



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 AM UTC

PDB ID : 1DAO / pdb_00001dao
Title : COVALENT ADDUCT OF D-AMINO ACID OXIDASE FROM PIG KIDNEY WITH 3-METHYL-2-OXO-VALERIC ACID
Authors : Todone, F.; Mattevi, A.
Deposited on : 1997-01-16
Resolution : 3.20 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

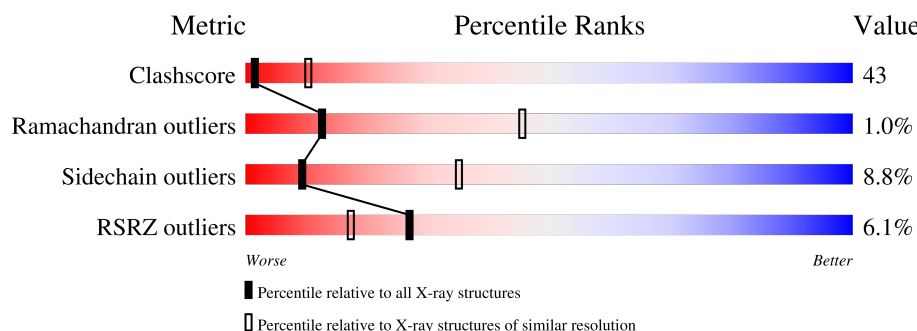
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	5% 37% 41% 18% ..
1	B	347	5% 36% 42% 18% ..
1	C	347	5% 34% 45% 17% ..
1	D	347	8% 35% 45% 16% ..
1	E	347	6% 34% 46% 16% ..
1	F	347	7% 38% 42% 16% ..

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Mol	Chain	Length	Quality of chain
1	G	347	5% 35% 44% 16% ••
1	H	347	6% 35% 45% 16% ••

2 Entry composition

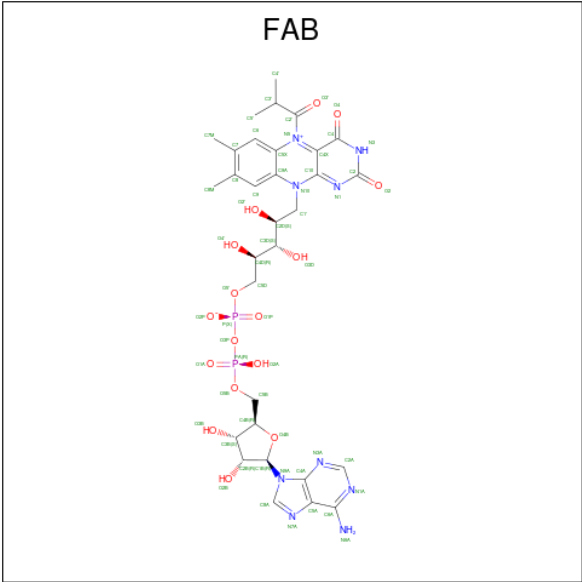
There are 3 unique types of molecules in this entry. The entry contains 22232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-AMINO ACID OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	103	0	0
			2720	1749	473	489	9			
1	B	339	Total	C	N	O	S	104	0	0
			2720	1749	473	489	9			
1	C	339	Total	C	N	O	S	109	0	0
			2720	1749	473	489	9			
1	D	339	Total	C	N	O	S	99	0	0
			2720	1749	473	489	9			
1	E	339	Total	C	N	O	S	113	0	0
			2720	1749	473	489	9			
1	F	339	Total	C	N	O	S	111	0	0
			2720	1749	473	489	9			
1	G	339	Total	C	N	O	S	116	0	0
			2720	1749	473	489	9			
1	H	339	Total	C	N	O	S	112	0	0
			2720	1749	473	489	9			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE-N5-ISOBUTYL KETONE (CCD ID: FAB) (formula: C₃₁H₃₉N₉O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	B	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	C	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	D	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	E	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	F	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	G	1	Total	C	N	O	P	0	0
			58	31	9	16	2		
2	H	1	Total	C	N	O	P	0	0
			58	31	9	16	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

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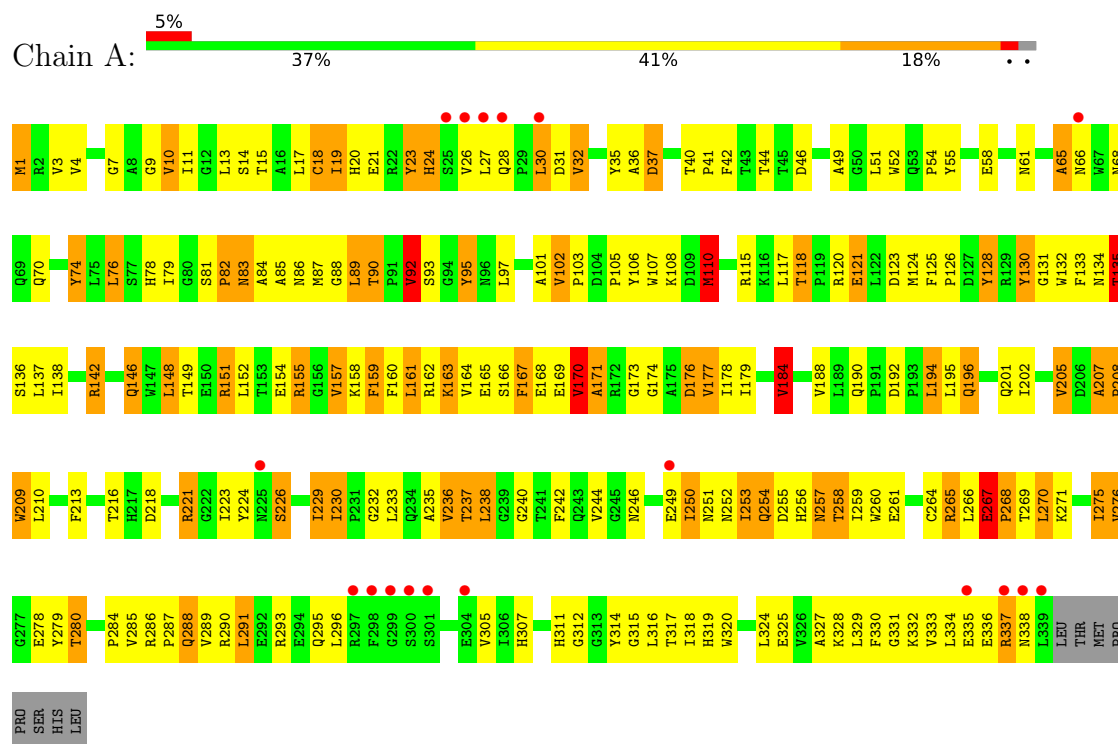
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0

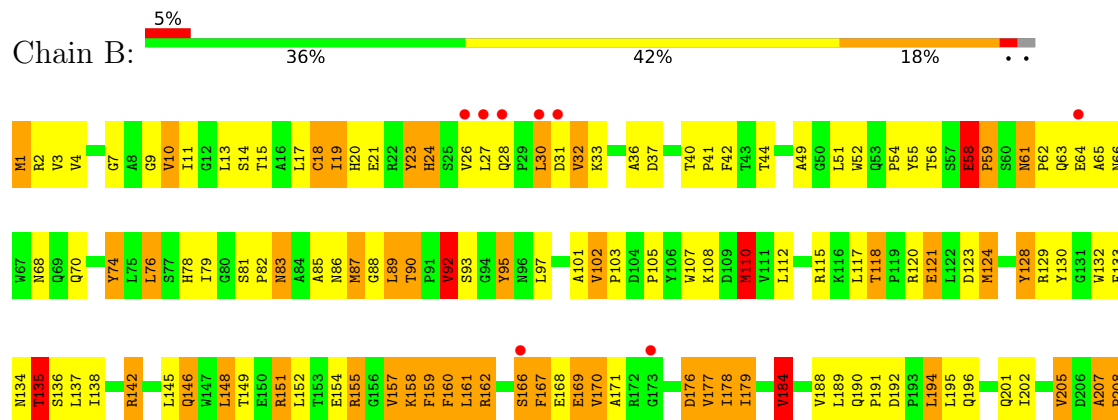
3 Residue-property plots

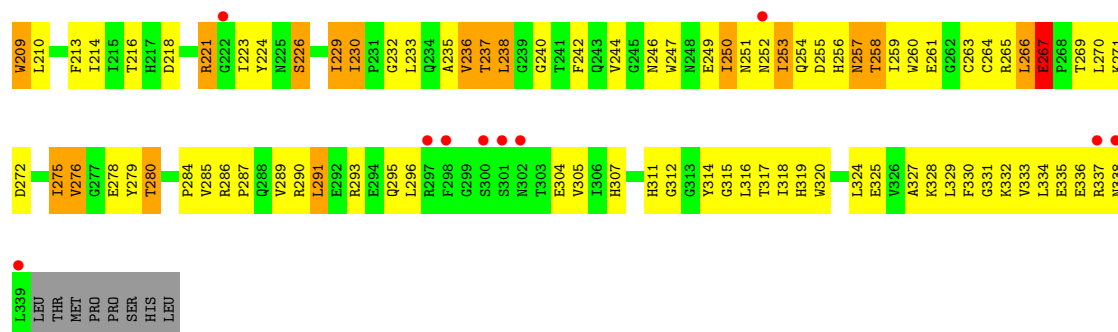
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: D-AMINO ACID OXIDASE

