	500 (88%)	71 (12%)	4	20
2	H	571/584 (98%)	502 (88%)	69 (12%)	5	21
All	All	3640/3724 (98%)	3118 (86%)	522 (14%)	3	16

All (522) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	THR
1	A	12	ARG
1	A	20	THR
1	A	25	GLU
1	A	26	LEU
1	A	33	THR
1	A	36	LYS
1	A	40	ASN
1	A	41	GLU
1	A	43	ASP
1	A	61	ASN
1	A	65	MET
1	A	66	MET
1	A	68	PRO
1	A	79	GLU
1	A	85	ASP
1	A	87	ARG
1	A	96	ILE
1	A	128	LEU
1	A	143	LEU
1	A	165	THR
1	A	198	GLU
1	A	209	SER
1	A	210	LEU

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Mol	Chain	Res	Type
1	A	212	VAL
1	A	231	LEU
1	A	233	GLN
1	A	237	THR
1	A	257	GLU
1	A	281	ILE
1	A	291	ILE
1	A	309	ARG
1	A	316	MET
1	A	337	GLU
1	A	348	LEU
1	A	349	ARG
1	A	359	GLN
1	A	361	ILE
1	A	362	SER
1	A	371	THR
1	A	375	SER
1	A	376	LYS
1	A	379	THR
1	A	381	ARG
1	A	390	VAL
1	A	393	ARG
1	A	401	LEU
1	A	423	THR
1	A	425	LEU
1	A	435	ARG
1	A	447	VAL
1	A	451	SER
1	A	455	VAL
1	A	457	VAL
2	B	2	SER
2	B	3	VAL
2	B	10	ASP
2	B	16	VAL
2	B	23	LEU
2	B	39	LEU
2	B	40	SER
2	B	48	THR
2	B	53	GLU
2	B	62	ILE
2	B	66	THR
2	B	77	SER

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Mol	Chain	Res	Type
2	B	90	GLU
2	B	105	SER
2	B	129	LEU
2	B	130	ASP
2	B	133	LEU
2	B	148	ARG
2	B	151	VAL
2	B	152	GLU
2	B	161	LEU
2	B	163	GLU
2	B	165	CYS
2	B	175	TYR
2	B	190	VAL
2	B	196	SER
2	B	200	SER
2	B	204	HIS
2	B	221	MET
2	B	222	ARG
2	B	234	GLN
2	B	237	HIS
2	B	247	ARG
2	B	264	VAL
2	B	268	LYS
2	B	296	ARG
2	B	313	LEU
2	B	330	ARG
2	B	355	ARG
2	B	357	ILE
2	B	364	MET
2	B	381	GLU
2	B	398	LYS
2	B	399	LYS
2	B	423	LYS
2	B	424	SER
2	B	426	ASN
2	B	429	THR
2	B	431	ARG
2	B	448	ILE
2	B	450	LEU
2	B	452	PRO
2	B	458	SER
2	B	461	LEU

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Mol	Chain	Res	Type
2	B	481	LEU
2	B	492	LEU
2	B	512	ARG
2	B	513	ILE
2	B	530	SER
2	B	548	ARG
2	B	558	ARG
2	B	561	CYS
2	B	566	VAL
2	B	574	GLN
2	B	576	SER
2	B	611	ARG
2	B	617	ARG
2	B	618	PRO
2	B	632	VAL
2	B	634	ASP
2	B	635	ARG
2	B	641	ARG
2	B	647	ILE
2	B	650	ASP
2	B	697	LYS
2	B	704	ARG
2	B	724	ARG
2	B	741	LEU
2	B	743	LEU
2	B	744	HIS
1	C	11	THR
1	C	15	ARG
1	C	20	THR
1	C	25	GLU
1	C	26	LEU
1	C	33	THR
1	C	36	LYS
1	C	40	ASN
1	C	41	GLU
1	C	61	ASN
1	C	69	GLN
1	C	79	GLU
1	C	87	ARG
1	C	91	VAL
1	C	113	SER
1	C	128	LEU

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Mol	Chain	Res	Type
1	C	143	LEU
1	C	165	THR
1	C	198	GLU
1	C	209	SER
1	C	210	LEU
1	C	212	VAL
1	C	221	GLU
1	C	231	LEU
1	C	237	THR
1	C	239	ASP
1	C	257	GLU
1	C	281	ILE
1	C	291	ILE
1	C	309	ARG
1	C	316	MET
1	C	331	ARG
1	C	337	GLU
1	C	344	SER
1	C	349	ARG
1	C	354	SER
1	C	355	LYS
1	C	361	ILE
1	C	375	SER
1	C	376	LYS
1	C	379	THR
1	C	381	ARG
1	C	392	LYS
1	C	393	ARG
1	C	425	LEU
1	C	447	VAL
1	C	451	SER
1	C	455	VAL
1	C	457	VAL
2	D	2	SER
2	D	10	ASP
2	D	16	VAL
2	D	39	LEU
2	D	48	THR
2	D	66	THR
2	D	129	LEU
2	D	130	ASP
2	D	148	ARG

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Mol	Chain	Res	Type
2	D	151	VAL
2	D	163	GLU
2	D	165	CYS
2	D	175	TYR
2	D	190	VAL
2	D	196	SER
2	D	221	MET
2	D	222	ARG
2	D	234	GLN
2	D	237	HIS
2	D	247	ARG
2	D	268	LYS
2	D	278	ILE
2	D	296	ARG
2	D	313	LEU
2	D	330	ARG
2	D	355	ARG
2	D	398	LYS
2	D	399	LYS
2	D	407	GLN
2	D	416	GLU
2	D	423	LYS
2	D	426	ASN
2	D	429	THR
2	D	431	ARG
2	D	441	ASN
2	D	450	LEU
2	D	451	SER
2	D	452	PRO
2	D	454	LYS
2	D	458	SER
2	D	461	LEU
2	D	465	ASN
2	D	466	GLN
2	D	478	SER
2	D	496	MET
2	D	498	GLN
2	D	512	ARG
2	D	513	ILE
2	D	520	LYS
2	D	541	LYS
2	D	547	LEU

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Mol	Chain	Res	Type
2	D	558	ARG
2	D	574	GLN
2	D	576	SER
2	D	608	SER
2	D	610	ASP
2	D	611	ARG
2	D	617	ARG
2	D	618	PRO
2	D	632	VAL
2	D	634	ASP
2	D	635	ARG
2	D	641	ARG
2	D	690	THR
2	D	694	SER
2	D	697	LYS
2	D	702	SER
2	D	704	ARG
2	D	707	ILE
2	D	724	ARG
2	D	741	LEU
2	D	743	LEU
2	D	744	HIS
1	E	1	MET
1	E	11	THR
1	E	12	ARG
1	E	20	THR
1	E	25	GLU
1	E	26	LEU
1	E	33	THR
1	E	36	LYS
1	E	40	ASN
1	E	43	ASP
1	E	58	ARG
1	E	60	VAL
1	E	61	ASN
1	E	65	MET
1	E	66	MET
1	E	69	GLN
1	E	79	GLU
1	E	90	PRO
1	E	93	GLN
1	E	96	ILE

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Mol	Chain	Res	Type
1	E	101	SER
1	E	113	SER
1	E	121	ASP
1	E	128	LEU
1	E	142	ILE
1	E	143	LEU
1	E	159	GLN
1	E	165	THR
1	E	179	PRO
1	E	198	GLU
1	E	209	SER
1	E	212	VAL
1	E	221	GLU
1	E	225	LEU
1	E	231	LEU
1	E	237	THR
1	E	239	ASP
1	E	247	VAL
1	E	257	GLU
1	E	291	ILE
1	E	308	ARG
1	E	309	ARG
1	E	316	MET
1	E	337	GLU
1	E	339	VAL
1	E	341	LEU
1	E	344	SER
1	E	348	LEU
1	E	349	ARG
1	E	354	SER
1	E	355	LYS
1	E	359	GLN
1	E	375	SER
1	E	390	VAL
1	E	393	ARG
1	E	401	LEU
1	E	408	GLU
1	E	425	LEU
1	E	435	ARG
1	E	447	VAL
1	E	451	SER
1	E	455	VAL

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Mol	Chain	Res	Type
2	F	2	SER
2	F	10	ASP
2	F	16	VAL
2	F	39	LEU
2	F	40	SER
2	F	48	THR
2	F	53	GLU
2	F	66	THR
2	F	129	LEU
2	F	130	ASP
2	F	148	ARG
2	F	151	VAL
2	F	175	TYR
2	F	190	VAL
2	F	196	SER
2	F	221	MET
2	F	222	ARG
2	F	234	GLN
2	F	237	HIS
2	F	247	ARG
2	F	251	ARG
2	F	264	VAL
2	F	268	LYS
2	F	274	ILE
2	F	296	ARG
2	F	313	LEU
2	F	319	TYR
2	F	330	ARG
2	F	355	ARG
2	F	398	LYS
2	F	399	LYS
2	F	407	GLN
2	F	416	GLU
2	F	426	ASN
2	F	428	THR
2	F	429	THR
2	F	442	ARG
2	F	450	LEU
2	F	451	SER
2	F	452	PRO
2	F	454	LYS
2	F	461	LEU