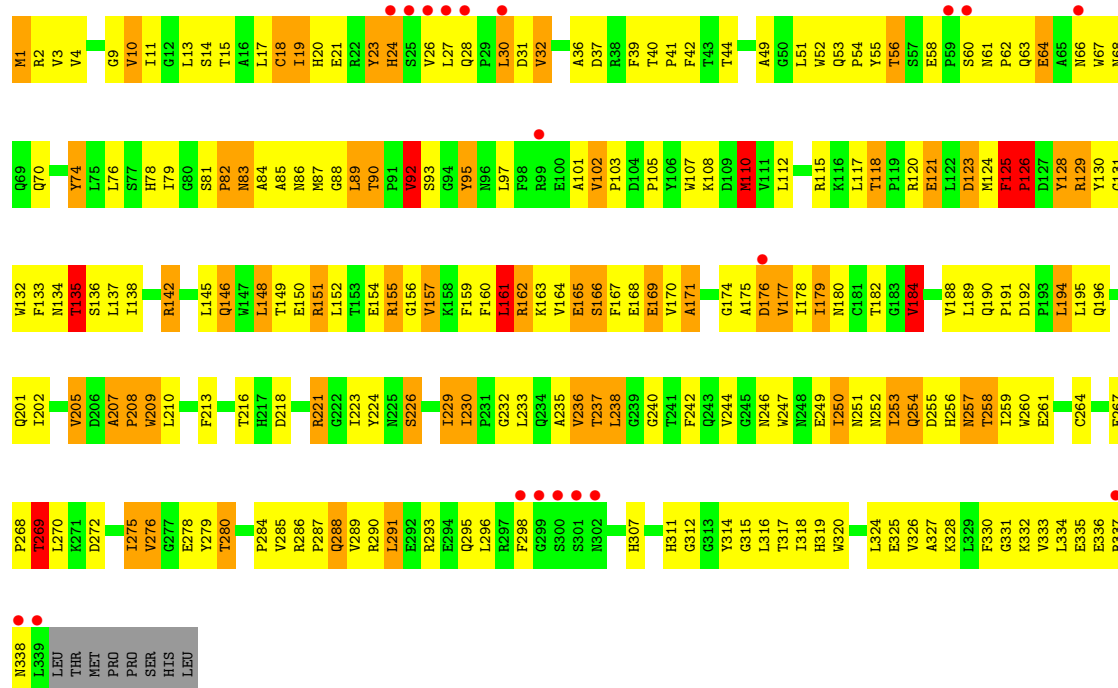


• Molecule 1: D-AMINO ACID OXIDASE

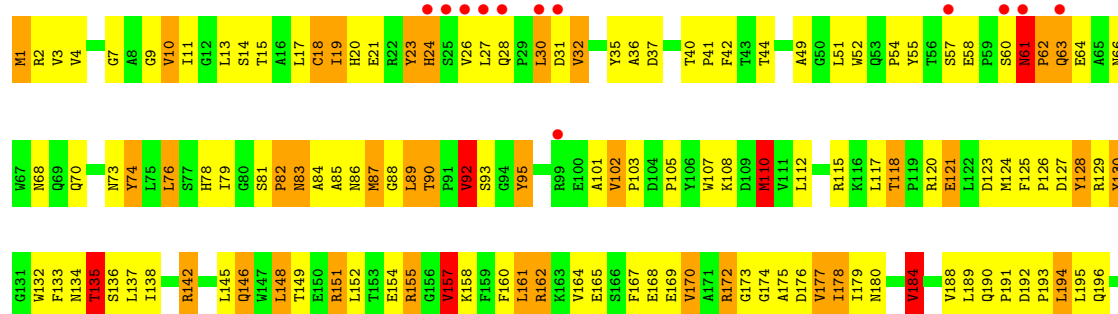


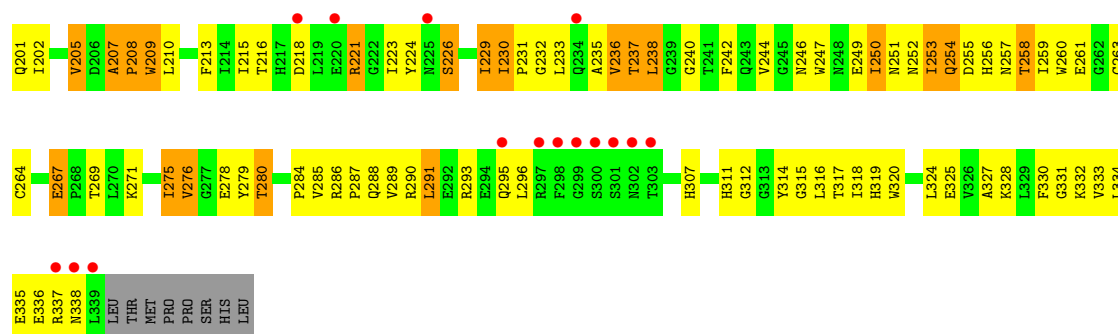


- Molecule 1: D-AMINO ACID OXIDASE



- Molecule 1: D-AMINO ACID OXIDASE

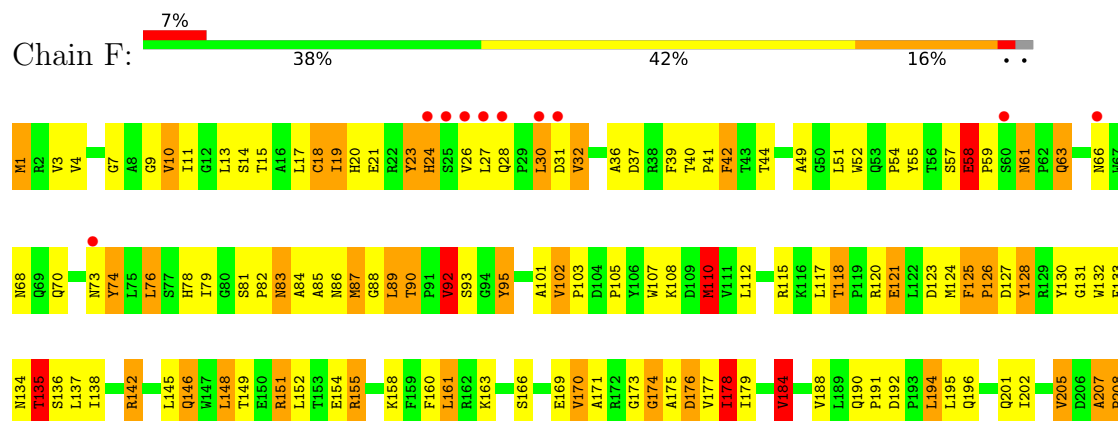


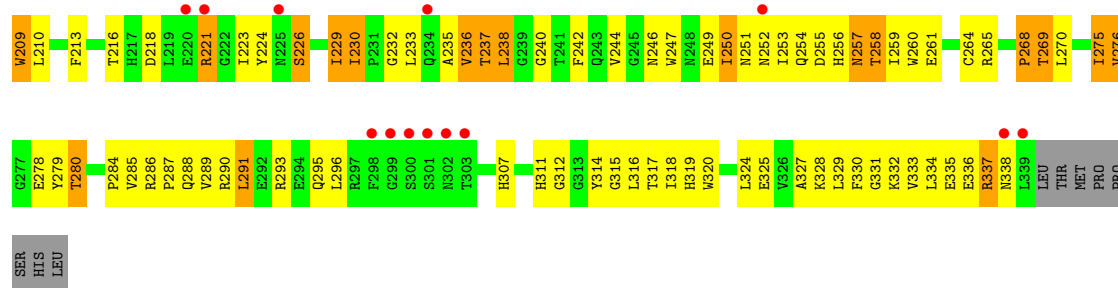


• Molecule 1: D-AMINO ACID OXIDASE

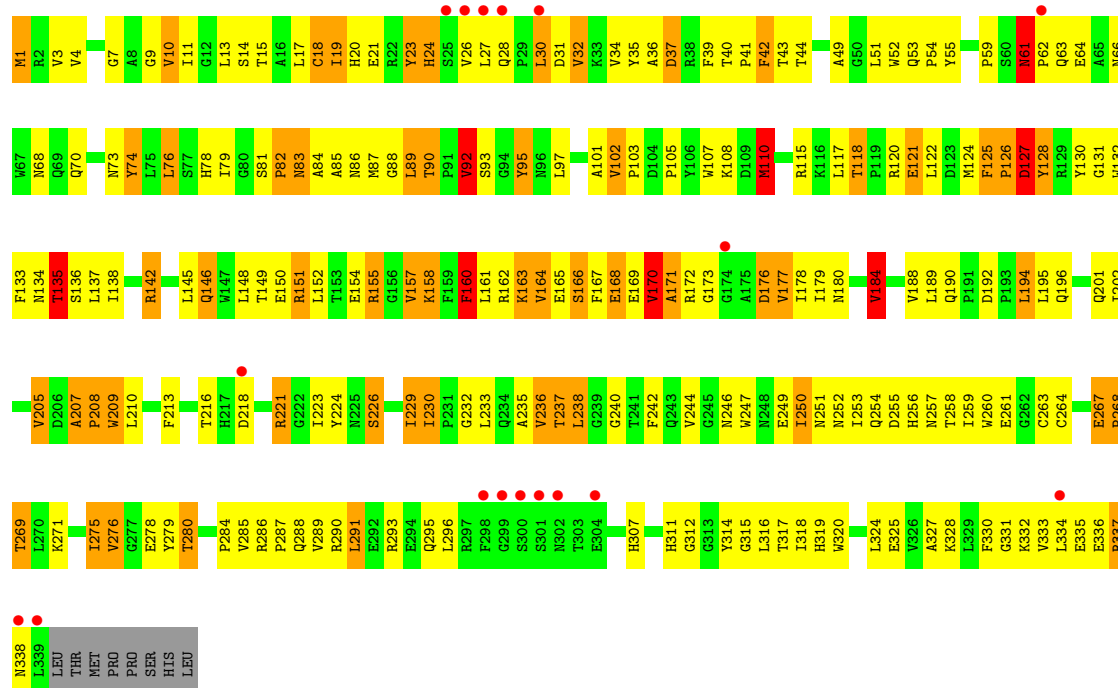


• Molecule 1: D-AMINO ACID OXIDASE

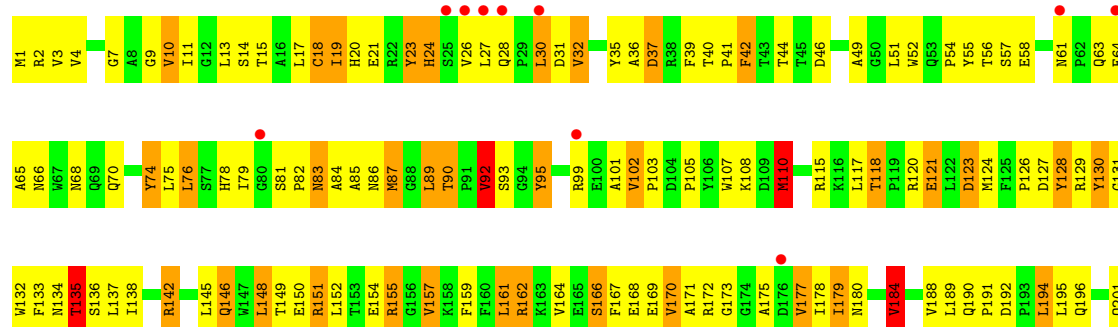


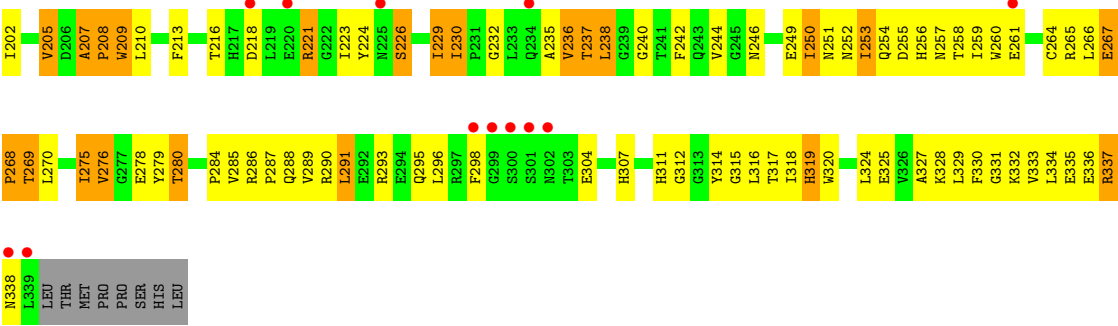


• Molecule 1: D-AMINO ACID OXIDASE



• Molecule 1: D-AMINO ACID OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	326.40Å 136.90Å 196.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-3.20) 99.3 (20.00-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.14 (at 3.22Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.232 , 0.260 0.249 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 110.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	22232	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAB

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	1.11	12/2796 (0.4%)	1.98	99/3808 (2.6%)
1	B	1.06	11/2796 (0.4%)	1.94	93/3808 (2.4%)
1	C	1.06	8/2796 (0.3%)	1.98	105/3808 (2.8%)
1	D	1.09	11/2796 (0.4%)	2.02	97/3808 (2.5%)
1	E	1.07	9/2796 (0.3%)	1.97	97/3808 (2.5%)
1	F	1.08	8/2796 (0.3%)	1.94	92/3808 (2.4%)
1	G	1.08	8/2796 (0.3%)	1.96	93/3808 (2.4%)
1	H	1.08	11/2796 (0.4%)	1.96	93/3808 (2.4%)
All	All	1.08	78/22368 (0.3%)	1.97	769/30464 (2.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
All	All	0	3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	163	LYS	CE-NZ	-12.96	1.10	1.49
1	E	276	VAL	CA-CB	-7.59	1.46	1.54
1	H	276	VAL	CA-CB	-7.57	1.46	1.54
1	F	276	VAL	CA-CB	-7.56	1.46	1.54
1	A	276	VAL	CA-CB	-7.51	1.46	1.54
1	D	276	VAL	CA-CB	-7.49	1.46	1.54
1	G	276	VAL	CA-CB	-7.48	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	276	VAL	CA-CB	-7.47	1.46	1.54
1	B	276	VAL	CA-CB	-7.47	1.46	1.54
1	E	230	ILE	CA-CB	-7.41	1.48	1.54
1	F	230	ILE	CA-CB	-7.37	1.48	1.54
1	B	230	ILE	CA-CB	-7.37	1.48	1.54
1	H	188	VAL	CA-CB	-7.36	1.45	1.54
1	F	188	VAL	CA-CB	-7.35	1.45	1.54
1	G	188	VAL	CA-CB	-7.35	1.45	1.54
1	H	230	ILE	CA-CB	-7.35	1.48	1.54
1	E	188	VAL	CA-CB	-7.33	1.45	1.54
1	A	230	ILE	CA-CB	-7.32	1.48	1.54
1	C	188	VAL	CA-CB	-7.32	1.45	1.54
1	A	188	VAL	CA-CB	-7.31	1.45	1.54
1	D	230	ILE	CA-CB	-7.29	1.48	1.54
1	D	188	VAL	CA-CB	-7.28	1.45	1.54
1	C	230	ILE	CA-CB	-7.27	1.49	1.54
1	B	188	VAL	CA-CB	-7.26	1.45	1.54
1	G	230	ILE	CA-CB	-7.26	1.49	1.54
1	D	178	ILE	CA-CB	-6.99	1.45	1.54
1	D	129	ARG	CA-C	-6.85	1.44	1.52
1	B	124	MET	C-N	-6.26	1.24	1.33
1	C	56	THR	CA-CB	6.19	1.63	1.53
1	A	179	ILE	CA-CB	-6.04	1.46	1.53
1	B	244	VAL	CA-CB	-5.91	1.47	1.54
1	E	157	VAL	CA-CB	-5.88	1.47	1.54
1	C	244	VAL	CA-CB	-5.88	1.47	1.54
1	G	237	THR	CA-CB	-5.87	1.45	1.53
1	C	237	THR	CA-CB	-5.86	1.45	1.53
1	B	237	THR	CA-CB	-5.85	1.45	1.53
1	F	244	VAL	CA-CB	-5.85	1.47	1.54
1	H	237	THR	CA-CB	-5.85	1.45	1.53
1	E	237	THR	CA-CB	-5.84	1.45	1.53
1	H	244	VAL	CA-CB	-5.84	1.47	1.54
1	G	244	VAL	CA-CB	-5.83	1.47	1.54
1	F	237	THR	CA-CB	-5.83	1.45	1.53
1	D	237	THR	CA-CB	-5.83	1.45	1.53
1	A	244	VAL	CA-CB	-5.82	1.47	1.54
1	E	244	VAL	CA-CB	-5.82	1.47	1.54
1	A	237	THR	CA-CB	-5.82	1.45	1.53
1	D	244	VAL	CA-CB	-5.81	1.47	1.54
1	H	65	ALA	CA-CB	-5.78	1.44	1.53
1	E	171	ALA	CA-C	-5.78	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	164	VAL	CA-CB	-5.76	1.47	1.54
1	A	170	VAL	CA-CB	-5.72	1.46	1.54
1	C	254	GLN	C-N	-5.69	1.26	1.33
1	A	164	VAL	CA-CB	-5.64	1.47	1.54
1	D	254	GLN	C-N	-5.63	1.26	1.33
1	B	178	ILE	CA-CB	-5.59	1.47	1.54
1	B	65	ALA	CA-CB	-5.56	1.44	1.53
1	F	63	GLN	CA-C	-5.47	1.45	1.52
1	B	157	VAL	CA-CB	-5.38	1.47	1.54
1	G	157	VAL	CA-CB	-5.36	1.47	1.54
1	F	275	ILE	CA-CB	-5.34	1.47	1.54
1	C	275	ILE	CA-CB	-5.33	1.47	1.54
1	D	179	ILE	CA-CB	-5.31	1.47	1.53
1	E	275	ILE	CA-CB	-5.29	1.48	1.54
1	A	275	ILE	CA-CB	-5.28	1.48	1.54
1	G	275	ILE	CA-CB	-5.27	1.48	1.54
1	B	275	ILE	CA-CB	-5.27	1.48	1.54
1	H	275	ILE	CA-CB	-5.26	1.48	1.54
1	H	267	GLU	C-N	-5.25	1.27	1.33
1	H	179	ILE	CA-C	-5.25	1.45	1.52
1	D	275	ILE	CA-CB	-5.24	1.48	1.54
1	B	159	PHE	CA-C	-5.19	1.46	1.52
1	E	179	ILE	CA-CB	-5.18	1.47	1.53
1	F	179	ILE	CA-C	-5.17	1.46	1.52
1	D	254	GLN	CA-C	-5.10	1.46	1.52
1	A	65	ALA	CA-CB	-5.09	1.45	1.53
1	H	268	PRO	N-CA	-5.06	1.40	1.47
1	A	268	PRO	C-O	-5.05	1.17	1.24
1	A	177	VAL	CA-CB	-5.02	1.47	1.54

All (769) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	ARG	NE-CZ-NH1	-16.16	105.34	121.50
1	D	126	PRO	CA-C-N	-13.93	96.76	120.58
1	D	126	PRO	C-N-CA	-13.93	96.76	120.58
1	D	129	ARG	NE-CZ-NH2	12.97	130.87	119.20
1	B	61	ASN	N-CA-C	-12.89	92.50	110.29
1	E	167	PHE	N-CA-C	-11.26	99.09	111.36
1	H	170	VAL	CB-CA-C	-10.74	98.23	111.97
1	D	127	ASP	N-CA-C	10.55	124.67	111.69
1	A	176	ASP	N-CA-C	-9.71	98.71	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42	PHE	N-CA-C	9.71	125.13	113.28
1	C	42	PHE	N-CA-C	9.70	125.11	113.28
1	C	92	VAL	CB-CA-C	-9.70	93.72	111.18
1	E	42	PHE	N-CA-C	9.69	125.11	113.28
1	F	92	VAL	CB-CA-C	-9.69	93.74	111.18
1	A	42	PHE	N-CA-C	9.68	125.09	113.28
1	A	92	VAL	CB-CA-C	-9.68	93.76	111.18
1	B	92	VAL	CB-CA-C	-9.67	93.77	111.18
1	E	92	VAL	CB-CA-C	-9.67	93.77	111.18
1	F	42	PHE	N-CA-C	9.67	125.08	113.28
1	G	42	PHE	N-CA-C	9.67	125.08	113.28
1	D	92	VAL	CB-CA-C	-9.67	93.77	111.18
1	G	92	VAL	CB-CA-C	-9.67	93.78	111.18
1	H	42	PHE	N-CA-C	9.66	125.07	113.28
1	H	92	VAL	CB-CA-C	-9.65	93.81	111.18
1	B	42	PHE	N-CA-C	9.64	125.04	113.28
1	G	127	ASP	N-CA-C	-9.44	100.71	112.88
1	D	179	ILE	CB-CA-C	9.32	124.57	111.81
1	G	171	ALA	N-CA-C	-9.08	100.21	111.11
1	B	266	LEU	N-CA-C	-9.04	101.51	112.54
1	D	62	PRO	N-CA-C	-9.01	102.60	113.86
1	A	161	LEU	N-CA-C	-8.69	96.81	109.59
1	A	126	PRO	CA-C-N	-8.62	108.72	120.44
1	A	126	PRO	C-N-CA	-8.62	108.72	120.44
1	B	19	ILE	CB-CA-C	-8.57	101.00	111.97
1	H	19	ILE	CB-CA-C	-8.57	101.00	111.97
1	B	90	THR	N-CA-CB	8.56	125.61	110.37
1	D	19	ILE	CB-CA-C	-8.56	101.01	111.97
1	A	19	ILE	CB-CA-C	-8.56	101.02	111.97
1	F	19	ILE	CB-CA-C	-8.55	101.02	111.97
1	C	19	ILE	CB-CA-C	-8.55	101.03	111.97
1	E	19	ILE	CB-CA-C	-8.55	101.02	111.97
1	E	90	THR	N-CA-CB	8.54	125.57	110.37
1	D	90	THR	N-CA-CB	8.54	125.57	110.37
1	A	90	THR	N-CA-CB	8.54	125.56	110.37
1	C	90	THR	N-CA-CB	8.53	125.56	110.37
1	G	19	ILE	CB-CA-C	-8.53	101.05	111.97
1	H	90	THR	N-CA-CB	8.52	125.53	110.37
1	F	90	THR	N-CA-CB	8.51	125.52	110.37
1	G	90	THR	N-CA-CB	8.50	125.51	110.37
1	A	163	LYS	N-CA-C	-8.46	92.95	108.02
1	G	164	VAL	N-CA-C	-8.46	96.27	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	163	LYS	CG-CD-CE	8.39	130.59	111.30
1	G	267	GLU	CA-C-O	8.32	129.16	121.34
1	H	166	SER	CA-C-N	-8.32	108.30	120.28
1	H	166	SER	C-N-CA	-8.32	108.30	120.28
1	G	61	ASN	N-CA-C	-8.31	99.62	109.93
1	E	127	ASP	CA-C-N	-8.15	108.44	123.03
1	E	127	ASP	C-N-CA	-8.15	108.44	123.03
1	H	184	VAL	CB-CA-C	-8.09	99.62	112.16
1	D	175	ALA	N-CA-C	8.08	122.14	110.10
1	A	130	TYR	CA-C-O	8.08	129.78	120.89
1	D	184	VAL	CB-CA-C	-8.08	99.64	112.16
1	G	184	VAL	CB-CA-C	-8.07	99.64	112.16
1	A	184	VAL	CB-CA-C	-8.06	99.66	112.16
1	F	184	VAL	CB-CA-C	-8.06	99.66	112.16
1	E	184	VAL	CB-CA-C	-8.05	99.68	112.16
1	C	184	VAL	CB-CA-C	-8.04	99.70	112.16
1	A	171	ALA	CA-C-O	-8.04	112.62	120.90
1	B	184	VAL	CB-CA-C	-8.03	99.71	112.16
1	F	176	ASP	N-CA-C	-7.98	101.66	111.40
1	H	44	THR	N-CA-C	-7.98	102.58	111.28
1	D	44	THR	N-CA-C	-7.97	102.60	111.28
1	E	129	ARG	CA-C-N	-7.97	108.18	121.80
1	E	129	ARG	C-N-CA	-7.97	108.18	121.80
1	C	44	THR	N-CA-C	-7.96	102.60	111.28
1	A	44	THR	N-CA-C	-7.95	102.61	111.28
1	E	44	THR	N-CA-C	-7.95	102.62	111.28
1	F	44	THR	N-CA-C	-7.93	102.64	111.28
1	B	44	THR	N-CA-C	-7.92	102.64	111.28
1	G	44	THR	N-CA-C	-7.92	102.65	111.28
1	A	167	PHE	N-CA-C	-7.86	102.70	111.82
1	C	229	ILE	CA-C-N	-7.67	116.17	122.85
1	C	229	ILE	C-N-CA	-7.67	116.17	122.85
1	H	127	ASP	N-CA-C	-7.67	103.72	113.23
1	G	229	ILE	CA-C-N	-7.66	116.19	122.85
1	G	229	ILE	C-N-CA	-7.66	116.19	122.85
1	E	130	TYR	CA-C-O	-7.65	113.27	121.38
1	E	229	ILE	CA-C-N	-7.65	116.19	122.85
1	E	229	ILE	C-N-CA	-7.65	116.19	122.85
1	F	229	ILE	CA-C-N	-7.65	116.20	122.85
1	F	229	ILE	C-N-CA	-7.65	116.20	122.85
1	F	178	ILE	CB-CA-C	-7.64	98.75	111.29
1	D	177	VAL	CA-C-N	-7.64	112.38	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	VAL	C-N-CA	-7.64	112.38	122.99
1	H	229	ILE	CA-C-N	-7.64	116.21	122.85
1	H	229	ILE	C-N-CA	-7.64	116.21	122.85
1	D	229	ILE	CA-C-N	-7.63	116.21	122.85
1	D	229	ILE	C-N-CA	-7.63	116.21	122.85
1	B	229	ILE	CA-C-N	-7.62	116.22	122.85
1	B	229	ILE	C-N-CA	-7.62	116.22	122.85
1	A	229	ILE	CA-C-N	-7.62	116.22	122.85
1	A	229	ILE	C-N-CA	-7.62	116.22	122.85
1	H	267	GLU	CB-CA-C	-7.59	99.41	111.02
1	C	160	PHE	CA-C-N	-7.56	111.30	122.41
1	C	160	PHE	C-N-CA	-7.56	111.30	122.41
1	B	58	GLU	N-CA-C	-7.54	99.68	110.08
1	C	164	VAL	N-CA-C	-7.51	99.89	109.58
1	A	168	GLU	O-C-N	7.51	129.90	122.09
1	C	129	ARG	N-CA-C	7.50	123.57	113.97
1	B	128	TYR	N-CA-C	7.45	120.62	110.35
1	E	164	VAL	CB-CA-C	-7.44	101.02	111.28
1	C	176	ASP	N-CA-C	7.40	118.98	111.07
1	E	83	ASN	N-CA-C	7.39	122.13	113.18
1	H	83	ASN	N-CA-C	7.39	122.13	113.18
1	C	83	ASN	N-CA-C	7.39	122.12	113.18
1	G	83	ASN	N-CA-C	7.39	122.12	113.18
1	B	83	ASN	N-CA-C	7.38	122.12	113.18
1	G	177	VAL	CB-CA-C	-7.38	97.50	110.71
1	A	83	ASN	N-CA-C	7.38	122.11	113.18
1	D	83	ASN	N-CA-C	7.37	122.10	113.18
1	F	83	ASN	N-CA-C	7.37	122.09	113.18
1	H	250	ILE	CB-CA-C	-7.34	100.22	111.31
1	D	250	ILE	CB-CA-C	-7.34	100.23	111.31
1	B	250	ILE	CB-CA-C	-7.33	100.24	111.31
1	G	250	ILE	CB-CA-C	-7.33	100.24	111.31
1	A	250	ILE	CB-CA-C	-7.33	100.25	111.31
1	F	250	ILE	CB-CA-C	-7.33	100.25	111.31
1	E	250	ILE	CB-CA-C	-7.33	100.25	111.31
1	C	250	ILE	CB-CA-C	-7.31	100.27	111.31
1	A	128	TYR	CA-CB-CG	-7.26	100.83	113.90
1	B	128	TYR	N-CA-CB	-7.22	100.41	110.38
1	D	288	GLN	N-CA-C	-7.19	97.35	108.42
1	D	172	ARG	N-CA-C	-7.19	103.44	111.71
1	C	156	GLY	CA-C-N	-7.18	111.75	121.66
1	C	156	GLY	C-N-CA	-7.18	111.75	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	176	ASP	N-CA-C	-7.18	102.86	111.69
1	A	58	GLU	CA-C-N	7.17	127.17	119.78
1	A	58	GLU	C-N-CA	7.17	127.17	119.78
1	G	128	TYR	N-CA-CB	7.16	121.88	110.85
1	D	244	VAL	N-CA-C	7.14	118.80	109.58
1	G	244	VAL	N-CA-C	7.14	118.80	109.58
1	E	244	VAL	N-CA-C	7.13	118.78	109.58
1	B	244	VAL	N-CA-C	7.12	118.77	109.58
1	F	244	VAL	N-CA-C	7.12	118.76	109.58
1	H	244	VAL	N-CA-C	7.12	118.76	109.58
1	D	174	GLY	N-CA-C	7.11	123.33	114.37
1	C	244	VAL	N-CA-C	7.10	118.75	109.58
1	A	244	VAL	N-CA-C	7.10	118.74	109.58
1	H	126	PRO	N-CA-C	7.10	122.76	114.03
1	H	157	VAL	CB-CA-C	-7.09	101.94	111.15
1	A	130	TYR	O-C-N	-7.05	115.58	123.48
1	E	65	ALA	CA-C-N	-6.95	111.41	120.44
1	E	65	ALA	C-N-CA	-6.95	111.41	120.44
1	C	165	GLU	N-CA-C	6.91	121.96	112.90
1	F	61	ASN	N-CA-C	-6.87	100.99	109.65
1	B	202	ILE	CB-CA-C	-6.87	98.50	110.38
1	H	202	ILE	CB-CA-C	-6.86	98.51	110.38
1	C	202	ILE	CB-CA-C	-6.86	98.52	110.38
1	E	202	ILE	CB-CA-C	-6.85	98.53	110.38
1	E	120	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	F	202	ILE	CB-CA-C	-6.84	98.54	110.38
1	D	202	ILE	CB-CA-C	-6.84	98.54	110.38
1	G	202	ILE	CB-CA-C	-6.84	98.54	110.38
1	A	202	ILE	CB-CA-C	-6.83	98.57	110.38
1	A	120	ARG	NE-CZ-NH1	-6.82	114.68	121.50
1	C	120	ARG	NE-CZ-NH1	-6.82	114.69	121.50
1	D	120	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	C	169	GLU	CA-C-N	-6.81	110.75	120.42
1	C	169	GLU	C-N-CA	-6.81	110.75	120.42
1	B	120	ARG	NE-CZ-NH1	-6.80	114.70	121.50
1	H	120	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	G	120	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	F	120	ARG	NE-CZ-NH1	-6.78	114.72	121.50
1	E	178	ILE	CB-CA-C	-6.77	100.74	110.83
1	F	74	TYR	CA-C-N	-6.67	111.77	120.44
1	F	74	TYR	C-N-CA	-6.67	111.77	120.44
1	B	89	LEU	N-CA-C	6.67	120.70	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	89	LEU	N-CA-C	6.67	120.70	109.76
1	G	89	LEU	N-CA-C	6.67	120.70	109.76
1	A	74	TYR	CA-C-N	-6.67	111.77	120.44
1	A	74	TYR	C-N-CA	-6.67	111.77	120.44
1	G	288	GLN	CA-C-O	-6.67	113.52	120.99
1	H	89	LEU	N-CA-C	6.66	120.69	109.76
1	E	89	LEU	N-CA-C	6.66	120.68	109.76
1	B	74	TYR	CA-C-N	-6.66	111.78	120.44
1	B	74	TYR	C-N-CA	-6.66	111.78	120.44
1	C	89	LEU	N-CA-C	6.66	120.68	109.76
1	C	74	TYR	CA-C-N	-6.66	111.79	120.44
1	C	74	TYR	C-N-CA	-6.66	111.79	120.44
1	A	89	LEU	N-CA-C	6.65	120.67	109.76
1	G	74	TYR	CA-C-N	-6.65	111.79	120.44
1	G	74	TYR	C-N-CA	-6.65	111.79	120.44
1	H	288	GLN	N-CA-C	-6.65	98.96	109.07
1	D	89	LEU	N-CA-C	6.65	120.66	109.76
1	D	74	TYR	CA-C-N	-6.62	111.83	120.44
1	D	74	TYR	C-N-CA	-6.62	111.83	120.44
1	H	74	TYR	CA-C-N	-6.62	111.83	120.44
1	H	74	TYR	C-N-CA	-6.62	111.83	120.44
1	D	129	ARG	CB-CA-C	-6.62	99.15	109.80
1	E	74	TYR	CA-C-N	-6.60	111.86	120.44
1	E	74	TYR	C-N-CA	-6.60	111.86	120.44
1	C	18	CYS	N-CA-CB	-6.59	100.18	110.06
1	F	18	CYS	N-CA-CB	-6.58	100.19	110.06
1	D	18	CYS	N-CA-CB	-6.57	100.21	110.06
1	A	18	CYS	N-CA-CB	-6.57	100.21	110.06
1	B	18	CYS	N-CA-CB	-6.56	100.22	110.06
1	G	18	CYS	N-CA-CB	-6.54	100.24	110.06
1	E	18	CYS	N-CA-CB	-6.54	100.25	110.06
1	H	18	CYS	N-CA-CB	-6.54	100.26	110.06
1	A	177	VAL	CA-CB-CG2	-6.53	99.29	110.40
1	E	89	LEU	CB-CA-C	-6.48	98.60	109.48
1	C	89	LEU	CB-CA-C	-6.48	98.60	109.48
1	A	89	LEU	CB-CA-C	-6.47	98.61	109.48
1	H	89	LEU	CB-CA-C	-6.46	98.62	109.48
1	C	149	THR	N-CA-C	6.46	117.98	111.07
1	G	288	GLN	O-C-N	6.45	130.62	123.33
1	A	149	THR	N-CA-C	6.45	117.97	111.07
1	B	89	LEU	CB-CA-C	-6.45	98.65	109.48
1	G	89	LEU	CB-CA-C	-6.45	98.65	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	LEU	CB-CA-C	-6.44	98.66	109.48
1	G	149	THR	N-CA-C	6.44	117.96	111.07
1	G	168	GLU	N-CA-C	-6.44	104.18	111.07
1	F	89	LEU	CB-CA-C	-6.44	98.67	109.48
1	B	149	THR	N-CA-C	6.43	117.95	111.07
1	E	149	THR	N-CA-C	6.43	117.95	111.07
1	F	149	THR	N-CA-C	6.42	117.94	111.07
1	D	61	ASN	N-CA-C	-6.42	97.83	108.23
1	H	149	THR	N-CA-C	6.40	117.92	111.07
1	B	167	PHE	CA-C-O	6.40	127.34	119.79
1	C	159	PHE	CB-CA-C	-6.39	97.02	109.68
1	C	269	THR	OG1-CB-CG2	-6.39	96.53	109.30
1	D	149	THR	N-CA-C	6.38	117.90	111.07
1	C	126	PRO	CA-C-N	-6.33	110.15	120.72
1	C	126	PRO	C-N-CA	-6.33	110.15	120.72
1	C	166	SER	CA-C-N	-6.31	110.18	120.72
1	C	166	SER	C-N-CA	-6.31	110.18	120.72
1	F	128	TYR	CA-CB-CG	-6.30	102.55	113.90
1	H	128	TYR	CA-CB-CG	-6.30	102.56	113.90
1	A	267	GLU	CA-C-N	6.30	126.77	119.47
1	A	267	GLU	C-N-CA	6.30	126.77	119.47
1	C	125	PHE	CB-CA-C	-6.26	100.82	111.15
1	D	128	TYR	CB-CA-C	6.26	122.87	110.42
1	B	266	LEU	CB-CG-CD1	-6.25	91.93	110.70
1	D	58	GLU	CA-C-N	6.23	126.19	120.21
1	D	58	GLU	C-N-CA	6.23	126.19	120.21
1	H	162	ARG	CA-C-N	-6.19	113.46	122.19
1	H	162	ARG	C-N-CA	-6.19	113.46	122.19
1	E	159	PHE	N-CA-C	6.19	119.78	109.95
1	C	128	TYR	CA-CB-CG	-6.18	102.77	113.90
1	F	125	PHE	C-N-CD	-6.18	99.66	125.00
1	B	59	PRO	N-CA-C	6.16	121.96	111.68
1	B	179	ILE	CB-CA-C	6.15	119.74	111.19
1	B	95	TYR	N-CA-C	6.13	119.65	110.14
1	C	95	TYR	N-CA-C	6.13	119.64	110.14
1	H	162	ARG	CG-CD-NE	-6.13	98.51	112.00
1	D	95	TYR	N-CA-C	6.13	119.64	110.14
1	G	95	TYR	N-CA-C	6.12	119.63	110.14
1	A	61	ASN	N-CA-C	-6.12	97.52	108.47