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Mol	Chain	Res	Type
2	F	465	ASN
2	F	506	ILE
2	F	512	ARG
2	F	541	LYS
2	F	558	ARG
2	F	566	VAL
2	F	574	GLN
2	F	578	LYS
2	F	579	SER
2	F	581	ARG
2	F	611	ARG
2	F	617	ARG
2	F	618	PRO
2	F	624	TYR
2	F	628	ILE
2	F	632	VAL
2	F	633	ILE
2	F	650	ASP
2	F	697	LYS
2	F	702	SER
2	F	703	ASP
2	F	704	ARG
2	F	707	ILE
2	F	718	ARG
2	F	724	ARG
2	F	741	LEU
2	F	743	LEU
2	F	744	HIS
2	F	757	LEU
1	G	12	ARG
1	G	14	VAL
1	G	20	THR
1	G	25	GLU
1	G	26	LEU
1	G	33	THR
1	G	35	THR
1	G	40	ASN
1	G	58	ARG
1	G	61	ASN
1	G	65	MET
1	G	66	MET
1	G	67	LEU

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Mol	Chain	Res	Type
1	G	68	PRO
1	G	69	GLN
1	G	78	ILE
1	G	79	GLU
1	G	85	ASP
1	G	87	ARG
1	G	89	HIS
1	G	90	PRO
1	G	91	VAL
1	G	93	GLN
1	G	96	ILE
1	G	128	LEU
1	G	133	LEU
1	G	143	LEU
1	G	179	PRO
1	G	198	GLU
1	G	209	SER
1	G	210	LEU
1	G	212	VAL
1	G	221	GLU
1	G	231	LEU
1	G	237	THR
1	G	247	VAL
1	G	257	GLU
1	G	281	ILE
1	G	291	ILE
1	G	295	PRO
1	G	309	ARG
1	G	316	MET
1	G	327	LYS
1	G	331	ARG
1	G	337	GLU
1	G	343	LYS
1	G	348	LEU
1	G	349	ARG
1	G	355	LYS
1	G	361	ILE
1	G	362	SER
1	G	371	THR
1	G	375	SER
1	G	379	THR
1	G	381	ARG

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Mol	Chain	Res	Type
1	G	393	ARG
1	G	401	LEU
1	G	408	GLU
1	G	409	ASP
1	G	425	LEU
1	G	435	ARG
1	G	455	VAL
1	G	457	VAL
2	H	2	SER
2	H	10	ASP
2	H	16	VAL
2	H	23	LEU
2	H	39	LEU
2	H	40	SER
2	H	48	THR
2	H	53	GLU
2	H	66	THR
2	H	105	SER
2	H	129	LEU
2	H	130	ASP
2	H	148	ARG
2	H	151	VAL
2	H	165	CYS
2	H	175	TYR
2	H	190	VAL
2	H	196	SER
2	H	221	MET
2	H	222	ARG
2	H	234	GLN
2	H	237	HIS
2	H	247	ARG
2	H	260	ASP
2	H	268	LYS
2	H	296	ARG
2	H	313	LEU
2	H	319	TYR
2	H	330	ARG
2	H	355	ARG
2	H	357	ILE
2	H	364	MET
2	H	381	GLU
2	H	398	LYS

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Mol	Chain	Res	Type
2	H	399	LYS
2	H	416	GLU
2	H	424	SER
2	H	426	ASN
2	H	429	THR
2	H	431	ARG
2	H	450	LEU
2	H	454	LYS
2	H	458	SER
2	H	461	LEU
2	H	465	ASN
2	H	496	MET
2	H	506	ILE
2	H	512	ARG
2	H	517	ASP
2	H	530	SER
2	H	541	LYS
2	H	555	VAL
2	H	558	ARG
2	H	561	CYS
2	H	574	GLN
2	H	611	ARG
2	H	617	ARG
2	H	618	PRO
2	H	632	VAL
2	H	661	ILE
2	H	697	LYS
2	H	699	PRO
2	H	704	ARG
2	H	718	ARG
2	H	724	ARG
2	H	741	LEU
2	H	743	LEU
2	H	744	HIS
2	H	760	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	61	ASN
1	A	118	HIS

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Mol	Chain	Res	Type
1	A	159	GLN
1	A	196	HIS
1	A	328	GLN
1	A	359	GLN
2	B	34	HIS
2	B	72	HIS
2	B	160	HIS
2	B	236	ASN
2	B	293	HIS
2	B	359	HIS
2	B	426	ASN
2	B	744	HIS
2	B	753	HIS
1	C	40	ASN
1	C	61	ASN
1	C	118	HIS
1	C	196	HIS
2	D	72	HIS
2	D	160	HIS
2	D	204	HIS
2	D	234	GLN
2	D	236	ASN
2	D	359	HIS
2	D	426	ASN
2	D	441	ASN
2	D	498	GLN
2	D	649	HIS
2	D	691	HIS
2	D	744	HIS
2	D	753	HIS
1	E	40	ASN
1	E	61	ASN
1	E	118	HIS
1	E	196	HIS
1	E	359	GLN
2	F	160	HIS
2	F	204	HIS
2	F	236	ASN
2	F	293	HIS
2	F	359	HIS
2	F	441	ASN
2	F	663	GLN