1	G	125	PHE	CA-C-O	6.12	125.79	119.49
1	A	95	TYR	N-CA-C	6.11	119.62	110.14
1	F	95	TYR	N-CA-C	6.11	119.61	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	254	GLN	CA-CB-CG	6.11	126.32	114.10
1	H	95	TYR	N-CA-C	6.11	119.60	110.14
1	E	95	TYR	N-CA-C	6.10	119.60	110.14
1	E	270	LEU	N-CA-C	-6.02	105.64	112.87
1	H	37	ASP	N-CA-C	-6.02	105.43	112.89
1	E	37	ASP	N-CA-C	-6.01	105.44	112.89
1	B	37	ASP	N-CA-C	-5.99	105.46	112.89
1	D	37	ASP	N-CA-C	-5.99	105.46	112.89
1	A	37	ASP	N-CA-C	-5.98	105.47	112.89
1	H	166	SER	N-CA-C	5.98	118.21	108.76
1	F	37	ASP	N-CA-C	-5.98	105.48	112.89
1	G	37	ASP	N-CA-C	-5.97	105.48	112.89
1	H	275	ILE	CB-CA-C	-5.96	102.45	111.33
1	D	275	ILE	CB-CA-C	-5.95	102.46	111.33
1	F	170	VAL	O-C-N	5.95	127.65	121.87
1	E	275	ILE	CB-CA-C	-5.95	102.47	111.33
1	A	275	ILE	CB-CA-C	-5.95	102.47	111.33
1	G	275	ILE	CB-CA-C	-5.95	102.47	111.33
1	B	275	ILE	CB-CA-C	-5.95	102.47	111.33
1	D	9	GLY	N-CA-C	-5.95	102.86	112.31
1	B	266	LEU	CB-CG-CD2	5.94	128.53	110.70
1	C	37	ASP	N-CA-C	-5.94	105.52	112.89
1	C	161	LEU	CB-CG-CD1	5.94	128.53	110.70
1	C	275	ILE	CB-CA-C	-5.94	102.48	111.33
1	B	155	ARG	N-CA-C	-5.93	106.00	113.18
1	D	155	ARG	N-CA-C	-5.93	106.00	113.18
1	B	208	PRO	CA-C-N	-5.93	110.02	121.58
1	B	208	PRO	C-N-CA	-5.93	110.02	121.58
1	D	208	PRO	CA-C-N	-5.93	110.02	121.58
1	D	208	PRO	C-N-CA	-5.93	110.02	121.58
1	G	9	GLY	N-CA-C	-5.92	102.89	112.31
1	G	173	GLY	N-CA-C	5.92	121.31	113.37
1	H	9	GLY	N-CA-C	-5.92	102.89	112.31
1	E	58	GLU	CA-C-N	5.92	125.83	119.85
1	E	58	GLU	C-N-CA	5.92	125.83	119.85
1	F	9	GLY	N-CA-C	-5.92	102.89	112.31
1	G	208	PRO	CA-C-N	-5.92	110.03	121.58
1	G	208	PRO	C-N-CA	-5.92	110.03	121.58
1	A	208	PRO	CA-C-N	-5.92	110.04	121.58
1	A	208	PRO	C-N-CA	-5.92	110.04	121.58
1	C	208	PRO	CA-C-N	-5.92	110.04	121.58
1	C	208	PRO	C-N-CA	-5.92	110.04	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	208	PRO	CA-C-N	-5.92	110.04	121.58
1	F	208	PRO	C-N-CA	-5.92	110.04	121.58
1	C	9	GLY	N-CA-C	-5.92	102.90	112.31
1	C	275	ILE	CA-C-N	-5.92	114.71	122.16
1	C	275	ILE	C-N-CA	-5.92	114.71	122.16
1	F	275	ILE	CB-CA-C	-5.92	102.52	111.33
1	G	155	ARG	N-CA-C	-5.92	106.02	113.18
1	A	155	ARG	N-CA-C	-5.91	106.03	113.18
1	B	267	GLU	CA-C-N	5.91	125.62	119.82
1	B	267	GLU	C-N-CA	5.91	125.62	119.82
1	E	82	PRO	CB-CA-C	-5.91	103.48	112.11
1	E	155	ARG	N-CA-C	-5.91	106.02	113.18
1	A	9	GLY	N-CA-C	-5.91	102.91	112.31
1	H	208	PRO	CA-C-N	-5.91	110.05	121.58
1	H	208	PRO	C-N-CA	-5.91	110.05	121.58
1	E	9	GLY	N-CA-C	-5.91	102.92	112.31
1	F	82	PRO	CB-CA-C	-5.90	103.49	112.11
1	H	82	PRO	CB-CA-C	-5.90	103.49	112.11
1	G	275	ILE	CA-C-N	-5.90	114.72	122.16
1	G	275	ILE	C-N-CA	-5.90	114.72	122.16
1	E	208	PRO	CA-C-N	-5.90	110.08	121.58
1	E	208	PRO	C-N-CA	-5.90	110.08	121.58
1	E	171	ALA	O-C-N	5.90	128.87	122.15
1	G	82	PRO	CB-CA-C	-5.90	103.50	112.11
1	A	82	PRO	CB-CA-C	-5.89	103.50	112.11
1	H	130	TYR	N-CA-CB	-5.89	102.60	111.56
1	B	82	PRO	CB-CA-C	-5.89	103.51	112.11
1	H	155	ARG	N-CA-C	-5.89	106.06	113.18
1	B	275	ILE	CA-C-N	-5.88	114.75	122.16
1	B	275	ILE	C-N-CA	-5.88	114.75	122.16
1	H	266	LEU	CA-C-N	5.88	129.66	122.42
1	H	266	LEU	C-N-CA	5.88	129.66	122.42
1	D	82	PRO	CB-CA-C	-5.88	103.52	112.11
1	B	9	GLY	N-CA-C	-5.88	102.96	112.31
1	A	275	ILE	CA-C-N	-5.88	114.75	122.16
1	A	275	ILE	C-N-CA	-5.88	114.75	122.16
1	F	155	ARG	N-CA-C	-5.88	106.07	113.18
1	C	82	PRO	CB-CA-C	-5.88	103.53	112.11
1	C	155	ARG	N-CA-C	-5.88	106.07	113.18
1	F	275	ILE	CA-C-N	-5.88	114.76	122.16
1	F	275	ILE	C-N-CA	-5.88	114.76	122.16
1	A	268	PRO	N-CD-CG	-5.88	94.39	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	275	ILE	CA-C-N	-5.87	114.76	122.16
1	H	275	ILE	C-N-CA	-5.87	114.76	122.16
1	C	254	GLN	CA-C-O	5.87	127.53	121.07
1	D	275	ILE	CA-C-N	-5.87	114.77	122.16
1	D	275	ILE	C-N-CA	-5.87	114.77	122.16
1	E	275	ILE	CA-C-N	-5.85	114.79	122.16
1	E	275	ILE	C-N-CA	-5.85	114.79	122.16
1	G	180	ASN	N-CA-C	5.83	117.80	108.41
1	B	157	VAL	CB-CA-C	-5.83	103.57	111.15
1	H	179	ILE	O-C-N	5.82	128.68	123.03
1	B	13	LEU	N-CA-C	5.81	117.29	111.07
1	D	63	GLN	CB-CA-C	-5.81	101.72	110.90
1	C	13	LEU	N-CA-C	5.81	117.28	111.07
1	B	160	PHE	CB-CA-C	-5.80	99.41	109.86
1	E	13	LEU	N-CA-C	5.80	117.28	111.07
1	A	13	LEU	N-CA-C	5.79	117.27	111.07
1	C	177	VAL	CB-CA-C	-5.79	100.34	110.71
1	B	65	ALA	CB-CA-C	-5.79	101.13	110.74
1	H	13	LEU	N-CA-C	5.79	117.26	111.07
1	D	13	LEU	N-CA-C	5.78	117.25	111.07
1	G	13	LEU	N-CA-C	5.77	117.24	111.07
1	D	173	GLY	CA-C-N	-5.76	115.30	123.08
1	D	173	GLY	C-N-CA	-5.76	115.30	123.08
1	F	13	LEU	N-CA-C	5.76	117.24	111.07
1	G	158	LYS	N-CA-C	5.76	119.35	110.42
1	G	32	VAL	N-CA-C	5.76	116.88	108.53
1	H	32	VAL	N-CA-C	5.76	116.88	108.53
1	D	32	VAL	N-CA-C	5.75	116.87	108.53
1	D	157	VAL	CB-CA-C	-5.74	103.69	111.15
1	C	32	VAL	N-CA-C	5.74	116.85	108.53
1	A	32	VAL	N-CA-C	5.74	116.84	108.53
1	F	85	ALA	N-CA-C	-5.73	105.78	112.89
1	E	32	VAL	N-CA-C	5.72	116.82	108.53
1	B	32	VAL	N-CA-C	5.71	116.82	108.53
1	B	85	ALA	N-CA-C	-5.71	105.81	112.89
1	F	32	VAL	N-CA-C	5.70	116.80	108.53
1	E	126	PRO	N-CA-C	5.70	122.07	113.81
1	A	85	ALA	N-CA-C	-5.70	105.83	112.89
1	G	85	ALA	N-CA-C	-5.70	105.83	112.89
1	E	269	THR	N-CA-CB	5.69	119.84	110.39
1	D	85	ALA	N-CA-C	-5.68	105.85	112.89
1	D	127	ASP	CA-C-O	5.67	126.54	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	85	ALA	N-CA-C	-5.67	105.85	112.89
1	C	85	ALA	N-CA-C	-5.67	105.86	112.89
1	A	267	GLU	N-CA-CB	-5.66	103.22	111.20
1	H	85	ALA	N-CA-C	-5.66	105.87	112.89
1	C	125	PHE	CA-C-N	5.64	125.31	119.56
1	C	125	PHE	C-N-CA	5.64	125.31	119.56
1	C	62	PRO	CB-CA-C	-5.63	103.46	111.68
1	C	64	GLU	N-CA-C	-5.63	104.84	110.97
1	A	288	GLN	O-C-N	-5.62	117.41	123.42
1	A	164	VAL	N-CA-C	-5.59	101.61	109.21
1	B	209	TRP	CA-C-N	-5.59	114.76	122.30
1	B	209	TRP	C-N-CA	-5.59	114.76	122.30
1	H	135	THR	CB-CA-C	5.58	119.58	109.37
1	E	209	TRP	CA-C-N	-5.58	114.77	122.30
1	E	209	TRP	C-N-CA	-5.58	114.77	122.30
1	D	135	THR	CB-CA-C	5.58	119.57	109.37
1	B	162	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	A	209	TRP	CA-C-N	-5.57	114.78	122.30
1	A	209	TRP	C-N-CA	-5.57	114.78	122.30
1	H	209	TRP	CA-C-N	-5.57	114.78	122.30
1	H	209	TRP	C-N-CA	-5.57	114.78	122.30
1	G	209	TRP	CA-C-N	-5.56	114.79	122.30
1	G	209	TRP	C-N-CA	-5.56	114.79	122.30
1	C	135	THR	CB-CA-C	5.56	119.54	109.37
1	D	209	TRP	CA-C-N	-5.56	114.79	122.30
1	D	209	TRP	C-N-CA	-5.56	114.79	122.30
1	A	135	THR	CB-CA-C	5.56	119.54	109.37
1	E	135	THR	CB-CA-C	5.55	119.53	109.37
1	E	120	ARG	CB-CA-C	-5.55	101.25	110.68
1	G	135	THR	CB-CA-C	5.55	119.52	109.37
1	E	129	ARG	N-CA-C	-5.54	105.29	113.61
1	F	135	THR	CB-CA-C	5.54	119.51	109.37
1	B	135	THR	CB-CA-C	5.54	119.50	109.37
1	D	164	VAL	O-C-N	5.54	129.26	122.95
1	B	120	ARG	CB-CA-C	-5.53	101.28	110.68
1	C	120	ARG	CB-CA-C	-5.53	101.28	110.68
1	D	120	ARG	CB-CA-C	-5.53	101.28	110.68
1	D	179	ILE	CA-CB-CG1	-5.53	101.00	110.40
1	F	120	ARG	CB-CA-C	-5.53	101.28	110.68
1	G	166	SER	N-CA-CB	-5.53	101.72	111.39
1	A	120	ARG	CB-CA-C	-5.53	101.28	110.68
1	E	64	GLU	CA-C-N	-5.53	111.91	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	64	GLU	C-N-CA	-5.53	111.91	120.31
1	G	1	MET	CA-CB-CG	-5.52	103.07	114.10
1	C	166	SER	CB-CA-C	-5.51	101.11	109.99
1	F	209	TRP	CA-C-N	-5.51	114.86	122.30
1	F	209	TRP	C-N-CA	-5.51	114.86	122.30
1	H	120	ARG	CB-CA-C	-5.51	101.31	110.68
1	B	1	MET	CA-CB-CG	-5.51	103.08	114.10
1	E	1	MET	CA-CB-CG	-5.51	103.08	114.10
1	D	1	MET	CA-CB-CG	-5.51	103.08	114.10
1	F	1	MET	CA-CB-CG	-5.51	103.08	114.10
1	G	120	ARG	CB-CA-C	-5.51	101.32	110.68
1	A	1	MET	CA-CB-CG	-5.51	103.09	114.10
1	C	209	TRP	CA-C-N	-5.50	114.87	122.30
1	C	209	TRP	C-N-CA	-5.50	114.87	122.30
1	H	1	MET	CA-CB-CG	-5.50	103.09	114.10
1	C	1	MET	CA-CB-CG	-5.50	103.10	114.10
1	G	163	LYS	N-CA-C	-5.50	101.51	110.20
1	B	158	LYS	CA-C-N	-5.50	113.96	122.59
1	B	158	LYS	C-N-CA	-5.50	113.96	122.59
1	G	126	PRO	CA-C-N	-5.50	114.03	122.60
1	G	126	PRO	C-N-CA	-5.50	114.03	122.60
1	C	267	GLU	N-CA-CB	-5.49	104.29	111.09
1	D	289	VAL	CA-C-N	-5.48	115.48	122.77
1	D	289	VAL	C-N-CA	-5.48	115.48	122.77
1	A	289	VAL	CA-C-N	-5.47	115.49	122.77
1	A	289	VAL	C-N-CA	-5.47	115.49	122.77
1	H	159	PHE	N-CA-C	5.47	118.38	109.24
1	D	180	ASN	N-CA-C	5.47	117.15	108.67
1	B	289	VAL	CA-C-N	-5.47	115.50	122.77
1	B	289	VAL	C-N-CA	-5.47	115.50	122.77
1	C	289	VAL	CA-C-N	-5.47	115.50	122.77
1	C	289	VAL	C-N-CA	-5.47	115.50	122.77
1	C	194	LEU	CA-CB-CG	-5.46	97.19	116.30
1	H	194	LEU	CA-CB-CG	-5.46	97.19	116.30
1	A	148	LEU	CA-C-N	-5.46	113.34	120.44
1	A	148	LEU	C-N-CA	-5.46	113.34	120.44
1	E	194	LEU	CA-CB-CG	-5.46	97.20	116.30
1	E	289	VAL	CA-C-N	-5.46	115.51	122.77
1	E	289	VAL	C-N-CA	-5.46	115.51	122.77
1	C	110	MET	N-CA-C	-5.46	105.75	112.90
1	D	194	LEU	CA-CB-CG	-5.46	97.21	116.30
1	A	194	LEU	CA-CB-CG	-5.45	97.22	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	LEU	CA-CB-CG	-5.45	97.23	116.30
1	G	194	LEU	CA-CB-CG	-5.45	97.23	116.30
1	E	110	MET	N-CA-C	-5.45	105.76	112.90
1	B	110	MET	N-CA-C	-5.45	105.76	112.90
1	H	289	VAL	CA-C-N	-5.45	115.53	122.77
1	H	289	VAL	C-N-CA	-5.45	115.53	122.77
1	G	110	MET	N-CA-C	-5.45	105.77	112.90
1	G	289	VAL	CA-C-N	-5.45	115.53	122.77
1	G	289	VAL	C-N-CA	-5.45	115.53	122.77
1	A	110	MET	N-CA-C	-5.44	105.77	112.90
1	B	257	ASN	CA-C-N	-5.44	112.45	120.28
1	B	257	ASN	C-N-CA	-5.44	112.45	120.28
1	F	110	MET	N-CA-C	-5.44	105.77	112.90
1	H	110	MET	N-CA-C	-5.44	105.77	112.90
1	D	257	ASN	CA-C-N	-5.44	112.45	120.28
1	D	257	ASN	C-N-CA	-5.44	112.45	120.28
1	F	194	LEU	CA-CB-CG	-5.44	97.26	116.30
1	D	110	MET	N-CA-C	-5.44	105.78	112.90
1	B	148	LEU	CA-C-N	-5.43	113.38	120.44
1	B	148	LEU	C-N-CA	-5.43	113.38	120.44
1	C	148	LEU	CA-C-N	-5.43	113.38	120.44
1	C	148	LEU	C-N-CA	-5.43	113.38	120.44
1	E	74	TYR	N-CA-C	-5.43	105.26	111.07
1	C	230	ILE	O-C-N	5.43	125.91	120.59
1	F	148	LEU	CA-C-N	-5.43	113.38	120.44
1	F	148	LEU	C-N-CA	-5.43	113.38	120.44
1	C	174	GLY	CA-C-N	5.43	130.39	122.85
1	C	174	GLY	C-N-CA	5.43	130.39	122.85
1	E	148	LEU	CA-C-N	-5.42	113.39	120.44
1	E	148	LEU	C-N-CA	-5.42	113.39	120.44
1	A	257	ASN	CA-C-N	-5.42	112.47	120.28
1	A	257	ASN	C-N-CA	-5.42	112.47	120.28
1	E	257	ASN	CA-C-N	-5.42	112.47	120.28
1	E	257	ASN	C-N-CA	-5.42	112.47	120.28
1	F	289	VAL	CA-C-N	-5.42	115.56	122.77
1	F	289	VAL	C-N-CA	-5.42	115.56	122.77
1	G	148	LEU	CA-C-N	-5.42	113.39	120.44
1	G	148	LEU	C-N-CA	-5.42	113.39	120.44
1	G	170	VAL	N-CA-C	-5.42	106.41	111.45
1	E	162	ARG	N-CA-CB	-5.42	101.43	111.13
1	D	230	ILE	O-C-N	5.42	125.90	120.59
1	F	257	ASN	CA-C-N	-5.42	112.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	257	ASN	C-N-CA	-5.42	112.48	120.28
1	H	257	ASN	CA-C-N	-5.41	112.48	120.28
1	H	257	ASN	C-N-CA	-5.41	112.48	120.28