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Mol	Chain	Res	Type
2	F	691	HIS
2	F	744	HIS
1	G	40	ASN
1	G	61	ASN
1	G	93	GLN
1	G	196	HIS
1	G	359	GLN
2	H	160	HIS
2	H	171	GLN
2	H	236	ASN
2	H	293	HIS
2	H	359	HIS
2	H	426	ASN
2	H	441	ASN
2	H	744	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FES	C	3001	1	0,4,4	-	-	-		
6	MTE	H	3003	7	21,26,26	6.13	11 (52%)	19,40,40	6.07	10 (52%)
4	FAD	A	3005	-	58,58,58	1.53	10 (17%)	85,89,89	2.48	36 (42%)
3	FES	E	3001	1	0,4,4	-	-	-		
6	MTE	B	3003	7	21,26,26	5.21	12 (57%)	19,40,40	6.11	13 (68%)
4	FAD	E	3005	-	58,58,58	1.62	13 (22%)	85,89,89	2.59	41 (48%)
4	FAD	C	3005	-	58,58,58	1.68	13 (22%)	85,89,89	2.66	39 (45%)
3	FES	G	3002	1	0,4,4	-	-	-		
3	FES	G	3001	1	0,4,4	-	-	-		
8	141	F	4000	7	11,12,12	3.57	5 (45%)	11,17,17	1.96	4 (36%)
7	MOS	B	3004	6,8	0,2,3	-	-	-		
8	141	D	4000	7	11,12,12	3.25	4 (36%)	11,17,17	1.69	3 (27%)
7	MOS	H	3004	6,8	0,2,3	-	-	-		
8	141	B	4000	7	11,12,12	3.23	6 (54%)	11,17,17	2.10	4 (36%)
3	FES	A	3001	1	0,4,4	-	-	-		
8	141	H	4000	7	11,12,12	3.16	5 (45%)	11,17,17	2.34	7 (63%)
3	FES	E	3002	1	0,4,4	-	-	-		
3	FES	C	3002	1	0,4,4	-	-	-		
7	MOS	F	3004	6,8,2	0,2,3	-	-	-		
4	FAD	G	3005	-	58,58,58	1.38	6 (10%)	85,89,89	2.30	35 (41%)
7	MOS	D	3004	6,8,2	0,2,3	-	-	-		
6	MTE	F	3003	7	21,26,26	5.55	13 (61%)	19,40,40	6.72	13 (68%)
3	FES	A	3002	1	0,4,4	-	-	-		
6	MTE	D	3003	7	21,26,26	5.56	13 (61%)	19,40,40	7.43	12 (63%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	C	3001	1	-	-	0/1/1/1
6	MTE	H	3003	7	-	2/6/34/34	0/3/3/3
4	FAD	A	3005	-	-	14/34/50/50	0/6/6/6
3	FES	E	3001	1	-	-	0/1/1/1
6	MTE	B	3003	7	-	0/6/34/34	0/3/3/3
4	FAD	E	3005	-	-	15/34/50/50	0/6/6/6
4	FAD	C	3005	-	-	14/34/50/50	0/6/6/6
3	FES	G	3002	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	G	3001	1	-	-	0/1/1/1
8	141	F	4000	7	-	-	0/2/2/2
8	141	D	4000	7	-	-	0/2/2/2
8	141	B	4000	7	-	-	0/2/2/2
3	FES	A	3001	1	-	-	0/1/1/1
8	141	H	4000	7	-	-	0/2/2/2
3	FES	E	3002	1	-	-	0/1/1/1
3	FES	C	3002	1	-	-	0/1/1/1
4	FAD	G	3005	-	-	17/34/50/50	0/6/6/6
6	MTE	F	3003	7	-	0/6/34/34	0/3/3/3
3	FES	A	3002	1	-	-	0/1/1/1
6	MTE	D	3003	7	-	5/6/34/34	0/3/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	3003	MTE	C7-C6	15.71	1.66	1.53
6	B	3003	MTE	C7-C6	13.70	1.64	1.53
6	H	3003	MTE	C9-C10	13.39	1.61	1.38
6	D	3003	MTE	C9-C10	13.19	1.61	1.38
6	F	3003	MTE	C7-C6	12.95	1.63	1.53
6	H	3003	MTE	C6-N5	12.41	1.60	1.46
6	F	3003	MTE	C6-N5	12.32	1.60	1.46
6	D	3003	MTE	C6-N5	11.43	1.59	1.46
6	F	3003	MTE	C9-C10	11.36	1.58	1.38
6	B	3003	MTE	C9-C10	10.97	1.57	1.38
6	D	3003	MTE	C7-C6	10.25	1.61	1.53
8	F	4000	141	O6-C6	9.16	1.40	1.23
6	B	3003	MTE	C6-N5	8.91	1.56	1.46
8	H	4000	141	O6-C6	8.23	1.39	1.23
8	D	4000	141	O6-C6	8.16	1.39	1.23
8	B	4000	141	O6-C6	7.69	1.38	1.23
6	H	3003	MTE	P-O4'	-7.46	1.36	1.60
6	D	3003	MTE	P-O4'	-7.08	1.38	1.60
6	D	3003	MTE	C4'-C3'	-6.76	1.42	1.51
6	H	3003	MTE	C4'-C3'	-6.51	1.42	1.51
6	B	3003	MTE	P-O4'	-6.40	1.40	1.60
6	B	3003	MTE	C4'-C3'	-6.38	1.43	1.51
6	F	3003	MTE	P-O4'	-6.21	1.40	1.60
6	D	3003	MTE	P-O3P	-6.02	1.32	1.54
6	F	3003	MTE	C4'-C3'	-5.84	1.43	1.51
6	B	3003	MTE	P-O3P	-5.80	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3003	MTE	O4-C4	5.78	1.34	1.23
6	H	3003	MTE	P-O3P	-5.73	1.33	1.54
6	F	3003	MTE	P-O3P	-5.63	1.33	1.54
6	D	3003	MTE	C9-N5	5.59	1.51	1.37
6	H	3003	MTE	C9-N5	5.43	1.50	1.37
6	F	3003	MTE	O4-C4	5.40	1.33	1.23
6	F	3003	MTE	C9-N5	5.12	1.49	1.37
4	C	3005	FAD	C2'-C3'	-4.99	1.44	1.53
8	F	4000	141	C7-C5	4.80	1.46	1.38
4	A	3005	FAD	C4X-N5	4.69	1.40	1.30
6	H	3003	MTE	O4-C4	4.67	1.32	1.23
8	B	4000	141	C5-C4	-4.54	1.37	1.45
6	B	3003	MTE	C9-N5	4.53	1.48	1.37
8	D	4000	141	C5-C4	-4.48	1.37	1.45
4	C	3005	FAD	C9A-C5X	-4.33	1.34	1.41
6	B	3003	MTE	O4-C4	4.15	1.31	1.23
4	G	3005	FAD	C4X-N5	4.09	1.39	1.30
4	A	3005	FAD	O4B-C4B	-3.72	1.36	1.45
4	C	3005	FAD	C4X-N5	3.70	1.38	1.30
8	D	4000	141	C7-C5	3.68	1.44	1.38
8	F	4000	141	C4-N3	3.67	1.39	1.32
4	E	3005	FAD	C2'-C3'	-3.44	1.47	1.53
4	E	3005	FAD	PA-O3P	3.36	1.63	1.59
4	E	3005	FAD	C4X-N5	3.34	1.38	1.30
6	D	3003	MTE	C2-N1	3.22	1.41	1.33
8	H	4000	141	C5-C4	-3.19	1.39	1.45
4	E	3005	FAD	C10-N1	3.18	1.39	1.33
8	H	4000	141	C4-N3	3.16	1.38	1.32
8	B	4000	141	C7-N8	-3.13	1.31	1.33
4	E	3005	FAD	C2A-N1A	3.12	1.39	1.33
6	H	3003	MTE	C10-N1	-3.12	1.31	1.36
4	E	3005	FAD	C9A-N10	-3.03	1.35	1.41
8	B	4000	141	C4-N3	3.02	1.38	1.32
4	G	3005	FAD	C8A-N7A	2.95	1.37	1.31
8	H	4000	141	C2-N3	-2.88	1.30	1.36
4	C	3005	FAD	O2B-C2B	-2.87	1.35	1.43
6	F	3003	MTE	C2-N3	-2.85	1.30	1.37
4	C	3005	FAD	C9A-N10	-2.76	1.36	1.41
8	F	4000	141	C5-C4	-2.74	1.40	1.45
4	E	3005	FAD	C2A-N3A	2.69	1.38	1.33
6	F	3003	MTE	C10-N8	2.68	1.38	1.35
4	G	3005	FAD	C5A-N7A	-2.66	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3005	FAD	O2B-C2B	-2.66	1.36	1.43
4	A	3005	FAD	C5A-N7A	-2.65	1.34	1.39
8	F	4000	141	C2-N3	-2.62	1.30	1.36
8	B	4000	141	C2-N3	-2.60	1.30	1.36
4	C	3005	FAD	C4X-C10	-2.59	1.36	1.44
4	C	3005	FAD	C4-N3	-2.56	1.34	1.38
6	B	3003	MTE	C2-N3	-2.53	1.31	1.37
4	C	3005	FAD	C5X-N5	-2.51	1.34	1.39
4	E	3005	FAD	C8-C7	-2.49	1.34	1.40
4	E	3005	FAD	P-O3P	2.48	1.62	1.59
6	D	3003	MTE	C9-C4	2.48	1.49	1.41
4	C	3005	FAD	C8A-N7A	2.47	1.36	1.31
6	B	3003	MTE	C10-N1	-2.47	1.32	1.36
4	A	3005	FAD	C9A-N10	-2.44	1.36	1.41
4	C	3005	FAD	C6-C5X	-2.37	1.36	1.40
4	A	3005	FAD	C8A-N7A	2.37	1.36	1.31
4	A	3005	FAD	C4X-C4	-2.37	1.35	1.44
8	D	4000	141	C2-N3	-2.36	1.31	1.36
6	B	3003	MTE	C2-N1	2.35	1.38	1.33
6	D	3003	MTE	C2-N3	-2.35	1.31	1.37
4	E	3005	FAD	C5A-N7A	-2.35	1.34	1.39
4	G	3005	FAD	O4B-C4B	-2.34	1.39	1.45
4	C	3005	FAD	C2B-C1B	-2.33	1.46	1.53
4	E	3005	FAD	C2B-C3B	-2.32	1.47	1.53
6	F	3003	MTE	P-O2P	-2.32	1.46	1.54
6	F	3003	MTE	P-O1P	2.30	1.57	1.50
8	B	4000	141	C7-C5	2.28	1.42	1.38
4	C	3005	FAD	C8-C7	-2.24	1.35	1.40
4	A	3005	FAD	C2A-N1A	2.23	1.37	1.33
6	B	3003	MTE	P-O2P	-2.22	1.46	1.54
6	F	3003	MTE	C9-C4	2.18	1.48	1.41
4	A	3005	FAD	C2B-C1B	-2.17	1.46	1.53
6	H	3003	MTE	C2-N1	2.17	1.38	1.33
6	H	3003	MTE	C9-C4	2.15	1.48	1.41
8	H	4000	141	C7-N8	-2.12	1.32	1.33
6	D	3003	MTE	C10-N8	2.11	1.37	1.35
4	G	3005	FAD	C4'-C3'	2.10	1.57	1.53
4	A	3005	FAD	C2A-N3A	2.09	1.37	1.33
4	E	3005	FAD	C7M-C7	2.09	1.54	1.51
6	D	3003	MTE	P-O2P	-2.09	1.47	1.54
4	G	3005	FAD	C2A-N1A	2.07	1.37	1.33
4	A	3005	FAD	C4-N3	-2.05	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3005	FAD	O3B-C3B	-2.00	1.38	1.43