1	G	257	ASN	CA-C-N	-5.41	112.49	120.28
1	G	257	ASN	C-N-CA	-5.41	112.49	120.28
1	A	65	ALA	CA-C-N	-5.41	113.08	120.44
1	A	65	ALA	C-N-CA	-5.41	113.08	120.44
1	B	207	ALA	CA-C-N	5.41	125.08	119.56
1	B	207	ALA	C-N-CA	5.41	125.08	119.56
1	F	230	ILE	O-C-N	5.41	125.89	120.59
1	A	288	GLN	CA-C-O	5.41	127.02	121.23
1	B	230	ILE	O-C-N	5.41	125.89	120.59
1	A	74	TYR	N-CA-C	-5.40	105.29	111.07
1	D	148	LEU	CA-C-N	-5.40	113.42	120.44
1	D	148	LEU	C-N-CA	-5.40	113.42	120.44
1	C	257	ASN	CA-C-N	-5.40	112.51	120.28
1	C	257	ASN	C-N-CA	-5.40	112.51	120.28
1	H	207	ALA	CA-C-N	5.39	125.06	119.56
1	H	207	ALA	C-N-CA	5.39	125.06	119.56
1	H	148	LEU	CA-C-N	-5.39	113.43	120.44
1	H	148	LEU	C-N-CA	-5.39	113.43	120.44
1	D	74	TYR	N-CA-C	-5.39	105.30	111.07
1	F	74	TYR	N-CA-C	-5.39	105.31	111.07
1	H	74	TYR	N-CA-C	-5.39	105.31	111.07
1	C	58	GLU	CB-CA-C	5.38	117.94	109.27
1	C	74	TYR	N-CA-C	-5.38	105.31	111.07
1	F	207	ALA	CA-C-N	5.38	125.04	119.56
1	F	207	ALA	C-N-CA	5.38	125.04	119.56
1	G	74	TYR	N-CA-C	-5.38	105.32	111.07
1	C	207	ALA	CA-C-N	5.37	125.04	119.56
1	C	207	ALA	C-N-CA	5.37	125.04	119.56
1	E	230	ILE	O-C-N	5.37	125.86	120.59
1	A	230	ILE	O-C-N	5.37	125.85	120.59
1	A	268	PRO	CA-CB-CG	-5.37	94.30	104.50
1	F	61	ASN	CA-C-N	-5.37	113.50	119.19
1	F	61	ASN	C-N-CA	-5.37	113.50	119.19
1	F	176	ASP	CB-CA-C	5.37	119.81	110.79
1	C	23	TYR	CA-C-N	-5.36	113.33	120.79
1	C	23	TYR	C-N-CA	-5.36	113.33	120.79
1	B	74	TYR	N-CA-C	-5.36	105.33	111.07
1	H	230	ILE	O-C-N	5.36	125.84	120.59
1	G	230	ILE	O-C-N	5.36	125.84	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	169	GLU	N-CA-CB	-5.35	102.04	110.06
1	D	1	MET	CB-CG-SD	-5.35	96.66	112.70
1	F	1	MET	CB-CG-SD	-5.35	96.66	112.70
1	H	166	SER	CB-CA-C	-5.35	100.38	110.16
1	E	56	THR	OG1-CB-CG2	-5.34	98.61	109.30
1	F	95	TYR	N-CA-CB	-5.34	102.62	110.85
1	B	95	TYR	N-CA-CB	-5.34	102.62	110.85
1	F	23	TYR	CA-C-N	-5.34	113.37	120.79
1	F	23	TYR	C-N-CA	-5.34	113.37	120.79
1	G	1	MET	CB-CG-SD	-5.34	96.68	112.70
1	F	261	GLU	CA-C-N	-5.34	114.13	120.00
1	F	261	GLU	C-N-CA	-5.34	114.13	120.00
1	G	261	GLU	CA-C-N	-5.34	114.13	120.00
1	G	261	GLU	C-N-CA	-5.34	114.13	120.00
1	H	95	TYR	N-CA-CB	-5.34	102.63	110.85
1	A	207	ALA	CA-C-N	5.34	125.00	119.56
1	A	207	ALA	C-N-CA	5.34	125.00	119.56
1	B	1	MET	CB-CG-SD	-5.34	96.69	112.70
1	E	1	MET	CB-CG-SD	-5.34	96.69	112.70
1	G	95	TYR	N-CA-CB	-5.33	102.64	110.85
1	B	221	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	E	95	TYR	N-CA-CB	-5.33	102.64	110.85
1	C	1	MET	CB-CG-SD	-5.33	96.70	112.70
1	D	95	TYR	N-CA-CB	-5.33	102.64	110.85
1	A	1	MET	CB-CG-SD	-5.33	96.71	112.70
1	B	261	GLU	CA-C-N	-5.33	114.14	120.00
1	B	261	GLU	C-N-CA	-5.33	114.14	120.00
1	B	23	TYR	CA-C-N	-5.33	113.38	120.79
1	B	23	TYR	C-N-CA	-5.33	113.38	120.79
1	C	261	GLU	CA-C-N	-5.33	114.14	120.00
1	C	261	GLU	C-N-CA	-5.33	114.14	120.00
1	E	207	ALA	CA-C-N	5.33	124.99	119.56
1	E	207	ALA	C-N-CA	5.33	124.99	119.56
1	D	207	ALA	CA-C-N	5.33	124.99	119.56
1	D	207	ALA	C-N-CA	5.33	124.99	119.56
1	E	23	TYR	CA-C-N	-5.33	113.39	120.79
1	E	23	TYR	C-N-CA	-5.33	113.39	120.79
1	H	1	MET	CB-CG-SD	-5.33	96.72	112.70
1	H	261	GLU	CA-C-N	-5.33	114.14	120.00
1	H	261	GLU	C-N-CA	-5.33	114.14	120.00
1	D	23	TYR	CA-C-N	-5.32	113.39	120.79
1	D	23	TYR	C-N-CA	-5.32	113.39	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	207	ALA	CA-C-N	5.32	124.99	119.56
1	G	207	ALA	C-N-CA	5.32	124.99	119.56
1	E	337	ARG	N-CA-C	-5.32	106.76	113.20
1	A	95	TYR	N-CA-CB	-5.32	102.66	110.85
1	A	23	TYR	CA-C-N	-5.32	113.40	120.79
1	A	23	TYR	C-N-CA	-5.32	113.40	120.79
1	E	221	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	F	161	LEU	N-CA-C	-5.31	100.51	108.96
1	C	95	TYR	N-CA-CB	-5.31	102.67	110.85
1	G	23	TYR	CA-C-N	-5.31	113.41	120.79
1	G	23	TYR	C-N-CA	-5.31	113.41	120.79
1	D	261	GLU	CA-C-N	-5.30	114.17	120.00
1	D	261	GLU	C-N-CA	-5.30	114.17	120.00
1	A	261	GLU	CA-C-N	-5.30	114.17	120.00
1	A	261	GLU	C-N-CA	-5.30	114.17	120.00
1	D	337	ARG	N-CA-C	-5.30	106.79	113.20
1	H	23	TYR	CA-C-N	-5.30	113.43	120.79
1	H	23	TYR	C-N-CA	-5.30	113.43	120.79
1	G	337	ARG	N-CA-C	-5.29	106.80	113.20
1	B	337	ARG	N-CA-C	-5.29	106.80	113.20
1	E	261	GLU	CA-C-N	-5.29	114.18	120.00
1	E	261	GLU	C-N-CA	-5.29	114.18	120.00
1	F	158	LYS	N-CA-C	5.29	118.69	110.17
1	G	221	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	337	ARG	N-CA-C	-5.29	106.80	113.20
1	H	337	ARG	N-CA-C	-5.28	106.81	113.20
1	F	221	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	221	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	F	337	ARG	N-CA-C	-5.28	106.82	113.20
1	G	236	VAL	CB-CA-C	-5.27	102.80	110.81
1	B	10	VAL	CB-CA-C	-5.27	105.02	112.14
1	D	179	ILE	N-CA-C	5.27	114.89	106.88
1	B	236	VAL	CB-CA-C	-5.27	102.80	110.81
1	D	221	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	E	179	ILE	CA-C-N	-5.26	115.42	122.42
1	E	179	ILE	C-N-CA	-5.26	115.42	122.42
1	F	10	VAL	CB-CA-C	-5.26	105.03	112.14
1	G	158	LYS	CA-C-N	-5.26	113.49	122.33
1	G	158	LYS	C-N-CA	-5.26	113.49	122.33
1	E	10	VAL	CB-CA-C	-5.26	105.04	112.14
1	C	337	ARG	N-CA-C	-5.26	106.84	113.20
1	E	125	PHE	CA-C-N	5.26	125.57	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	PHE	C-N-CA	5.26	125.57	119.47
1	H	221	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	D	236	VAL	CB-CA-C	-5.26	102.82	110.81
1	A	236	VAL	CB-CA-C	-5.25	102.82	110.81
1	E	236	VAL	CB-CA-C	-5.25	102.82	110.81
1	A	270	LEU	CB-CG-CD1	-5.25	94.94	110.70
1	C	56	THR	N-CA-C	5.25	117.08	111.36
1	F	236	VAL	CB-CA-C	-5.25	102.83	110.81
1	G	10	VAL	CB-CA-C	-5.25	105.05	112.14
1	F	58	GLU	CA-C-N	5.25	125.16	119.85
1	F	58	GLU	C-N-CA	5.25	125.16	119.85
1	A	10	VAL	CB-CA-C	-5.25	105.05	112.14
1	E	180	ASN	N-CA-C	5.25	116.86	108.41
1	A	158	LYS	N-CA-C	5.25	118.37	109.76
1	H	236	VAL	CB-CA-C	-5.24	102.84	110.81
1	H	254	GLN	CA-C-N	5.24	127.26	120.44
1	H	254	GLN	C-N-CA	5.24	127.26	120.44
1	C	221	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	H	10	VAL	CB-CA-C	-5.24	105.07	112.14
1	C	236	VAL	CB-CA-C	-5.24	102.85	110.81
1	C	10	VAL	CB-CA-C	-5.23	105.08	112.14
1	D	10	VAL	CB-CA-C	-5.22	105.09	112.14
1	F	127	ASP	N-CA-CB	5.22	118.16	110.33
1	B	64	GLU	CA-CB-CG	-5.21	103.67	114.10
1	A	161	LEU	CA-CB-CG	-5.21	98.07	116.30
1	D	23	TYR	CB-CA-C	-5.20	100.81	109.75
1	C	60	SER	N-CA-C	-5.20	104.54	111.24
1	F	24	HIS	CA-CB-CG	-5.20	108.60	113.80
1	F	63	GLN	CB-CA-C	-5.20	99.36	110.32
1	F	270	LEU	O-C-N	5.20	129.34	122.43
1	C	23	TYR	CB-CA-C	-5.19	100.82	109.75
1	D	235	ALA	N-CA-C	5.19	117.23	110.53
1	G	23	TYR	CB-CA-C	-5.19	100.82	109.75
1	F	23	TYR	CB-CA-C	-5.19	100.83	109.75
1	B	23	TYR	CB-CA-C	-5.18	100.83	109.75
1	C	171	ALA	N-CA-C	5.18	116.62	110.97
1	E	23	TYR	CB-CA-C	-5.18	100.84	109.75
1	A	23	TYR	CB-CA-C	-5.18	100.84	109.75
1	H	23	TYR	CB-CA-C	-5.18	100.84	109.75
1	A	24	HIS	CA-CB-CG	-5.17	108.63	113.80
1	G	235	ALA	N-CA-C	5.17	117.20	110.53
1	G	24	HIS	CA-CB-CG	-5.17	108.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	177	VAL	N-CA-C	5.17	116.09	108.45
1	B	235	ALA	N-CA-C	5.16	117.19	110.53
1	C	24	HIS	CA-CB-CG	-5.16	108.64	113.80
1	C	235	ALA	N-CA-C	5.16	117.19	110.53
1	H	170	VAL	O-C-N	5.16	126.96	121.91
1	B	159	PHE	CB-CA-C	-5.16	99.22	109.79
1	A	235	ALA	N-CA-C	5.15	117.17	110.53
1	E	235	ALA	N-CA-C	5.15	117.17	110.53
1	G	268	PRO	CA-C-N	-5.15	112.36	120.60
1	G	268	PRO	C-N-CA	-5.15	112.36	120.60
1	D	24	HIS	CA-CB-CG	-5.15	108.65	113.80
1	B	177	VAL	CA-C-N	-5.14	115.96	123.06
1	B	177	VAL	C-N-CA	-5.14	115.96	123.06
1	B	24	HIS	CA-CB-CG	-5.14	108.66	113.80
1	H	235	ALA	N-CA-C	5.14	117.16	110.53
1	F	235	ALA	N-CA-C	5.13	117.15	110.53
1	G	249	GLU	N-CA-CB	5.13	118.06	110.56
1	D	1	MET	CA-C-N	-5.13	115.60	122.42
1	D	1	MET	C-N-CA	-5.13	115.60	122.42
1	E	24	HIS	CA-CB-CG	-5.13	108.67	113.80
1	A	249	GLU	N-CA-CB	5.12	118.04	110.56
1	B	249	GLU	N-CA-CB	5.12	118.04	110.56
1	C	1	MET	CA-C-N	-5.12	115.61	122.42
1	C	1	MET	C-N-CA	-5.12	115.61	122.42
1	H	24	HIS	CA-CB-CG	-5.12	108.68	113.80
1	C	249	GLU	N-CA-CB	5.11	118.03	110.56
1	G	160	PHE	CA-CB-CG	-5.11	108.69	113.80
1	H	1	MET	CA-C-N	-5.11	115.62	122.42
1	H	1	MET	C-N-CA	-5.11	115.62	122.42
1	F	1	MET	CA-C-N	-5.11	115.63	122.42
1	F	1	MET	C-N-CA	-5.11	115.63	122.42
1	A	1	MET	CA-C-N	-5.11	115.63	122.42
1	A	1	MET	C-N-CA	-5.11	115.63	122.42
1	D	249	GLU	N-CA-CB	5.10	118.01	110.56
1	H	249	GLU	N-CA-CB	5.10	118.01	110.56
1	E	249	GLU	N-CA-CB	5.10	118.00	110.56
1	F	249	GLU	N-CA-CB	5.10	118.00	110.56
1	F	179	ILE	CA-C-O	-5.09	115.12	120.57
1	B	166	SER	CA-C-N	-5.09	112.02	120.68
1	B	166	SER	C-N-CA	-5.09	112.02	120.68
1	E	1	MET	CA-C-N	-5.09	115.65	122.42
1	E	1	MET	C-N-CA	-5.09	115.65	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	GLU	CB-CA-C	-5.08	102.30	110.74
1	G	1	MET	CA-C-N	-5.08	115.66	122.42
1	G	1	MET	C-N-CA	-5.08	115.66	122.42
1	C	179	ILE	CB-CG1-CD1	5.08	124.47	113.80
1	B	121	GLU	CG-CD-OE1	-5.08	106.72	118.40
1	B	1	MET	CA-C-N	-5.08	115.67	122.42
1	B	1	MET	C-N-CA	-5.08	115.67	122.42
1	D	121	GLU	CG-CD-OE1	-5.07	106.74	118.40
1	E	121	GLU	CG-CD-OE1	-5.07	106.74	118.40
1	F	102	VAL	N-CA-CB	-5.07	104.11	111.21
1	F	163	LYS	CA-C-N	-5.07	114.66	121.66
1	F	163	LYS	C-N-CA	-5.07	114.66	121.66
1	A	121	GLU	CG-CD-OE1	-5.07	106.74	118.40
1	C	121	GLU	CG-CD-OE1	-5.07	106.74	118.40
1	B	102	VAL	N-CA-CB	-5.06	104.13	111.21
1	C	102	VAL	N-CA-CB	-5.06	104.13	111.21
1	F	121	GLU	CG-CD-OE1	-5.06	106.76	118.40
1	H	121	GLU	CG-CD-OE1	-5.06	106.76	118.40
1	C	163	LYS	N-CA-C	-5.06	99.55	108.20
1	G	121	GLU	CG-CD-OE1	-5.05	106.78	118.40
1	D	102	VAL	N-CA-CB	-5.05	104.14	111.21
1	H	123	ASP	N-CA-C	-5.05	106.38	112.54
1	A	102	VAL	N-CA-CB	-5.05	104.15	111.21
1	D	64	GLU	N-CA-C	-5.04	106.23	112.38
1	E	102	VAL	N-CA-CB	-5.04	104.15	111.21
1	H	102	VAL	N-CA-CB	-5.04	104.15	111.21
1	A	130	TYR	N-CA-CB	-5.04	102.57	111.39
1	G	102	VAL	N-CA-CB	-5.04	104.16	111.21
1	F	123	ASP	N-CA-C	-5.03	106.41	112.54
1	B	123	ASP	N-CA-C	-5.03	106.41	112.54
1	A	123	ASP	N-CA-C	-5.02	106.41	112.54
1	A	265	ARG	CB-CA-C	-5.02	101.51	110.70
1	H	87	MET	N-CA-C	-5.02	107.10	113.18
1	C	161	LEU	CB-CA-C	5.01	119.82	111.30
1	C	123	ASP	N-CA-C	-5.01	106.42	112.54
1	F	173	GLY	N-CA-C	-5.01	106.69	112.50
1	F	87	MET	N-CA-C	-5.01	107.12	113.18
1	D	123	ASP	N-CA-C	-5.01	106.43	112.54
1	F	176	ASP	CA-C-N	-5.01	115.81	122.77
1	F	176	ASP	C-N-CA	-5.01	115.81	122.77
1	B	87	MET	N-CA-C	-5.00	107.12	113.18
1	A	196	GLN	O-C-N	5.00	125.30	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	265	ARG	N-CA-C	-5.00	105.54	111.69
1	H	319	HIS	N-CA-C	5.00	117.11	111.11
1	D	87	MET	N-CA-C	-5.00	107.13	113.18
1	E	123	ASP	N-CA-C	-5.00	106.44	112.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	PHE	Sidechain
1	C	125	PHE	Sidechain
1	G	160	PHE	Sidechain

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	2720	0	2675	238	0
1	B	2720	0	2675	232	0
1	C	2720	0	2675	229	3
1	D	2720	0	2675	223	1
1	E	2720	0	2675	250	1
1	F	2720	0	2675	222	1
1	G	2720	0	2675	238	1
1	H	2720	0	2675	222	3
2	A	58	0	38	6	0
2	B	58	0	38	7	0
2	C	58	0	38	5	0
2	D	58	0	38	6	0
2	E	58	0	38	7	0
2	F	58	0	38	7	0
2	G	58	0	38	6	0
2	H	58	0	38	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	1	0
3	H	1	0	0	0	0
All	All	22232	0	21704	1803	5

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 43.

All (1803) 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)
1:E:61:ASN:ND2	1:E:63:GLN:HG3	1.11	1.38
1:E:61:ASN:ND2	1:E:63:GLN:CG	1.89	1.35
1:E:61:ASN:HD21	1:E:63:GLN:NE2	1.40	1.19
1:A:253:ILE:HG13	1:F:42:PHE:CD1	1.88	1.08
1:G:78:HIS:CD2	1:G:87:MET:HE1	1.92	1.05
1:C:78:HIS:CD2	1:C:87:MET:HE1	1.92	1.05
1:D:78:HIS:CD2	1:D:87:MET:HE1	1.92	1.05
1:H:78:HIS:CD2	1:H:87:MET:HE1	1.92	1.05
1:A:78:HIS:CD2	1:A:87:MET:HE1	1.92	1.04
1:B:78:HIS:CD2	1:B:87:MET:HE1	1.92	1.04
1:E:78:HIS:CD2	1:E:87:MET:HE1	1.92	1.04
1:B:250:ILE:HD11	1:E:250:ILE:CD1	1.88	1.04
1:F:1:MET:CE	1:F:177:VAL:HG23	1.90	1.02
1:F:78:HIS:CD2	1:F:87:MET:HE1	1.92	1.02
1:E:61:ASN:ND2	1:E:63:GLN:HE21	1.56	1.02
1:B:23:TYR:HD1	1:B:26:VAL:HG11	1.26	1.01
1:A:23:TYR:HD1	1:A:26:VAL:HG11	1.25	1.00
1:C:23:TYR:HD1	1:C:26:VAL:HG11	1.25	1.00
1:H:23:TYR:HD1	1:H:26:VAL:HG11	1.25	1.00
1:B:253:ILE:HG13	1:E:42:PHE:CD1	1.96	0.99
1:G:23:TYR:HD1	1:G:26:VAL:HG11	1.25	0.98
1:D:23:TYR:HD1	1:D:26:VAL:HG11	1.25	0.97
1:E:23:TYR:HD1	1:E:26:VAL:HG11	1.26	0.97
1:F:23:TYR:HD1	1:F:26:VAL:HG11	1.26	0.97
1:E:61:ASN:HD21	1:E:63:GLN:CD	1.71	0.97
1:G:53:GLN:HG2	3:G:349:HOH:O	1.65	0.96
1:C:101:ALA:HA	1:C:130:TYR:CD2	1.99	0.96
1:B:250:ILE:HD11	1:E:250:ILE:HD11	1.48	0.94
1:F:61:ASN:OD1	1:F:63:GLN:HG3	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:HIS:ND1	1:F:278:GLU:OE2	2.01	0.93
1:G:167:PHE:CE1	1:G:189:LEU:HB3	2.02	0.93
1:E:256:HIS:ND1	1:E:278:GLU:OE2	2.01	0.93
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.34	0.93
1:A:142:ARG:HH11	1:A:142:ARG:HG3	1.34	0.93
1:C:256:HIS:ND1	1:C:278:GLU:OE2	2.02	0.93
1:F:1:MET:HE2	1:F:177:VAL:HG23	1.47	0.93
1:B:256:HIS:ND1	1:B:278:GLU:OE2	2.02	0.93
1:D:142:ARG:HH11	1:D:142:ARG:HG3	1.34	0.93
1:G:142:ARG:HH11	1:G:142:ARG:HG3	1.34	0.93
1:A:256:HIS:ND1	1:A:278:GLU:OE2	2.01	0.93
1:G:256:HIS:ND1	1:G:278:GLU:OE2	2.01	0.92
1:H:256:HIS:ND1	1:H:278:GLU:OE2	2.01	0.92
1:E:61:ASN:CG	1:E:63:GLN:CG	2.42	0.92
1:F:142:ARG:HG3	1:F:142:ARG:HH11	1.34	0.92
1:D:256:HIS:ND1	1:D:278:GLU:OE2	2.02	0.91
1:H:142:ARG:HH11	1:H:142:ARG:HG3	1.34	0.91
1:E:61:ASN:HD22	1:E:63:GLN:HG3	1.32	0.91
1:C:142:ARG:HG3	1:C:142:ARG:HH11	1.34	0.90
1:E:61:ASN:HD21	1:E:63:GLN:HE21	1.04	0.90
1:E:61:ASN:ND2	1:E:63:GLN:NE2	2.14	0.90
1:E:61:ASN:CG	1:E:63:GLN:HG3	1.96	0.90
1:E:142:ARG:HH11	1:E:142:ARG:HG3	1.34	0.90
1:E:93:SER:OG	1:E:135:THR:HB	1.73	0.89
1:D:93:SER:OG	1:D:135:THR:HB	1.73	0.89
1:G:93:SER:OG	1:G:135:THR:HB	1.72	0.89
1:A:93:SER:OG	1:A:135:THR:HB	1.73	0.89
1:C:93:SER:OG	1:C:135:THR:HB	1.73	0.89
1:B:250:ILE:CD1	1:E:250:ILE:CD1	2.51	0.88
1:F:93:SER:OG	1:F:135:THR:HB	1.72	0.88
1:B:93:SER:OG	1:B:135:THR:HB	1.73	0.88
1:H:167:PHE:CE2	1:H:189:LEU:HB3	2.08	0.88
1:E:92:VAL:CG2	1:E:138:ILE:HG13	2.04	0.88
1:E:252:ASN:HD21	1:E:255:ASP:CG	1.83	0.87
1:D:252:ASN:HD21	1:D:255:ASP:CG	1.83	0.87
1:B:252:ASN:HD21	1:B:255:ASP:CG	1.83	0.87
1:D:92:VAL:CG2	1:D:138:ILE:HG13	2.04	0.87
1:G:252:ASN:HD21	1:G:255:ASP:CG	1.83	0.87
1:F:252:ASN:HD21	1:F:255:ASP:CG	1.83	0.87
1:H:93:SER:OG	1:H:135:THR:HB	1.72	0.87
1:G:92:VAL:CG2	1:G:138:ILE:HG13	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:CG2	1:A:138:ILE:HG13	2.04	0.86
1:B:92:VAL:CG2	1:B:138:ILE:HG13	2.04	0.86
1:A:23:TYR:CD1	1:A:26:VAL:HG11	2.10	0.86
1:C:23:TYR:CD1	1:C:26:VAL:HG11	2.10	0.86
1:E:23:TYR:CD1	1:E:26:VAL:HG11	2.10	0.86
1:C:92:VAL:CG2	1:C:138:ILE:HG13	2.04	0.86
1:H:92:VAL:CG2	1:H:138:ILE:HG13	2.04	0.86
1:F:92:VAL:CG2	1:F:138:ILE:HG13	2.04	0.86
1:B:33:LYS:HB3	1:B:160:PHE:HE1	1.41	0.86
1:D:23:TYR:CD1	1:D:26:VAL:HG11	2.10	0.86
1:B:23:TYR:CD1	1:B:26:VAL:HG11	2.10	0.86
1:H:23:TYR:CD1	1:H:26:VAL:HG11	2.10	0.85
1:H:252:ASN:HD21	1:H:255:ASP:CG	1.83	0.85
1:C:252:ASN:HD21	1:C:255:ASP:CG	1.83	0.85
1:A:252:ASN:HD21	1:A:255:ASP:CG	1.83	0.85
1:F:125:PHE:N	1:F:126:PRO:HD3	1.92	0.85
1:C:1:MET:HE2	1:C:177:VAL:HG23	1.56	0.84
1:F:23:TYR:CD1	1:F:26:VAL:HG11	2.10	0.84
1:G:23:TYR:CD1	1:G:26:VAL:HG11	2.10	0.84
1:C:20:HIS:CE1	1:C:155:ARG:HH11	1.95	0.84
1:A:20:HIS:CE1	1:A:155:ARG:HH11	1.95	0.84
1:B:20:HIS:CE1	1:B:155:ARG:HH11	1.95	0.84
1:H:20:HIS:CE1	1:H:155:ARG:HH11	1.95	0.84
1:B:21:GLU:HG3	1:B:155:ARG:NH2	1.93	0.84
1:D:20:HIS:CE1	1:D:155:ARG:HH11	1.95	0.84
1:F:21:GLU:HG3	1:F:155:ARG:NH2	1.93	0.84
1:C:21:GLU:HG3	1:C:155:ARG:NH2	1.93	0.84
1:F:20:HIS:CE1	1:F:155:ARG:HH11	1.95	0.83
1:D:60:SER:C	1:D:61:ASN:HD22	1.86	0.83
1:E:20:HIS:CE1	1:E:155:ARG:HH11	1.95	0.83
1:G:21:GLU:HG3	1:G:155:ARG:NH2	1.93	0.83
1:A:24:HIS:HA	1:A:30:LEU:HD23	1.61	0.83
1:E:21:GLU:HG3	1:E:155:ARG:NH2	1.93	0.83
1:F:24:HIS:HA	1:F:30:LEU:HD23	1.61	0.83
1:G:20:HIS:CE1	1:G:155:ARG:HH11	1.95	0.83
1:D:21:GLU:HG3	1:D:155:ARG:NH2	1.92	0.83
1:G:24:HIS:HA	1:G:30:LEU:HD23	1.61	0.83
1:H:21:GLU:HG3	1:H:155:ARG:NH2	1.93	0.83
1:A:21:GLU:HG3	1:A:155:ARG:NH2	1.92	0.82
1:B:24:HIS:HA	1:B:30:LEU:HD23	1.61	0.82
1:A:250:ILE:HD11	1:F:250:ILE:CD1	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ILE:CG1	1:F:42:PHE:CD1	2.63	0.82
1:D:82:PRO:HA	1:H:268:PRO:HB2	1.60	0.82
1:H:24:HIS:HA	1:H:30:LEU:HD23	1.61	0.82
1:E:24:HIS:HA	1:E:30:LEU:HD23	1.61	0.81
1:B:128:TYR:N	1:B:128:TYR:CD1	2.45	0.81
1:H:118:THR:HG23	1:H:121:GLU:OE1	1.81	0.81
1:C:24:HIS:HA	1:C:30:LEU:HD23	1.61	0.81
1:F:118:THR:HG23	1:F:121:GLU:OE1	1.81	0.81
1:A:118:THR:HG23	1:A:121:GLU:OE1	1.81	0.81
1:D:79:ILE:HG21	1:H:124:MET:HE3	1.61	0.81
1:H:168:GLU:O	1:H:171:ALA:HB3	1.81	0.81
1:C:118:THR:HG23	1:C:121:GLU:OE1	1.81	0.81
1:E:118:THR:HG23	1:E:121:GLU:OE1	1.81	0.81
1:G:118:THR:HG23	1:G:121:GLU:OE1	1.81	0.81
1:B:250:ILE:HD11	1:E:250:ILE:HD13	1.63	0.81
1:B:118:THR:HG23	1:B:121:GLU:OE1	1.81	0.80
1:D:24:HIS:HA	1:D:30:LEU:HD23	1.61	0.80
1:D:2:ARG:O	1:D:176:ASP:N	2.13	0.80
1:C:61:ASN:HB3	1:C:64:GLU:HG3	1.64	0.80
1:D:167:PHE:HE1	1:D:189:LEU:HD13	1.46	0.80
1:D:118:THR:HG23	1:D:121:GLU:OE1	1.81	0.80
1:B:253:ILE:CG1	1:E:42:PHE:CD1	2.65	0.79
1:C:54:PRO:HG2	1:C:107:TRP:CD1	2.18	0.79
1:D:124:MET:HE3	1:H:79:ILE:HG21	1.63	0.79
1:E:54:PRO:HG2	1:E:107:TRP:CD1	2.18	0.79
1:F:1:MET:CE	1:F:177:VAL:CG2	2.60	0.79
1:B:54:PRO:HG2	1:B:107:TRP:CD1	2.18	0.79
1:H:54:PRO:HG2	1:H:107:TRP:CD1	2.18	0.79
1:A:101:ALA:HA	1:A:130:TYR:CD2	2.18	0.78
1:A:124:MET:HE3	1:E:79:ILE:HG21	1.65	0.78
1:D:54:PRO:HG2	1:D:107:TRP:CD1	2.18	0.78
1:A:54:PRO:HG2	1:A:107:TRP:CD1	2.18	0.78
1:D:286:ARG:HG2	1:D:287:PRO:HD2	1.65	0.78
1:B:250:ILE:CD1	1:E:250:ILE:HD13	2.13	0.78
1:F:115:ARG:NH2	1:F:121:GLU:OE1	2.17	0.78
1:G:54:PRO:HG2	1:G:107:TRP:CD1	2.18	0.78
1:A:286:ARG:HG2	1:A:287:PRO:HD2	1.66	0.78
1:F:286:ARG:HG2	1:F:287:PRO:HD2	1.66	0.78
1:G:286:ARG:HG2	1:G:287:PRO:HD2	1.66	0.78
1:F:54:PRO:HG2	1:F:107:TRP:CD1	2.18	0.77
1:E:61:ASN:ND2	1:E:63:GLN:CD	2.37	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:ALA:O	1:F:161:LEU:HD12	1.84	0.77
1:A:115:ARG:NH2	1:A:121:GLU:OE1	2.17	0.77
1:E:115:ARG:HH22	1:E:121:GLU:CD	1.93	0.77
1:C:115:ARG:HH22	1:C:121:GLU:CD	1.93	0.77
1:A:115:ARG:HH22	1:A:121:GLU:CD	1.93	0.77
1:E:286:ARG:HG2	1:E:287:PRO:HD2	1.65	0.77
1:H:115:ARG:HH22	1:H:121:GLU:CD	1.93	0.77
1:H:286:ARG:HG2	1:H:287:PRO:HD2	1.65	0.77
1:C:115:ARG:NH2	1:C:121:GLU:OE1	2.17	0.77
1:G:115:ARG:NH2	1:G:121:GLU:OE1	2.17	0.77
1:H:115:ARG:NH2	1:H:121:GLU:OE1	2.17	0.77
1:B:115:ARG:NH2	1:B:121:GLU:OE1	2.17	0.77
1:G:177:VAL:HG12	1:G:178:ILE:N	1.99	0.77
1:D:115:ARG:NH2	1:D:121:GLU:OE1	2.17	0.77
1:E:115:ARG:NH2	1:E:121:GLU:OE1	2.17	0.77
1:B:115:ARG:HH22	1:B:121:GLU:CD	1.93	0.76
1:E:266:LEU:HD12	1:E:266:LEU:O	1.84	0.76
1:A:286:ARG:CG	1:A:287:PRO:HD2	2.16	0.76
1:D:115:ARG:HH22	1:D:121:GLU:CD	1.93	0.76
1:H:286:ARG:CG	1:H:287:PRO:HD2	2.16	0.76
1:F:115:ARG:HH22	1:F:121:GLU:CD	1.93	0.76
1:B:286:ARG:HG2	1:B:287:PRO:HD2	1.66	0.76
1:C:286:ARG:CG	1:C:287:PRO:HD2	2.16	0.76
1:E:286:ARG:CG	1:E:287:PRO:HD2	2.16	0.76
1:C:286:ARG:HG2	1:C:287:PRO:HD2	1.66	0.76
1:E:61:ASN:OD1	1:E:62:PRO:HD2	1.84	0.76
1:B:214:ILE:HG21	1:B:266:LEU:HD21	1.66	0.76
1:D:286:ARG:CG	1:D:287:PRO:HD2	2.16	0.75
1:B:286:ARG:CG	1:B:287:PRO:HD2	2.16	0.75
1:G:286:ARG:CG	1:G:287:PRO:HD2	2.16	0.75
1:G:115:ARG:HH22	1:G:121:GLU:CD	1.93	0.75
1:B:124:MET:HE3	1:F:79:ILE:HG21	1.67	0.75
1:F:286:ARG:CG	1:F:287:PRO:HD2	2.16	0.75
1:D:252:ASN:OD1	1:D:254:GLN:HB2	1.87	0.74
1:B:252:ASN:OD1	1:B:254:GLN:HG2	1.86	0.74
1:D:253:ILE:HG13	1:G:42:PHE:CD1	2.22	0.74
1:D:167:PHE:HE1	1:D:189:LEU:CD1	1.99	0.74
1:A:51:LEU:HD12	1:A:52:TRP:H	1.53	0.73
1:F:51:LEU:HD12	1:F:52:TRP:H	1.53	0.73
1:G:51:LEU:HD12	1:G:52:TRP:H	1.53	0.73
1:G:61:ASN:HD22	1:G:62:PRO:N	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:ILE:HD12	1:G:179:ILE:N	2.02	0.73
1:B:20:HIS:ND1	1:B:155:ARG:NH1	2.37	0.73
1:G:66:ASN:O	1:G:70:GLN:HG3	1.89	0.73
1:A:20:HIS:ND1	1:A:155:ARG:NH1	2.37	0.73
1:G:177:VAL:CG1	1:G:178:ILE:N	2.51	0.73
1:B:51:LEU:HD12	1:B:52:TRP:H	1.53	0.72
1:D:66:ASN:O	1:D:70:GLN:HG3	1.89	0.72
1:D:167:PHE:CE1	1:D:189:LEU:HD13	2.23	0.72
1:H:20:HIS:ND1	1:H:155:ARG:NH1	2.37	0.72
1:H:92:VAL:HG21	1:H:138:ILE:HG13	1.71	0.72
1:A:255:ASP:O	1:A:259:ILE:HG13	1.89	0.72
1:D:51:LEU:HD12	1:D:52:TRP:H	1.53	0.72
1:F:1:MET:HE2	1:F:177:VAL:CG2	2.18	0.72
1:F:20:HIS:ND1	1:F:155:ARG:NH1	2.37	0.72
1:B:255:ASP:O	1:B:259:ILE:HG13	1.89	0.72
1:C:254:GLN:O	1:C:258:THR:HG23	1.90	0.72
1:D:161:LEU:C	1:D:161:LEU:HD12	2.13	0.72
1:D:255:ASP:O	1:D:259:ILE:HG13	1.89	0.72
1:E:66:ASN:O	1:E:70:GLN:HG3	1.89	0.72
1:A:92:VAL:HG22	1:A:138:ILE:HG13	1.72	0.72
1:C:66:ASN:O	1:C:70:GLN:HG3	1.89	0.72
1:C:92:VAL:HG22	1:C:138:ILE:HG13	1.71	0.72
1:D:20:HIS:ND1	1:D:155:ARG:NH1	2.37	0.72
1:G:255:ASP:O	1:G:259:ILE:HG13	1.89	0.72
1:C:130:TYR:CD1	1:C:131:GLY:N	2.58	0.72