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3003	MTE	O3'-C7-C6	-29.62	89.21	108.96
6	F	3003	MTE	O3'-C7-C6	-24.82	92.41	108.96
6	H	3003	MTE	O3'-C7-C6	-23.00	93.63	108.96
6	B	3003	MTE	O3'-C7-C6	-20.63	95.20	108.96
6	F	3003	MTE	C2-N1-C10	9.94	130.91	113.36
4	C	3005	FAD	O2'-C2'-C3'	-9.06	88.03	109.25
6	B	3003	MTE	C2-N1-C10	8.83	128.94	113.36
6	B	3003	MTE	O3'-C7-N8	-8.30	101.08	108.61
4	A	3005	FAD	C5X-C9A-N10	8.11	125.30	117.97
6	D	3003	MTE	C2-N1-C10	7.66	126.88	113.36
4	C	3005	FAD	O3'-C3'-C4'	7.40	125.75	108.93
4	C	3005	FAD	C1'-C2'-C3'	-7.35	89.73	109.66
4	G	3005	FAD	N3A-C2A-N1A	-7.20	117.68	128.58
6	H	3003	MTE	C2-N1-C10	7.03	125.77	113.36
4	A	3005	FAD	N3A-C2A-N1A	-6.91	118.12	128.58
4	E	3005	FAD	N3A-C2A-N1A	-6.47	118.79	128.58
4	E	3005	FAD	O3'-C3'-C4'	6.21	123.04	108.93
6	H	3003	MTE	O2P-P-O4'	6.15	122.72	106.67
4	E	3005	FAD	C2B-C1B-N9A	-5.24	100.29	113.30
4	E	3005	FAD	O3'-C3'-C2'	-5.22	97.07	108.93
6	B	3003	MTE	O4-C4-C9	-5.21	114.71	127.26
4	C	3005	FAD	C5A-C4A-N3A	-5.19	119.58	126.72
6	F	3003	MTE	O4'-C4'-C3'	5.13	121.24	108.58
6	B	3003	MTE	O2P-P-O4'	4.94	119.56	106.67
4	E	3005	FAD	C5'-C4'-C3'	-4.81	103.14	112.22
4	G	3005	FAD	O3B-C3B-C4B	-4.71	97.56	111.08
4	E	3005	FAD	C5A-C4A-N3A	-4.68	120.27	126.72
4	G	3005	FAD	C7M-C7-C8	-4.64	111.29	120.76
4	A	3005	FAD	N9A-C8A-N7A	-4.58	107.44	113.94
6	F	3003	MTE	O4-C4-C9	-4.52	116.35	127.26
4	A	3005	FAD	C5A-C4A-N3A	-4.46	120.57	126.72
4	A	3005	FAD	C9-C9A-N10	-4.45	115.87	121.85
4	C	3005	FAD	C4A-C5A-N7A	-4.42	105.53	110.58
4	E	3005	FAD	C1'-C2'-C3'	-4.36	97.84	109.66
4	E	3005	FAD	C8M-C8-C7	-4.33	111.92	120.76
4	E	3005	FAD	C4'-C3'-C2'	-4.31	106.40	113.57
4	E	3005	FAD	C7M-C7-C6	4.30	127.14	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3005	FAD	C4X-C10-N10	4.30	122.63	116.48
6	D	3003	MTE	O3'-C7-N8	-4.25	104.75	108.61
4	C	3005	FAD	O3'-C3'-C2'	-4.25	99.27	108.93
4	C	3005	FAD	C5A-C4A-N9A	4.07	110.24	105.81
6	D	3003	MTE	C4-C9-N5	4.06	127.33	116.27
4	G	3005	FAD	O5'-C5'-C4'	-4.05	98.56	109.36
4	G	3005	FAD	O2A-PA-O3P	4.04	118.20	107.27
4	A	3005	FAD	O5'-C5'-C4'	-4.04	98.57	109.36
6	D	3003	MTE	C7-C6-N5	-4.01	103.93	107.87
6	F	3003	MTE	C4-C9-N5	3.95	127.04	116.27
4	G	3005	FAD	C7M-C7-C6	3.95	126.53	119.57
4	G	3005	FAD	O3B-C3B-C2B	-3.95	99.17	111.82
4	E	3005	FAD	C5X-C9A-N10	3.90	121.49	117.97
4	E	3005	FAD	O3B-C3B-C2B	-3.89	99.34	111.82
6	B	3003	MTE	O3P-P-O4'	3.85	116.70	106.67
4	A	3005	FAD	O3B-C3B-C2B	-3.84	99.51	111.82
4	C	3005	FAD	C4B-O4B-C1B	3.83	117.93	109.47
4	A	3005	FAD	C2A-N3A-C4A	3.83	121.19	111.83
4	G	3005	FAD	O2B-C2B-C1B	-3.83	96.91	110.10
4	C	3005	FAD	C5X-C9A-N10	3.82	121.42	117.97
6	F	3003	MTE	N2-C2-N3	3.81	124.80	116.76
6	H	3003	MTE	O4-C4-C9	-3.80	118.09	127.26
4	G	3005	FAD	C5A-C4A-N3A	-3.79	121.49	126.72
4	A	3005	FAD	O4-C4-C4X	-3.78	116.54	126.53
4	E	3005	FAD	C2A-N3A-C4A	3.78	121.07	111.83
6	F	3003	MTE	O3P-P-O2P	-3.77	93.66	107.80
4	A	3005	FAD	O4B-C4B-C3B	-3.73	97.74	105.15
4	E	3005	FAD	N3A-C4A-N9A	3.73	133.51	127.17
4	A	3005	FAD	C9A-N10-C10	-3.72	115.08	120.75
4	G	3005	FAD	O4'-C4'-C5'	-3.71	101.80	109.99
6	B	3003	MTE	N2-C2-N3	3.69	124.54	116.76
4	A	3005	FAD	O4'-C4'-C3'	3.65	117.78	109.25
6	H	3003	MTE	C4-C9-N5	3.64	126.19	116.27
4	C	3005	FAD	N6A-C6A-N1A	-3.64	110.28	118.38
4	A	3005	FAD	O2'-C2'-C3'	-3.62	100.78	109.25
4	A	3005	FAD	C5A-N7A-C8A	3.58	109.08	103.45
4	G	3005	FAD	O4B-C1B-N9A	3.58	114.96	108.09
4	C	3005	FAD	O5'-C5'-C4'	-3.56	99.86	109.36
4	G	3005	FAD	C8M-C8-C7	-3.55	113.51	120.76
4	A	3005	FAD	C4X-C4-N3	3.54	122.25	113.25
4	G	3005	FAD	C2A-N3A-C4A	3.52	120.42	111.83
4	G	3005	FAD	O3'-C3'-C4'	3.50	116.88	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3005	FAD	C10-C4X-N5	-3.48	117.69	124.81
8	B	4000	141	C5-C7-N8	3.47	113.82	107.14
6	B	3003	MTE	C4-C9-N5	3.47	125.73	116.27
4	A	3005	FAD	O5B-PA-O1A	-3.46	95.24	108.94
4	C	3005	FAD	N9A-C8A-N7A	-3.45	109.03	113.94
4	A	3005	FAD	O4B-C4B-C5B	-3.43	98.36	109.33
4	E	3005	FAD	O4B-C1B-N9A	3.41	114.63	108.09
4	C	3005	FAD	C5A-N7A-C8A	3.40	108.79	103.45
4	C	3005	FAD	C2A-N3A-C4A	3.36	120.05	111.83
4	E	3005	FAD	C5A-C6A-N6A	-3.34	115.02	123.29
8	F	4000	141	C5-C7-N8	3.34	113.56	107.14
4	E	3005	FAD	O2A-PA-O3P	3.33	116.29	107.27
8	H	4000	141	O6-C6-C5	3.33	133.31	125.98
4	G	3005	FAD	C2B-C3B-C4B	3.31	109.01	102.61
4	A	3005	FAD	C4X-C10-N10	3.30	121.21	116.48
4	E	3005	FAD	N9A-C8A-N7A	-3.30	109.25	113.94
6	H	3003	MTE	N2-C2-N3	3.30	123.73	116.76
4	C	3005	FAD	C5'-C4'-C3'	-3.29	106.02	112.22
4	C	3005	FAD	N3A-C2A-N1A	-3.28	123.62	128.58
6	F	3003	MTE	O2P-P-O4'	3.27	115.19	106.67
4	A	3005	FAD	O2A-PA-O5B	3.25	122.32	107.57
6	D	3003	MTE	N2-C2-N3	3.22	123.55	116.76
4	E	3005	FAD	C7M-C7-C8	-3.21	114.21	120.76
6	B	3003	MTE	C9-C4-N3	3.19	120.90	112.13
4	E	3005	FAD	C4-N3-C2	-3.19	119.97	125.64
4	E	3005	FAD	N6A-C6A-N1A	3.18	125.46	118.38
4	A	3005	FAD	C4-N3-C2	-3.18	120.00	125.64
8	B	4000	141	C4-N9-N8	3.17	113.67	109.99
4	G	3005	FAD	C4-N3-C2	-3.17	120.01	125.64
4	C	3005	FAD	C9A-C5X-N5	-3.16	119.10	122.45
4	G	3005	FAD	O4B-C4B-C3B	-3.15	98.89	105.15
4	C	3005	FAD	O4B-C1B-N9A	-3.14	102.06	108.09
4	C	3005	FAD	C7M-C7-C6	3.11	125.05	119.57
6	D	3003	MTE	O3P-P-O1P	-3.11	98.74	110.83
4	A	3005	FAD	C5A-C6A-N6A	-3.08	115.65	123.29
8	D	4000	141	C4-N9-N8	3.07	113.55	109.99
4	E	3005	FAD	O2A-PA-O5B	3.03	121.32	107.57
6	H	3003	MTE	C9-C4-N3	3.02	120.42	112.13
4	C	3005	FAD	O4B-C1B-C2B	-3.01	100.17	106.62
4	G	3005	FAD	N9A-C8A-N7A	-3.01	109.67	113.94
6	F	3003	MTE	N3-C2-N1	-3.00	117.83	123.32
6	F	3003	MTE	O3P-P-O4'	3.00	114.49	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	4000	141	C7-N8-N9	-2.95	102.73	109.42
4	A	3005	FAD	N3A-C4A-N9A	2.94	132.17	127.17
4	E	3005	FAD	C6A-C5A-C4A	2.94	121.19	117.18
8	F	4000	141	C4-N9-N8	2.93	113.39	109.99
4	E	3005	FAD	C9A-C5X-N5	-2.92	119.35	122.45
8	H	4000	141	O2-C2-N1	-2.91	113.01	118.58
8	H	4000	141	N1-C2-N3	2.91	125.68	119.50
8	H	4000	141	C5-C7-N8	2.90	112.71	107.14
4	E	3005	FAD	O4-C4-C4X	-2.90	118.88	126.53
6	B	3003	MTE	O3P-P-O2P	-2.90	96.93	107.80
6	D	3003	MTE	O4-C4-C9	-2.89	120.29	127.26
6	H	3003	MTE	N2-C2-N1	-2.89	114.03	119.67
4	A	3005	FAD	O4B-C1B-N9A	2.87	113.60	108.09
4	A	3005	FAD	C8M-C8-C9	-2.86	114.53	119.57
4	C	3005	FAD	O4B-C4B-C3B	-2.86	99.48	105.15
8	D	4000	141	C7-N8-N9	-2.85	102.95	109.42
4	G	3005	FAD	O2-C2-N1	-2.85	117.07	121.80
4	G	3005	FAD	C2A-N1A-C6A	2.85	123.41	118.73
4	C	3005	FAD	C4X-C10-N10	2.83	120.53	116.48
8	D	4000	141	C5-C7-N8	2.82	112.56	107.14
4	G	3005	FAD	C5X-C9A-N10	2.79	120.49	117.97
6	H	3003	MTE	O4'-C4'-C3'	2.78	115.43	108.58
4	E	3005	FAD	C9-C8-C7	2.76	123.74	119.69
4	C	3005	FAD	O2B-C2B-C1B	-2.76	100.61	110.10
4	C	3005	FAD	O2'-C2'-C1'	2.74	121.48	110.20
4	G	3005	FAD	C10-C4X-N5	-2.70	119.29	124.81
4	A	3005	FAD	O2B-C2B-C3B	-2.70	103.17	111.82
4	E	3005	FAD	O2'-C2'-C1'	2.70	121.29	110.20
4	E	3005	FAD	O4B-C4B-C3B	-2.69	99.81	105.15
4	E	3005	FAD	C8M-C8-C9	2.69	124.31	119.57
6	F	3003	MTE	C9-C4-N3	2.69	119.50	112.13
4	A	3005	FAD	C7M-C7-C8	-2.68	115.29	120.76
8	F	4000	141	C7-N8-N9	-2.68	103.35	109.42
4	C	3005	FAD	C4-N3-C2	-2.66	120.92	125.64
4	C	3005	FAD	O4-C4-N3	-2.62	115.18	120.11
4	A	3005	FAD	C7M-C7-C6	2.61	124.16	119.57
6	D	3003	MTE	N3-C2-N1	-2.60	118.56	123.32
4	A	3005	FAD	C9A-C5X-N5	-2.60	119.70	122.45
8	B	4000	141	O6-C6-C5	2.58	131.66	125.98
6	D	3003	MTE	C9-C4-N3	2.56	119.17	112.13
8	H	4000	141	C4-N3-C2	-2.56	111.10	117.43
4	C	3005	FAD	O3P-P-O1P	2.55	118.36	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3003	MTE	N3-C2-N1	-2.51	118.72	123.32
4	C	3005	FAD	C4X-C10-N1	-2.49	118.49	124.59
4	E	3005	FAD	C1B-N9A-C8A	-2.47	121.62	127.09
4	C	3005	FAD	O2B-C2B-C3B	-2.47	103.90	111.82
4	C	3005	FAD	O3B-C3B-C4B	-2.45	104.04	111.08
4	A	3005	FAD	O3'-C3'-C4'	2.44	114.47	108.93
8	H	4000	141	O6-C6-N1	-2.43	115.54	120.11
6	D	3003	MTE	O2P-P-O1P	2.42	120.28	110.83
6	B	3003	MTE	C7-C6-N5	2.42	110.24	107.87
4	G	3005	FAD	C9A-C5X-N5	-2.42	119.89	122.45
4	C	3005	FAD	C4-C4X-N5	2.40	121.53	118.21
4	E	3005	FAD	C4X-C4-N3	2.38	119.31	113.25
4	G	3005	FAD	C8M-C8-C9	2.38	123.77	119.57
4	G	3005	FAD	C4-C4X-N5	2.37	121.49	118.21
4	C	3005	FAD	C5X-N5-C4X	2.37	121.93	118.09
4	C	3005	FAD	O5B-PA-O1A	-2.36	99.57	108.94
4	C	3005	FAD	O3B-C3B-C2B	-2.36	104.25	111.82
4	E	3005	FAD	O2P-P-O1P	-2.30	101.74	112.44
4	E	3005	FAD	O4-C4-N3	-2.29	115.81	120.11
4	A	3005	FAD	C5X-N5-C4X	-2.29	114.39	118.09
4	A	3005	FAD	O2B-C2B-C1B	-2.28	102.25	110.10
8	F	4000	141	O6-C6-C5	2.28	131.00	125.98
4	A	3005	FAD	C5B-C4B-C3B	-2.28	107.01	115.21
6	B	3003	MTE	O4-C4-N3	2.28	124.39	120.11
4	A	3005	FAD	C4A-N9A-C8A	2.27	108.12	105.74
4	E	3005	FAD	O2-C2-N3	-2.26	114.25	118.58
4	C	3005	FAD	O2A-PA-O3P	2.25	113.35	107.27
4	E	3005	FAD	C4-C4X-C10	2.24	120.78	116.93
4	G	3005	FAD	O2B-C2B-C3B	-2.24	104.64	111.82
4	G	3005	FAD	C5A-C4A-N9A	2.22	108.23	105.81
4	G	3005	FAD	C5A-N7A-C8A	2.21	106.93	103.45
4	C	3005	FAD	C4-C4X-C10	2.21	120.72	116.93
4	G	3005	FAD	O2'-C2'-C3'	-2.20	104.09	109.25
4	G	3005	FAD	O5'-P-O1P	2.19	117.60	108.94
4	E	3005	FAD	O2A-PA-O1A	-2.18	102.31	112.44
4	A	3005	FAD	C4A-C5A-N7A	-2.18	108.09	110.58
6	D	3003	MTE	O2P-P-O4'	2.16	112.30	106.67
4	E	3005	FAD	C9-C9A-N10	-2.15	118.97	121.85
4	G	3005	FAD	C6A-C5A-C4A	2.14	120.10	117.18
6	F	3003	MTE	O4-C4-N3	2.14	124.13	120.11
6	H	3003	MTE	O3'-C7-N8	-2.14	106.67	108.61
4	E	3005	FAD	O3P-P-O1P	2.12	117.10	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3005	FAD	P-O5'-C5'	-2.12	109.18	121.35
4	E	3005	FAD	O2'-C2'-C3'	-2.11	104.31	109.25
4	G	3005	FAD	C5A-C6A-N6A	-2.11	118.06	123.29
4	C	3005	FAD	C4X-C4-N3	2.10	118.60	113.25
4	G	3005	FAD	C4X-C4-N3	2.08	118.56	113.25
4	A	3005	FAD	O3P-P-O1P	-2.05	104.53	110.70
4	A	3005	FAD	C4B-O4B-C1B	2.05	113.99	109.47
4	E	3005	FAD	C4X-C10-N1	-2.05	119.58	124.59
6	F	3003	MTE	C7-C6-N5	-2.04	105.87	107.87
4	E	3005	FAD	C6A-C5A-N7A	-2.03	128.18	132.09
8	H	4000	141	C7-N8-N9	-2.02	104.84	109.42
4	C	3005	FAD	C6-C5X-C9A	2.00	121.80	119.05

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	FAD	C2'-C1'-N10-C10
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'
4	A	3005	FAD	C2'-C3'-C4'-O4'
4	A	3005	FAD	O3'-C3'-C4'-O4'
4	A	3005	FAD	C3'-C4'-C5'-O5'
4	A	3005	FAD	C5'-O5'-P-O2P
4	C	3005	FAD	C2'-C1'-N10-C10
4	C	3005	FAD	N10-C1'-C2'-O2'
4	C	3005	FAD	N10-C1'-C2'-C3'
4	C	3005	FAD	C2'-C3'-C4'-O4'
4	C	3005	FAD	C2'-C3'-C4'-C5'
4	C	3005	FAD	O3'-C3'-C4'-O4'
4	C	3005	FAD	O3'-C3'-C4'-C5'
4	C	3005	FAD	C3'-C4'-C5'-O5'
4	C	3005	FAD	O4'-C4'-C5'-O5'
4	E	3005	FAD	O4B-C4B-C5B-O5B
4	E	3005	FAD	C2'-C1'-N10-C10
4	E	3005	FAD	N10-C1'-C2'-O2'
4	E	3005	FAD	N10-C1'-C2'-C3'
4	E	3005	FAD	C2'-C3'-C4'-O4'
4	E	3005	FAD	O3'-C3'-C4'-O4'
4	E	3005	FAD	O3'-C3'-C4'-C5'
4	E	3005	FAD	C3'-C4'-C5'-O5'
4	E	3005	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	G	3005	FAD	N10-C1'-C2'-O2'
4	G	3005	FAD	N10-C1'-C2'-C3'
4	G	3005	FAD	C2'-C3'-C4'-O4'
4	G	3005	FAD	O3'-C3'-C4'-O4'
4	G	3005	FAD	C3'-C4'-C5'-O5'
4	G	3005	FAD	O4'-C4'-C5'-O5'
4	G	3005	FAD	C5'-O5'-P-O2P
6	D	3003	MTE	O3'-C3'-C4'-O4'
6	D	3003	MTE	C4'-O4'-P-O2P
4	C	3005	FAD	C3B-C4B-C5B-O5B
4	A	3005	FAD	O3'-C3'-C4'-C5'
4	G	3005	FAD	O3'-C3'-C4'-C5'
4	A	3005	FAD	C2'-C3'-C4'-C5'
4	E	3005	FAD	C2'-C3'-C4'-C5'
4	G	3005	FAD	C2'-C3'-C4'-C5'
4	E	3005	FAD	C3B-C4B-C5B-O5B
4	G	3005	FAD	O4B-C4B-C5B-O5B
4	G	3005	FAD	C3B-C4B-C5B-O5B
4	A	3005	FAD	O4'-C4'-C5'-O5'
4	A	3005	FAD	O4B-C4B-C5B-O5B
4	C	3005	FAD	O4B-C4B-C5B-O5B
6	H	3003	MTE	C4'-O4'-P-O2P
6	D	3003	MTE	C2'-C3'-C4'-O4'
4	A	3005	FAD	C5B-O5B-PA-O2A
4	A	3005	FAD	C5'-O5'-P-O1P
4	A	3005	FAD	C5'-O5'-P-O3P
4	C	3005	FAD	C5B-O5B-PA-O1A
4	C	3005	FAD	C5B-O5B-PA-O2A
4	C	3005	FAD	C5B-O5B-PA-O3P
4	E	3005	FAD	C5B-O5B-PA-O1A
4	E	3005	FAD	C5B-O5B-PA-O2A
4	E	3005	FAD	C5B-O5B-PA-O3P
4	G	3005	FAD	C5B-O5B-PA-O1A
4	G	3005	FAD	C5B-O5B-PA-O2A
4	G	3005	FAD	C5B-O5B-PA-O3P
4	G	3005	FAD	C2'-C1'-N10-C10
4	G	3005	FAD	C5'-O5'-P-O1P
4	G	3005	FAD	C5'-O5'-P-O3P
4	E	3005	FAD	C2B-C1B-N9A-C8A
6	H	3003	MTE	O3'-C3'-C4'-O4'
6	D	3003	MTE	C4'-O4'-P-O1P
6	D	3003	MTE	C4'-O4'-P-O3P