1:E:92:VAL:HG21	1:E:138:ILE:HG13	1.71	0.72
1:C:20:HIS:ND1	1:C:155:ARG:NH1	2.37	0.72
1:D:92:VAL:HG21	1:D:138:ILE:HG13	1.71	0.72
1:D:167:PHE:CE1	1:D:189:LEU:HB3	2.24	0.72
1:G:20:HIS:ND1	1:G:155:ARG:NH1	2.37	0.72
1:C:92:VAL:HG21	1:C:138:ILE:HG13	1.71	0.72
1:C:166:SER:OG	1:C:169:GLU:HB2	1.89	0.72
1:E:51:LEU:HD12	1:E:52:TRP:H	1.53	0.72
1:G:92:VAL:HG22	1:G:138:ILE:HG13	1.72	0.72
1:H:51:LEU:HD12	1:H:52:TRP:H	1.53	0.72
1:B:66:ASN:O	1:B:70:GLN:HG3	1.89	0.71
1:C:51:LEU:HD12	1:C:52:TRP:H	1.53	0.71
1:F:66:ASN:O	1:F:70:GLN:HG3	1.89	0.71
1:C:255:ASP:O	1:C:259:ILE:HG13	1.89	0.71
1:E:255:ASP:O	1:E:259:ILE:HG13	1.89	0.71
1:G:252:ASN:OD1	1:G:254:GLN:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:ASP:O	1:F:259:ILE:HG13	1.89	0.71
1:A:66:ASN:O	1:A:70:GLN:HG3	1.89	0.71
1:G:92:VAL:HG21	1:G:138:ILE:HG13	1.71	0.71
1:E:20:HIS:CE1	1:E:155:ARG:HD2	2.26	0.71
1:E:92:VAL:HG22	1:E:138:ILE:HG13	1.71	0.71
1:F:20:HIS:CE1	1:F:155:ARG:HD2	2.26	0.71
1:H:66:ASN:O	1:H:70:GLN:HG3	1.89	0.71
1:H:255:ASP:O	1:H:259:ILE:HG13	1.89	0.71
1:E:20:HIS:ND1	1:E:155:ARG:NH1	2.37	0.71
1:G:36:ALA:O	1:G:161:LEU:HD12	1.91	0.71
1:G:61:ASN:HD22	1:G:62:PRO:CD	2.04	0.71
1:F:92:VAL:HG22	1:F:138:ILE:HG13	1.72	0.71
1:G:20:HIS:CE1	1:G:155:ARG:HD2	2.26	0.71
1:A:20:HIS:CE1	1:A:155:ARG:HD2	2.26	0.71
1:A:165:GLU:N	1:A:169:GLU:OE1	2.19	0.71
1:A:166:SER:OG	1:A:169:GLU:HB2	1.91	0.71
1:D:20:HIS:CE1	1:D:155:ARG:HD2	2.26	0.71
1:F:92:VAL:HG21	1:F:138:ILE:HG13	1.71	0.71
1:E:49:ALA:HB3	2:E:348:FAB:H3'	1.73	0.71
1:E:164:VAL:HG12	1:E:165:GLU:N	2.06	0.71
1:B:49:ALA:HB3	2:B:348:FAB:H3'	1.73	0.70
1:B:92:VAL:HG21	1:B:138:ILE:HG13	1.71	0.70
1:F:49:ALA:HB3	2:F:348:FAB:H3'	1.73	0.70
1:A:92:VAL:HG21	1:A:138:ILE:HG13	1.71	0.70
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.26	0.70
1:B:105:PRO:HD3	1:B:132:TRP:CZ2	2.27	0.70
1:F:105:PRO:HD3	1:F:132:TRP:CZ2	2.26	0.70
1:H:166:SER:OG	1:H:169:GLU:N	2.22	0.70
1:C:162:ARG:HG3	1:C:162:ARG:HH11	1.55	0.70
1:D:92:VAL:HG22	1:D:138:ILE:HG13	1.72	0.70
1:H:101:ALA:HA	1:H:130:TYR:CD2	2.24	0.70
1:D:61:ASN:HD22	1:D:61:ASN:N	1.89	0.70
1:E:105:PRO:HD3	1:E:132:TRP:CZ2	2.27	0.70
1:C:20:HIS:CE1	1:C:155:ARG:HD2	2.26	0.70
1:D:161:LEU:HD12	1:D:162:ARG:N	2.06	0.70
1:F:254:GLN:O	1:F:258:THR:HG23	1.91	0.70
1:G:267:GLU:OE1	1:G:269:THR:HG23	1.92	0.70
1:H:105:PRO:HD3	1:H:132:TRP:CZ2	2.26	0.70
1:F:142:ARG:HH11	1:F:142:ARG:CG	2.05	0.70
1:H:20:HIS:CE1	1:H:155:ARG:HD2	2.26	0.70
1:G:105:PRO:HD3	1:G:132:TRP:CZ2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:HIS:CE1	1:B:155:ARG:HD2	2.26	0.70
1:A:250:ILE:HD11	1:F:250:ILE:HD13	1.74	0.70
1:C:105:PRO:HD3	1:C:132:TRP:CZ2	2.26	0.70
1:E:254:GLN:O	1:E:258:THR:HG23	1.92	0.70
1:H:92:VAL:HG22	1:H:138:ILE:HG13	1.72	0.70
1:A:49:ALA:HB3	2:A:348:FAB:H3'	1.73	0.69
1:D:49:ALA:HB3	2:D:348:FAB:H3'	1.73	0.69
1:B:92:VAL:HG22	1:B:138:ILE:HG13	1.72	0.69
1:B:253:ILE:HG12	1:E:42:PHE:CE1	2.27	0.69
1:C:23:TYR:HD1	1:C:26:VAL:CG1	2.05	0.69
1:D:23:TYR:HD1	1:D:26:VAL:CG1	2.04	0.69
1:C:49:ALA:HB3	2:C:348:FAB:H3'	1.73	0.69
1:G:61:ASN:ND2	1:G:63:GLN:H	1.91	0.69
1:G:142:ARG:HH11	1:G:142:ARG:CG	2.05	0.69
1:C:79:ILE:HG21	1:G:124:MET:HE3	1.74	0.69
1:D:105:PRO:HD3	1:D:132:TRP:CZ2	2.26	0.69
1:B:23:TYR:HD1	1:B:26:VAL:CG1	2.05	0.69
1:B:214:ILE:CG2	1:B:266:LEU:HD21	2.23	0.69
1:G:166:SER:O	1:G:170:VAL:HG23	1.93	0.69
1:E:266:LEU:HD12	1:E:266:LEU:C	2.16	0.69
1:G:35:TYR:HE1	1:G:160:PHE:CD2	2.11	0.69
1:H:40:THR:OG1	1:H:41:PRO:HA	1.93	0.69
1:H:49:ALA:HB3	2:H:348:FAB:H3'	1.73	0.69
1:C:40:THR:OG1	1:C:41:PRO:HA	1.93	0.69
1:A:250:ILE:HD11	1:F:250:ILE:HD11	1.74	0.69
1:C:39:PHE:CD2	1:C:161:LEU:HD23	2.27	0.69
1:D:40:THR:OG1	1:D:41:PRO:HA	1.93	0.69
1:A:152:LEU:O	1:A:157:VAL:HG23	1.93	0.68
1:C:253:ILE:HG13	1:H:42:PHE:CD1	2.29	0.68
1:G:39:PHE:CD2	1:G:161:LEU:HD13	2.28	0.68
1:G:40:THR:OG1	1:G:41:PRO:HA	1.93	0.68
1:B:142:ARG:HH11	1:B:142:ARG:CG	2.05	0.68
1:E:40:THR:OG1	1:E:41:PRO:HA	1.93	0.68
1:H:295:GLN:O	1:H:296:LEU:HD23	1.93	0.68
1:C:295:GLN:O	1:C:296:LEU:HD23	1.93	0.68
1:F:40:THR:OG1	1:F:41:PRO:HA	1.93	0.68
1:C:142:ARG:HH11	1:C:142:ARG:CG	2.05	0.68
1:G:49:ALA:HB3	2:G:348:FAB:H3'	1.73	0.68
1:F:251:ASN:HA	1:F:280:THR:HG21	1.76	0.68
1:B:251:ASN:HA	1:B:280:THR:HG21	1.76	0.68
1:D:142:ARG:HH11	1:D:142:ARG:CG	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:GLN:O	1:F:296:LEU:HD23	1.93	0.68
1:G:251:ASN:HA	1:G:280:THR:HG21	1.76	0.68
1:H:23:TYR:HD1	1:H:26:VAL:CG1	2.04	0.68
1:H:251:ASN:HA	1:H:280:THR:HG21	1.76	0.68
1:A:101:ALA:HA	1:A:130:TYR:CG	2.29	0.68
1:E:51:LEU:HD12	1:E:52:TRP:N	2.09	0.68
1:A:40:THR:OG1	1:A:41:PRO:HA	1.93	0.68
1:C:251:ASN:HA	1:C:280:THR:HG21	1.76	0.68
1:G:295:GLN:O	1:G:296:LEU:HD23	1.93	0.68
1:B:295:GLN:O	1:B:296:LEU:HD23	1.93	0.67
1:E:142:ARG:HH11	1:E:142:ARG:CG	2.05	0.67
1:E:295:GLN:O	1:E:296:LEU:HD23	1.93	0.67
1:A:51:LEU:HD12	1:A:52:TRP:N	2.09	0.67
1:A:79:ILE:HG21	1:E:124:MET:HE3	1.74	0.67
1:F:39:PHE:CD2	1:F:161:LEU:HD13	2.30	0.67
1:G:51:LEU:HD12	1:G:52:TRP:N	2.09	0.67
1:G:105:PRO:HD3	1:G:132:TRP:CH2	2.30	0.67
1:H:51:LEU:HD12	1:H:52:TRP:N	2.09	0.67
1:H:166:SER:OG	1:H:169:GLU:HB2	1.93	0.67
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.05	0.67
1:A:295:GLN:O	1:A:296:LEU:HD23	1.93	0.67
1:B:40:THR:OG1	1:B:41:PRO:HA	1.93	0.67
1:C:51:LEU:HD12	1:C:52:TRP:N	2.09	0.67
1:C:162:ARG:HH11	1:C:162:ARG:CG	2.07	0.67
1:D:1:MET:HG3	1:D:176:ASP:HB2	1.77	0.67
1:E:23:TYR:HD1	1:E:26:VAL:CG1	2.05	0.67
1:E:105:PRO:HD3	1:E:132:TRP:CH2	2.30	0.67
1:E:251:ASN:HA	1:E:280:THR:HG21	1.76	0.67
1:C:105:PRO:HD3	1:C:132:TRP:CH2	2.30	0.67
1:D:105:PRO:HD3	1:D:132:TRP:CH2	2.30	0.67
1:D:170:VAL:CG1	1:D:178:ILE:HD13	2.24	0.67
1:D:251:ASN:HA	1:D:280:THR:HG21	1.76	0.67
1:E:61:ASN:HB3	1:E:64:GLU:HG3	1.74	0.67
1:F:209:TRP:NE1	1:F:269:THR:OG1	2.19	0.67
1:D:51:LEU:HD12	1:D:52:TRP:N	2.09	0.67
1:A:253:ILE:HG12	1:F:42:PHE:CE1	2.30	0.67
1:E:2:ARG:O	1:E:176:ASP:HB2	1.95	0.67
1:H:142:ARG:HH11	1:H:142:ARG:CG	2.05	0.67
1:A:105:PRO:HD3	1:A:132:TRP:CH2	2.30	0.66
1:D:295:GLN:O	1:D:296:LEU:HD23	1.93	0.66
1:F:51:LEU:HD12	1:F:52:TRP:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:PHE:HD2	1:E:161:LEU:HD12	1.60	0.66
1:B:51:LEU:HD12	1:B:52:TRP:N	2.09	0.66
1:B:105:PRO:HD3	1:B:132:TRP:CH2	2.30	0.66
1:F:105:PRO:HD3	1:F:132:TRP:CH2	2.30	0.66
1:D:193:PRO:HG2	1:F:73:ASN:HB2	1.76	0.66
1:E:61:ASN:CG	1:E:63:GLN:HE21	2.03	0.66
1:C:124:MET:HE3	1:G:79:ILE:HG21	1.78	0.66
1:C:293:ARG:HH22	1:C:336:GLU:CD	2.04	0.66
1:H:105:PRO:HD3	1:H:132:TRP:CH2	2.30	0.66
1:E:293:ARG:HH22	1:E:336:GLU:CD	2.04	0.66
1:B:170:VAL:HG12	1:B:178:ILE:HD11	1.77	0.65
1:D:293:ARG:HH22	1:D:336:GLU:CD	2.04	0.65
1:A:253:ILE:CG1	1:F:42:PHE:CE1	2.79	0.65
1:B:293:ARG:HH22	1:B:336:GLU:CD	2.04	0.65
1:A:293:ARG:HH22	1:A:336:GLU:CD	2.04	0.65
1:F:293:ARG:HH22	1:F:336:GLU:CD	2.04	0.65
1:G:293:ARG:HH22	1:G:336:GLU:CD	2.04	0.65
1:G:127:ASP:OD1	1:G:127:ASP:N	2.28	0.65
1:H:293:ARG:HH22	1:H:336:GLU:CD	2.04	0.65
1:A:251:ASN:HA	1:A:280:THR:HG21	1.76	0.65
1:E:39:PHE:HE2	1:E:161:LEU:HA	1.60	0.65
1:G:23:TYR:HD1	1:G:26:VAL:CG1	2.04	0.65
1:G:196:GLN:O	1:G:285:VAL:HB	1.97	0.65
1:B:196:GLN:O	1:B:285:VAL:HB	1.97	0.65
1:D:208:PRO:HD2	1:D:209:TRP:CE3	2.32	0.65
1:D:254:GLN:O	1:D:258:THR:HG23	1.97	0.65
1:G:1:MET:CE	1:G:177:VAL:HG23	2.27	0.65
1:G:208:PRO:HD2	1:G:209:TRP:CE3	2.32	0.65
1:G:59:PRO:HB3	1:G:64:GLU:OE2	1.96	0.64
1:A:23:TYR:HD1	1:A:26:VAL:CG1	2.05	0.64
1:A:159:PHE:C	1:A:160:PHE:CD1	2.76	0.64
1:A:287:PRO:HB2	1:A:288:GLN:NE2	2.12	0.64
1:C:165:GLU:HB2	1:C:169:GLU:CD	2.22	0.64
1:C:196:GLN:O	1:C:285:VAL:HB	1.97	0.64
1:E:208:PRO:HD2	1:E:209:TRP:CE3	2.32	0.64
1:C:93:SER:HG	1:C:135:THR:HB	1.62	0.64
1:C:165:GLU:HB2	1:C:169:GLU:OE1	1.96	0.64
1:D:196:GLN:O	1:D:285:VAL:HB	1.97	0.64
1:F:208:PRO:HD2	1:F:209:TRP:CE3	2.32	0.64
1:E:196:GLN:O	1:E:285:VAL:HB	1.97	0.64
1:B:79:ILE:HG21	1:F:124:MET:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:TYR:HD1	1:F:26:VAL:CG1	2.04	0.64
1:H:107:TRP:HB3	1:H:110:MET:HE3	1.80	0.64
1:H:208:PRO:HD2	1:H:209:TRP:CE3	2.32	0.64
1:A:208:PRO:HD2	1:A:209:TRP:CE3	2.32	0.64
1:D:168:GLU:O	1:D:172:ARG:HG3	1.98	0.64
1:E:61:ASN:CG	1:E:63:GLN:HG2	2.23	0.64
1:B:208:PRO:HD2	1:B:209:TRP:CE3	2.32	0.64
1:C:107:TRP:HB3	1:C:110:MET:HE3	1.80	0.64
1:F:196:GLN:O	1:F:285:VAL:HB	1.97	0.64
1:A:159:PHE:N	1:A:159:PHE:HD1	1.96	0.64
1:A:196:GLN:O	1:A:285:VAL:HB	1.97	0.64
1:E:107:TRP:HB3	1:E:110:MET:HE3	1.80	0.64
1:F:39:PHE:CE2	1:F:161:LEU:HD13	2.33	0.63
1:H:196:GLN:O	1:H:285:VAL:HB	1.97	0.63
1:G:107:TRP:HB3	1:G:110:MET:HE3	1.80	0.63
1:D:128:TYR:CD1	1:D:128:TYR:N	2.64	0.63
1:A:177:VAL:HG12	1:A:178:ILE:N	2.14	0.63
1:D:177:VAL:HG12	1:D:178:ILE:N	2.11	0.63
1:C:208:PRO:HD2	1:C:209:TRP:CE3	2.32	0.63
1:H:267:GLU:O	1:H:270:LEU:HB2	1.98	0.63
1:A:250:ILE:CD1	1:F:250:ILE:CD1	2.76	0.62
1:F:224:TYR:HB2	1:F:242:PHE:HD2	1.64	0.62
1:H:168:GLU:OE2	1:H:172:ARG:NH1	2.32	0.62
1:A:107:TRP:HB3	1:A:110:MET:HE3	1.80	0.62
1:D:107:TRP:HB3	1:D:110:MET:HE3	1.80	0.62
1:C:325:GLU:O	1:C:328:LYS:HB3	2.00	0.62
1:D:325:GLU:O	1:D:328:LYS:HB3	2.00	0.62
1:D:20:HIS:ND1	1:D:155:ARG:HD2	2.15	0.62
1:D:177:VAL:CG1	1:D:178:ILE:N	2.63	0.62
1:E:224:TYR:HB2	1:E:242:PHE:HD2	1.64	0.62
1:F:107:TRP:HB3	1:F:110:MET:HE3	1.80	0.62
1:A:35:TYR:CD1	1:A:160:PHE:HB2	2.35	0.62
1:A:254:GLN:O	1:A:258:THR:HG23	2.00	0.62
1:B:253:ILE:HG13	1:E:42:PHE:CG	2.34	0.62
1:H:20:HIS:ND1	1:H:155:ARG:HD2	2.15	0.62
1:H:325:GLU:O	1:H:328:LYS:HB3	2.00	0.62
1:A:224:TYR:HB2	1:A:242:PHE:HD2	1.64	0.62
1:A:325:GLU:O	1:A:328:LYS:HB3	2.00	0.62
1:C:39:PHE:CE2	1:C:161:LEU:HD23	2.33	0.62
1:B:107:TRP:HB3	1:B:110:MET:HE3	1.80	0.61
1:E:325:GLU:O	1:E:328:LYS:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:GLU:O	1:F:328:LYS:HB3	2.00	0.61
1:G:20:HIS:ND1	1:G:155:ARG:HD2	2.15	0.61
1:C:1:MET:HE3	1:C:176:ASP:HB3	1.81	0.61
1:C:252:ASN:OD1	1:C:254:GLN:HB3	1.99	0.61
1:F:20:HIS:ND1	1:F:155:ARG:HD2	2.15	0.61
1:A:20:HIS:ND1	1:A:155:ARG:HD2	2.15	0.61
1:H:224:TYR:HB2	1:H:242:PHE:HD2	1.64	0.61
1:H:332:LYS:O	1:H:336:GLU:HG3	2.01	0.61
1:C:20:HIS:ND1	1:C:155:ARG:HD2	2.15	0.61
1:B:128:TYR:N	1:B:128:TYR:HD1	1.99	0.61
1:B:224:TYR:HB2	1:B:242:PHE:HD2	1.64	0.61