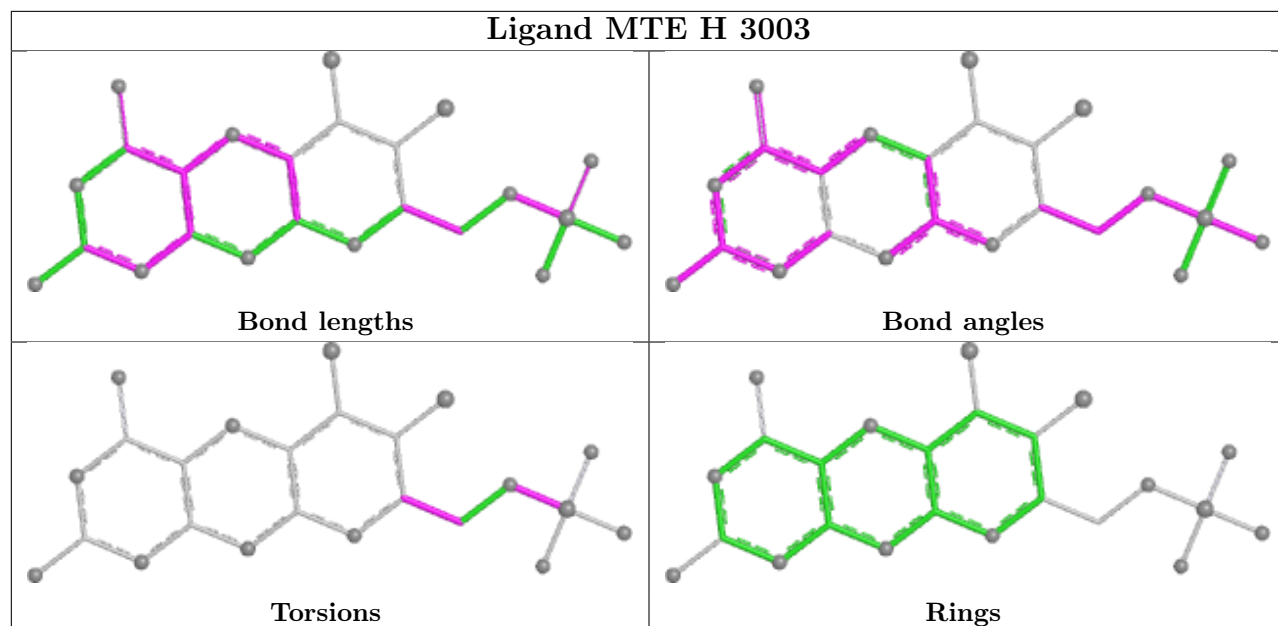
There are no ring outliers.

21 monomers are involved in 95 short contacts:

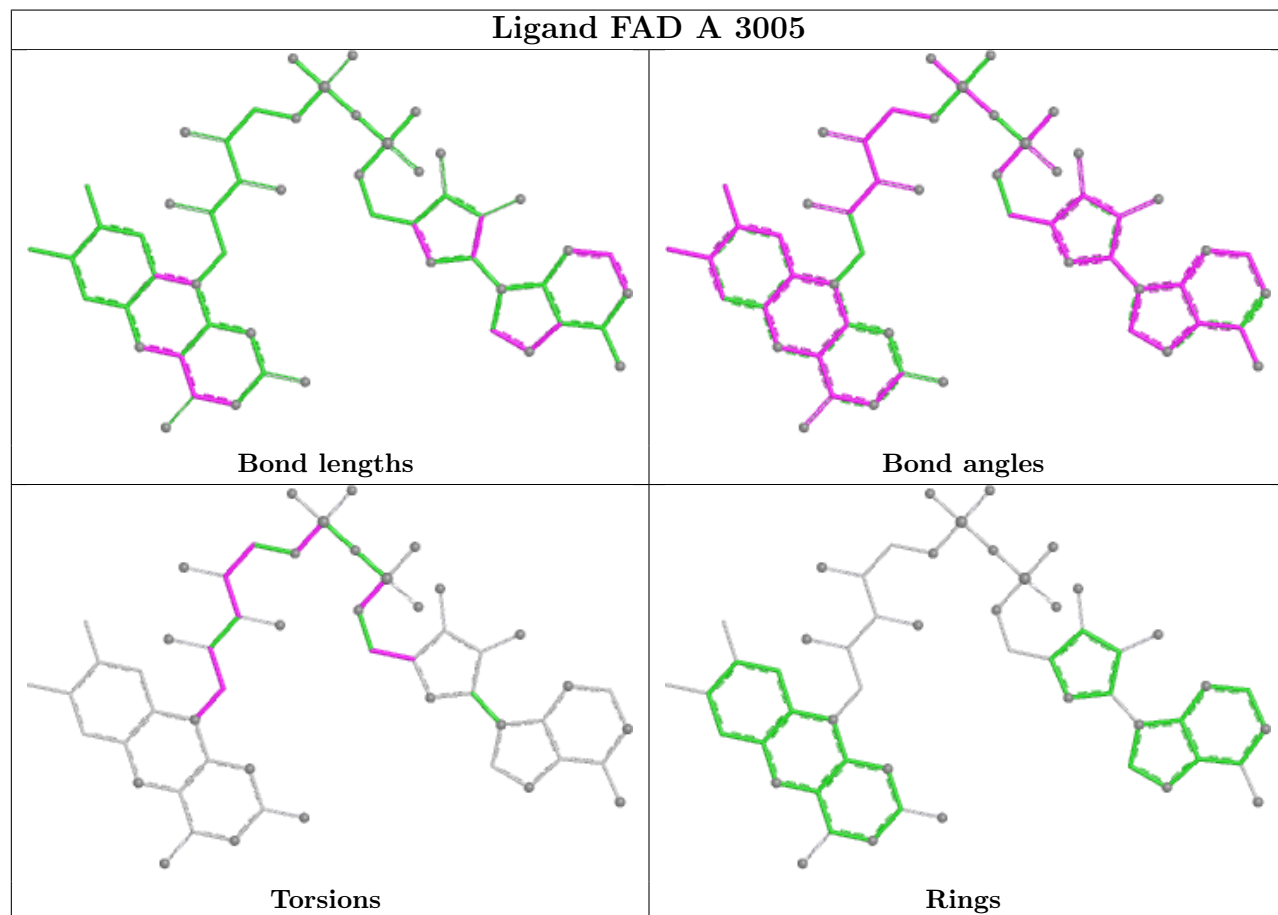
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	3003	MTE	7	0
4	A	3005	FAD	10	0
3	E	3001	FES	1	0
6	B	3003	MTE	4	0
4	E	3005	FAD	10	0
4	C	3005	FAD	3	0
3	G	3002	FES	1	0
3	G	3001	FES	2	0
8	F	4000	141	5	0
7	B	3004	MOS	4	0
8	D	4000	141	5	0
7	H	3004	MOS	5	0
8	B	4000	141	9	0
8	H	4000	141	4	0
3	E	3002	FES	5	0
7	F	3004	MOS	8	0
4	G	3005	FAD	9	0
7	D	3004	MOS	7	0
6	F	3003	MTE	7	0
3	A	3002	FES	1	0
6	D	3003	MTE	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

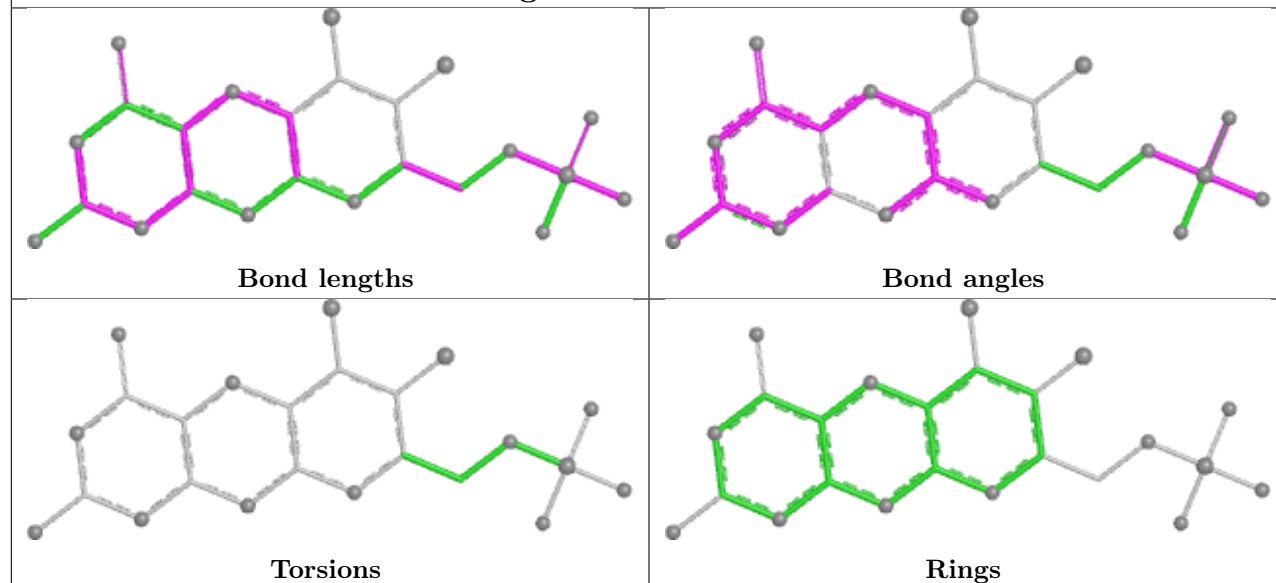
Ligand MTE H 3003



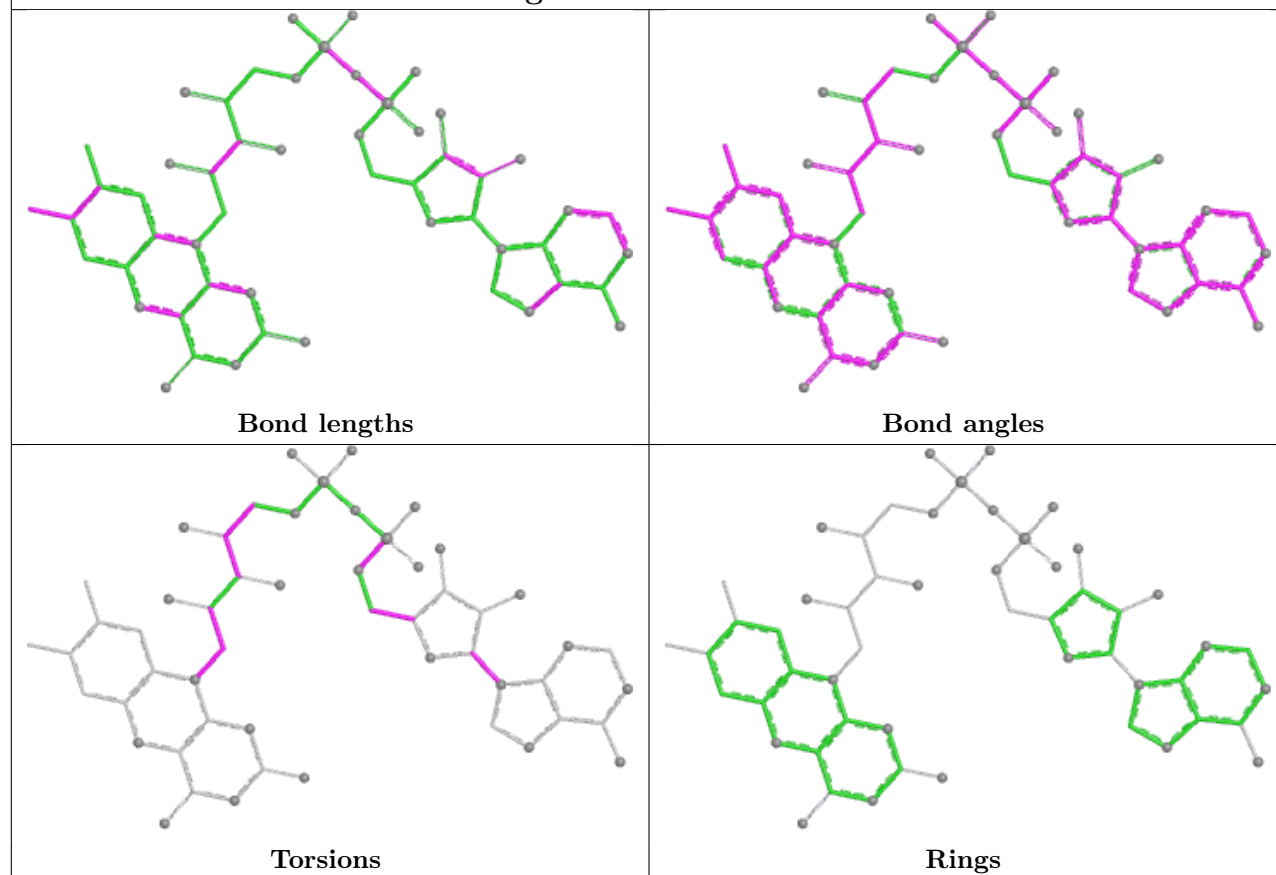
Ligand FAD A 3005

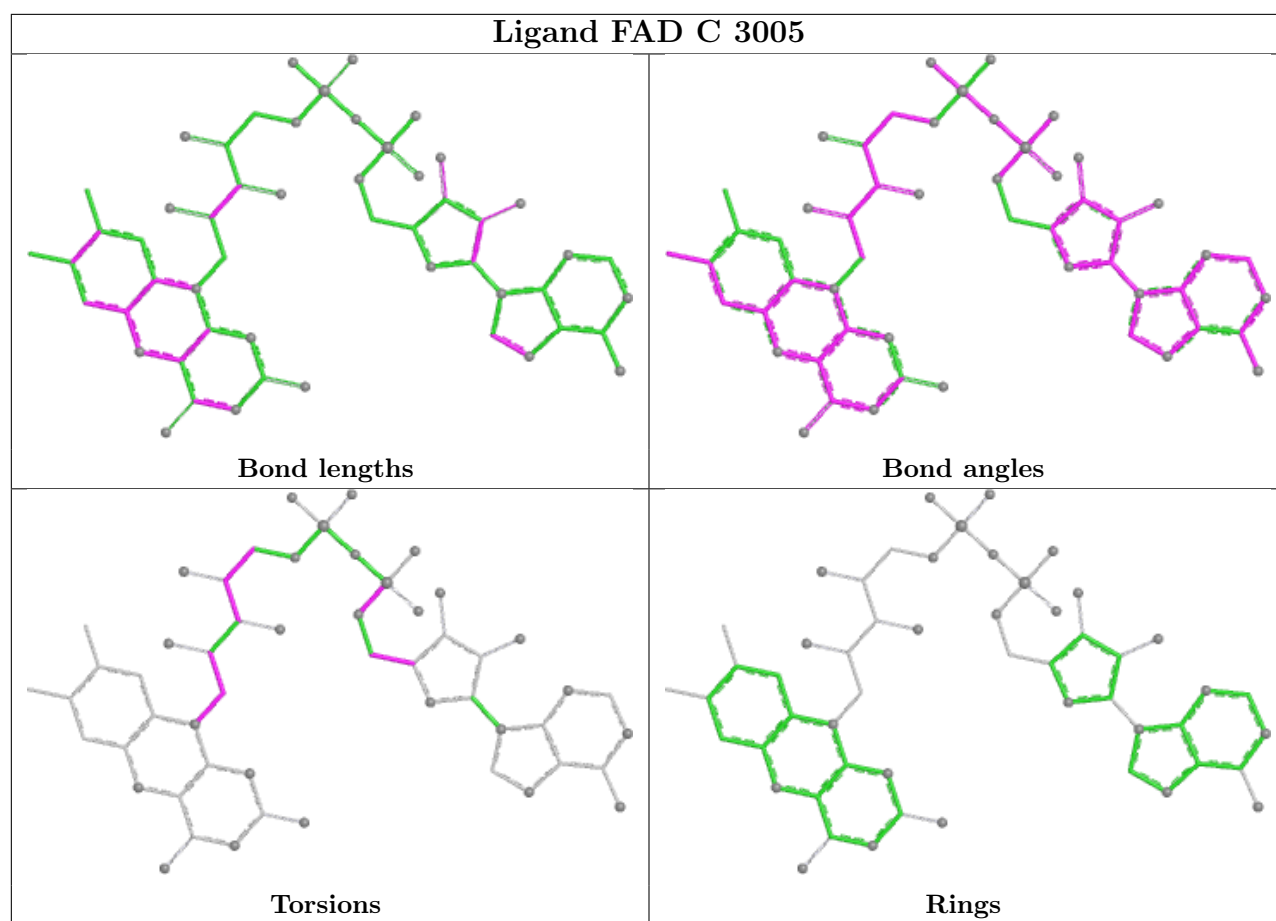


Ligand MTE B 3003

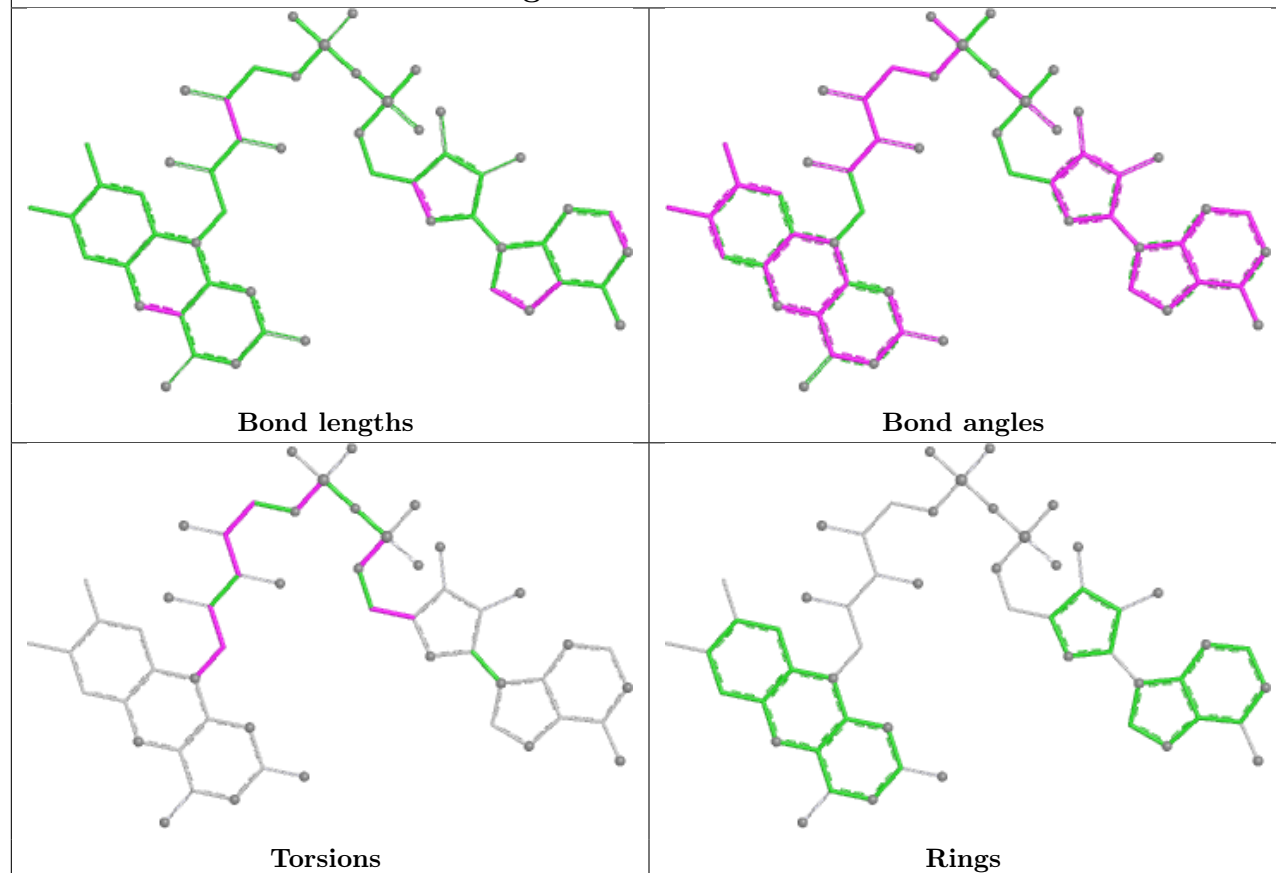


Ligand FAD E 3005

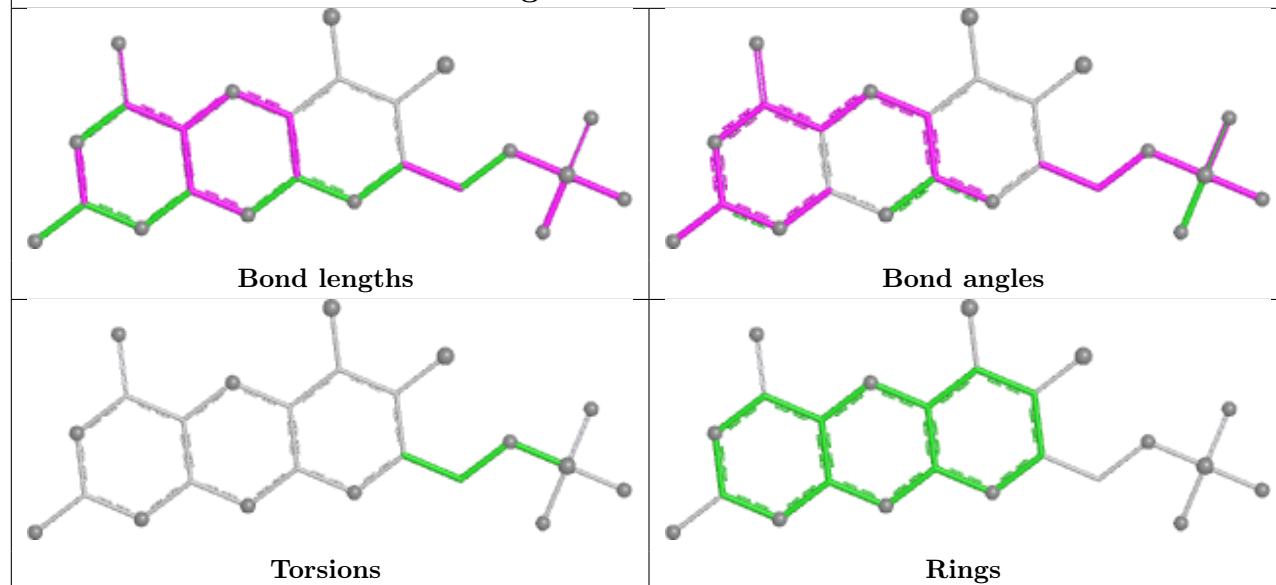


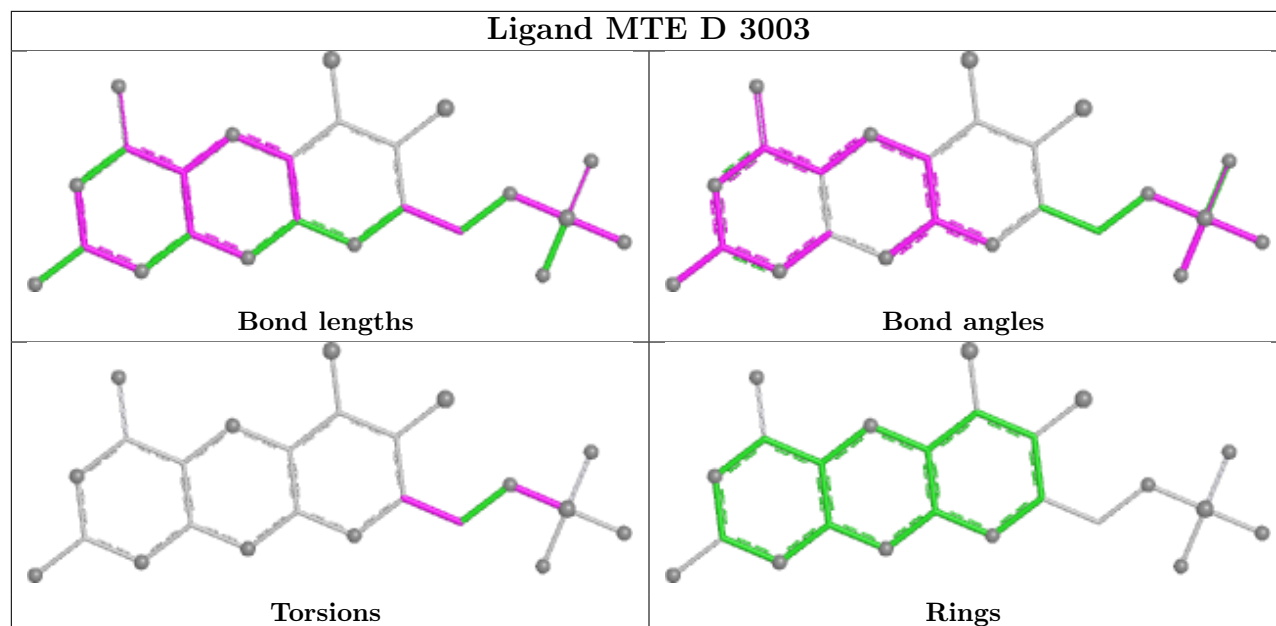


Ligand FAD G 3005



Ligand MTE F 3003





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.