1:G:325:GLU:O	1:G:328:LYS:HB3	2.00	0.61
1:C:224:TYR:HB2	1:C:242:PHE:HD2	1.64	0.61
1:G:35:TYR:CE1	1:G:160:PHE:CD2	2.89	0.61
1:A:159:PHE:N	1:A:159:PHE:CD1	2.67	0.61
1:B:325:GLU:O	1:B:328:LYS:HB3	2.00	0.61
1:G:224:TYR:HB2	1:G:242:PHE:HD2	1.64	0.61
1:A:332:LYS:O	1:A:336:GLU:HG3	2.01	0.61
1:E:332:LYS:O	1:E:336:GLU:HG3	2.01	0.61
1:B:20:HIS:ND1	1:B:155:ARG:HD2	2.15	0.60
1:E:20:HIS:ND1	1:E:155:ARG:HD2	2.15	0.60
1:G:61:ASN:ND2	1:G:63:GLN:HB2	2.16	0.60
1:B:332:LYS:O	1:B:336:GLU:HG3	2.01	0.60
1:F:1:MET:HE3	1:F:176:ASP:HB3	1.82	0.60
1:H:99:ARG:O	1:H:129:ARG:HB3	2.00	0.60
1:G:170:VAL:HB	1:G:178:ILE:CD1	2.31	0.60
1:B:269:THR:C	1:B:271:LYS:H	2.10	0.60
1:D:193:PRO:HG2	1:F:73:ASN:CB	2.30	0.60
1:D:224:TYR:HB2	1:D:242:PHE:HD2	1.65	0.60
1:A:1:MET:HE3	1:A:176:ASP:HB3	1.84	0.60
1:A:36:ALA:O	1:A:161:LEU:HD12	2.01	0.60
1:A:291:LEU:HA	1:A:307:HIS:O	2.02	0.60
1:C:332:LYS:O	1:C:336:GLU:HG3	2.01	0.60
1:G:291:LEU:HA	1:G:307:HIS:O	2.02	0.60
1:B:253:ILE:CG1	1:E:42:PHE:CE1	2.84	0.60
1:C:291:LEU:HA	1:C:307:HIS:O	2.02	0.60
1:F:166:SER:O	1:F:170:VAL:HG23	2.02	0.60
1:F:332:LYS:O	1:F:336:GLU:HG3	2.01	0.60
1:B:291:LEU:HA	1:B:307:HIS:O	2.02	0.60
1:B:201:GLN:HG3	1:B:280:THR:HG22	1.84	0.60
1:C:101:ALA:CA	1:C:130:TYR:CD2	2.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:GLN:HG3	1:D:280:THR:HG22	1.84	0.60
1:E:201:GLN:HG3	1:E:280:THR:HG22	1.84	0.60
1:G:332:LYS:O	1:G:336:GLU:HG3	2.01	0.60
1:C:130:TYR:HD1	1:C:131:GLY:N	2.00	0.59
1:H:291:LEU:HA	1:H:307:HIS:O	2.02	0.59
1:F:291:LEU:HA	1:F:307:HIS:O	2.02	0.59
1:C:101:ALA:HA	1:C:130:TYR:CG	2.38	0.59
1:C:125:PHE:N	1:C:126:PRO:HD3	2.17	0.59
1:G:102:VAL:HG13	1:G:103:PRO:HD2	1.84	0.59
1:H:267:GLU:OE1	1:H:269:THR:HG23	2.02	0.59
1:B:260:TRP:O	1:B:264:CYS:HB2	2.03	0.59
1:C:165:GLU:HB2	1:C:169:GLU:OE2	2.03	0.59
1:D:332:LYS:O	1:D:336:GLU:HG3	2.01	0.59
1:H:260:TRP:O	1:H:264:CYS:HB2	2.03	0.59
1:A:161:LEU:O	1:A:162:ARG:HG2	2.02	0.59
1:D:35:TYR:HE1	1:D:160:PHE:CD2	2.20	0.59
1:C:260:TRP:O	1:C:264:CYS:HB2	2.03	0.59
1:F:201:GLN:HG3	1:F:280:THR:HG22	1.84	0.59
1:G:201:GLN:HG3	1:G:280:THR:HG22	1.84	0.59
1:F:260:TRP:O	1:F:264:CYS:HB2	2.03	0.59
1:G:122:LEU:O	1:G:125:PHE:O	2.21	0.59
1:D:291:LEU:HA	1:D:307:HIS:O	2.02	0.59
1:H:201:GLN:HG3	1:H:280:THR:HG22	1.84	0.59
1:A:291:LEU:C	1:A:291:LEU:HD12	2.28	0.59
1:B:263:CYS:O	1:B:267:GLU:N	2.36	0.59
1:C:102:VAL:HG13	1:C:103:PRO:HD2	1.84	0.59
1:C:291:LEU:C	1:C:291:LEU:HD12	2.28	0.59
1:E:10:VAL:HG13	1:E:11:ILE:N	2.18	0.59
1:A:201:GLN:HG3	1:A:280:THR:HG22	1.84	0.58
1:B:250:ILE:CD1	1:E:250:ILE:HD11	2.24	0.58
1:H:102:VAL:HG13	1:H:103:PRO:HD2	1.84	0.58
1:B:291:LEU:C	1:B:291:LEU:HD12	2.28	0.58
1:C:61:ASN:OD1	1:C:63:GLN:N	2.35	0.58
1:E:291:LEU:C	1:E:291:LEU:HD12	2.28	0.58
1:E:291:LEU:HA	1:E:307:HIS:O	2.02	0.58
1:G:10:VAL:HG13	1:G:11:ILE:N	2.18	0.58
1:A:102:VAL:HG13	1:A:103:PRO:HD2	1.84	0.58
1:D:195:LEU:HD12	1:D:285:VAL:O	2.04	0.58
1:H:291:LEU:C	1:H:291:LEU:HD12	2.28	0.58
1:B:195:LEU:HD12	1:B:285:VAL:O	2.04	0.58
1:D:260:TRP:O	1:D:264:CYS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LEU:C	1:D:291:LEU:HD12	2.28	0.58
1:E:260:TRP:O	1:E:264:CYS:HB2	2.03	0.58
1:G:167:PHE:HE1	1:G:189:LEU:O	1.85	0.58
1:G:260:TRP:O	1:G:264:CYS:HB2	2.03	0.58
1:A:253:ILE:HA	1:F:42:PHE:CZ	2.39	0.58
1:A:260:TRP:O	1:A:264:CYS:HB2	2.03	0.58
1:D:102:VAL:HG13	1:D:103:PRO:HD2	1.84	0.58
1:F:128:TYR:N	1:F:128:TYR:CD1	2.72	0.58
1:F:291:LEU:C	1:F:291:LEU:HD12	2.28	0.58
1:G:195:LEU:HD12	1:G:285:VAL:O	2.04	0.58
1:C:205:VAL:HG23	1:C:275:ILE:HA	1.86	0.58
1:E:102:VAL:HG13	1:E:103:PRO:HD2	1.84	0.58
1:F:10:VAL:HG13	1:F:11:ILE:N	2.18	0.58
1:H:195:LEU:HD12	1:H:285:VAL:O	2.04	0.58
1:B:10:VAL:HG13	1:B:11:ILE:N	2.18	0.58
1:B:33:LYS:HB3	1:B:160:PHE:CE1	2.31	0.58
1:D:205:VAL:HG23	1:D:275:ILE:HA	1.86	0.58
1:G:166:SER:OG	1:G:169:GLU:HB2	2.02	0.58
1:C:201:GLN:HG3	1:C:280:THR:HG22	1.84	0.58
1:E:195:LEU:HD12	1:E:285:VAL:O	2.04	0.58
1:E:205:VAL:HG23	1:E:275:ILE:HA	1.86	0.58
1:G:1:MET:HE3	1:G:176:ASP:HB3	1.84	0.58
1:D:125:PHE:N	1:D:125:PHE:CD1	2.71	0.58
1:H:205:VAL:HG23	1:H:275:ILE:HA	1.86	0.58
1:F:124:MET:C	1:F:126:PRO:HD3	2.28	0.57
1:B:102:VAL:HG13	1:B:103:PRO:HD2	1.85	0.57
1:C:152:LEU:O	1:C:157:VAL:HG13	2.04	0.57
1:E:168:GLU:HG3	1:E:298:PHE:CE1	2.39	0.57
1:H:10:VAL:HG13	1:H:11:ILE:N	2.18	0.57
1:H:35:TYR:CZ	1:H:162:ARG:NH1	2.72	0.57
1:C:195:LEU:HD12	1:C:285:VAL:O	2.04	0.57
1:A:10:VAL:HG13	1:A:11:ILE:N	2.18	0.57
1:A:250:ILE:CD1	1:F:250:ILE:HD13	2.33	0.57
1:C:10:VAL:HG13	1:C:11:ILE:N	2.18	0.57
1:C:128:TYR:N	1:C:128:TYR:CD1	2.71	0.57
1:F:102:VAL:HG13	1:F:103:PRO:HD2	1.84	0.57
1:F:195:LEU:HD12	1:F:285:VAL:O	2.04	0.57
1:B:269:THR:C	1:B:271:LYS:N	2.57	0.57
1:D:10:VAL:HG13	1:D:11:ILE:N	2.18	0.57
1:F:24:HIS:C	1:F:24:HIS:CD2	2.81	0.57
1:G:291:LEU:C	1:G:291:LEU:HD12	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:TYR:CD1	1:H:131:GLY:N	2.73	0.57
1:H:293:ARG:NH2	1:H:336:GLU:OE1	2.38	0.57
1:A:195:LEU:HD12	1:A:285:VAL:O	2.04	0.57
1:C:1:MET:CE	1:C:177:VAL:HG23	2.32	0.57
1:D:293:ARG:NH2	1:D:336:GLU:OE1	2.38	0.57
1:D:170:VAL:HG11	1:D:178:ILE:HD13	1.87	0.57
1:F:293:ARG:NH2	1:F:336:GLU:OE1	2.38	0.57
1:G:130:TYR:CD1	1:G:131:GLY:N	2.73	0.57
1:D:165:GLU:OE1	1:D:165:GLU:HA	2.03	0.57
1:A:293:ARG:NH2	1:A:336:GLU:OE1	2.38	0.56
1:E:293:ARG:NH2	1:E:336:GLU:OE1	2.38	0.56
1:A:205:VAL:HG23	1:A:275:ILE:HA	1.86	0.56
1:C:293:ARG:NH2	1:C:336:GLU:OE1	2.38	0.56
1:D:170:VAL:HG12	1:D:178:ILE:HD13	1.87	0.56
1:E:1:MET:HE3	1:E:176:ASP:HB3	1.87	0.56
1:G:293:ARG:NH2	1:G:336:GLU:OE1	2.38	0.56
1:A:93:SER:HA	1:A:135:THR:HA	1.88	0.56
1:A:177:VAL:CG1	1:A:178:ILE:N	2.69	0.56
1:B:293:ARG:NH2	1:B:336:GLU:OE1	2.38	0.56
1:F:93:SER:HA	1:F:135:THR:HA	1.88	0.56
1:F:205:VAL:HG23	1:F:275:ILE:HA	1.86	0.56
1:H:128:TYR:N	1:H:128:TYR:CD1	2.73	0.56
1:H:152:LEU:HD22	1:H:157:VAL:HG21	1.87	0.56
1:B:24:HIS:C	1:B:24:HIS:CD2	2.81	0.56
1:E:24:HIS:C	1:E:24:HIS:CD2	2.81	0.56
1:E:93:SER:HG	1:E:135:THR:HB	1.70	0.56
1:G:205:VAL:HG23	1:G:275:ILE:HA	1.86	0.56
1:D:93:SER:HA	1:D:135:THR:HA	1.88	0.56
1:G:93:SER:HA	1:G:135:THR:HA	1.88	0.56
1:B:205:VAL:HG23	1:B:275:ILE:HA	1.86	0.56
1:C:256:HIS:HD1	1:C:278:GLU:CD	2.12	0.56
1:E:2:ARG:N	1:E:176:ASP:OD2	2.23	0.56
1:H:168:GLU:CG	1:H:172:ARG:HD2	2.35	0.56
1:D:78:HIS:CG	1:D:87:MET:HE1	2.41	0.56
1:D:236:VAL:HG12	1:D:237:THR:N	2.21	0.56
1:B:160:PHE:N	1:B:160:PHE:CD1	2.74	0.56
1:E:24:HIS:O	1:E:27:LEU:O	2.24	0.56
1:A:24:HIS:O	1:A:27:LEU:O	2.24	0.55
1:C:36:ALA:O	1:C:161:LEU:HD22	2.06	0.55
1:G:24:HIS:O	1:G:27:LEU:O	2.24	0.55
1:G:190:GLN:NE2	1:G:290:ARG:HH12	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:NE2	1:A:290:ARG:HH12	2.05	0.55
1:C:190:GLN:NE2	1:C:290:ARG:HH12	2.05	0.55
1:B:93:SER:HA	1:B:135:THR:HA	1.88	0.55
1:B:236:VAL:HG12	1:B:237:THR:N	2.21	0.55
1:D:24:HIS:O	1:D:27:LEU:O	2.24	0.55
1:H:190:GLN:NE2	1:H:290:ARG:HH12	2.05	0.55
1:B:24:HIS:O	1:B:27:LEU:O	2.24	0.55
1:D:124:MET:HB2	1:D:125:PHE:CE1	2.42	0.55
1:D:256:HIS:HD1	1:D:278:GLU:CD	2.12	0.55
1:F:190:GLN:NE2	1:F:290:ARG:HH12	2.05	0.55
1:F:256:HIS:HD1	1:F:278:GLU:CD	2.12	0.55
1:B:190:GLN:NE2	1:B:290:ARG:HH12	2.05	0.55
1:G:35:TYR:CG	1:G:162:ARG:HD2	2.42	0.55
1:E:93:SER:HA	1:E:135:THR:HA	1.88	0.55
1:F:101:ALA:HA	1:F:130:TYR:CD2	2.42	0.55
1:G:78:HIS:CG	1:G:87:MET:HE1	2.41	0.55
1:H:24:HIS:O	1:H:27:LEU:O	2.24	0.55
1:A:290:ARG:NH2	1:A:307:HIS:CE1	2.75	0.55
1:C:24:HIS:O	1:C:27:LEU:O	2.24	0.55
1:C:236:VAL:HG12	1:C:237:THR:N	2.21	0.55
1:E:190:GLN:NE2	1:E:290:ARG:HH12	2.05	0.55
1:F:142:ARG:HG3	1:F:142:ARG:NH1	2.14	0.55
1:G:290:ARG:NH2	1:G:307:HIS:CE1	2.75	0.55
1:B:290:ARG:NH2	1:B:307:HIS:CE1	2.75	0.55
1:D:128:TYR:H	1:D:128:TYR:HD1	1.54	0.55
1:E:61:ASN:CG	1:E:63:GLN:NE2	2.64	0.55
1:F:236:VAL:HG12	1:F:237:THR:N	2.21	0.55
1:B:166:SER:OG	1:B:169:GLU:HB3	2.06	0.55
1:C:290:ARG:NH2	1:C:307:HIS:CE1	2.75	0.55
1:D:138:ILE:HD13	1:D:232:GLY:HA2	1.89	0.55
1:E:128:TYR:N	1:E:128:TYR:CD1	2.74	0.55
1:E:138:ILE:HD13	1:E:232:GLY:HA2	1.89	0.55
1:E:164:VAL:CG1	1:E:165:GLU:N	2.69	0.55
1:E:256:HIS:HD1	1:E:278:GLU:CD	2.12	0.55
1:F:316:LEU:HB2	2:F:348:FAB:O2	2.07	0.55
1:A:236:VAL:HG12	1:A:237:THR:N	2.21	0.55
1:H:316:LEU:HB2	2:H:348:FAB:O2	2.07	0.55
1:E:236:VAL:HG12	1:E:237:THR:N	2.21	0.54
1:H:290:ARG:NH2	1:H:307:HIS:CE1	2.75	0.54
1:A:78:HIS:CG	1:A:87:MET:HE1	2.41	0.54
1:C:93:SER:HA	1:C:135:THR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:THR:O	1:D:19:ILE:HG12	2.08	0.54
1:D:316:LEU:HB2	2:D:348:FAB:O2	2.07	0.54
1:E:290:ARG:NH2	1:E:307:HIS:CE1	2.75	0.54
1:F:89:LEU:O	1:F:90:THR:HG23	2.08	0.54
1:G:15:THR:O	1:G:19:ILE:HG12	2.08	0.54
1:G:138:ILE:HD13	1:G:232:GLY:HA2	1.89	0.54
1:H:177:VAL:CG1	1:H:178:ILE:N	2.70	0.54
1:A:138:ILE:HD13	1:A:232:GLY:HA2	1.89	0.54
1:B:136:SER:O	1:B:137:LEU:HD23	2.08	0.54
1:D:136:SER:O	1:D:137:LEU:HD23	2.08	0.54
1:D:290:ARG:NH2	1:D:307:HIS:CE1	2.75	0.54
1:E:15:THR:O	1:E:19:ILE:HG12	2.08	0.54
1:F:290:ARG:NH2	1:F:307:HIS:CE1	2.75	0.54
1:H:37:ASP:O	1:H:161:LEU:HD11	2.07	0.54
1:H:93:SER:HA	1:H:135:THR:HA	1.88	0.54
1:H:136:SER:O	1:H:137:LEU:HD23	2.08	0.54
1:C:136:SER:O	1:C:137:LEU:HD23	2.08	0.54
1:E:180:ASN:HD22	1:E:307:HIS:CD2	2.26	0.54
1:G:316:LEU:HB2	2:G:348:FAB:O2	2.07	0.54
1:A:93:SER:HG	1:A:135:THR:HB	1.72	0.54
1:C:1:MET:HE3	1:C:176:ASP:CB	2.37	0.54
1:E:61:ASN:HD21	1:E:63:GLN:CG	1.75	0.54
1:E:316:LEU:HB2	2:E:348:FAB:O2	2.07	0.54
1:F:24:HIS:O	1:F:27:LEU:O	2.24	0.54
1:F:136:SER:O	1:F:137:LEU:HD23	2.08	0.54
1:F:138:ILE:HD13	1:F:232:GLY:HA2	1.89	0.54
1:A:165:GLU:HB3	1:A:169:GLU:OE1	2.07	0.54
1:C:316:LEU:HB2	2:C:348:FAB:O2	2.07	0.54
1:E:136:SER:O	1:E:137:LEU:HD23	2.08	0.54
1:G:136:SER:O	1:G:137:LEU:HD23	2.08	0.54
1:G:236:VAL:HG12	1:G:237:THR:N	2.21	0.54
1:D:24:HIS:O	1:D:24:HIS:CD2	2.61	0.54
1:D:89:LEU:O	1:D:90:THR:HG23	2.08	0.54
1:D:190:GLN:NE2	1:D:290:ARG:HH12	2.05	0.54
1:E:89:LEU:O	1:E:90:THR:HG23	2.08	0.54
1:F:78:HIS:CG	1:F:87:MET:HE1	2.41	0.54
1:H:236:VAL:HG12	1:H:237:THR:N	2.21	0.54
1:H:24:HIS:O	1:H:24:HIS:CD2	2.61	0.54
1:A:89:LEU:O	1:A:90:THR:HG23	2.08	0.54
1:B:15:THR:O	1:B:19:ILE:HG12	2.08	0.54
1:C:15:THR:O	1:C:19:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:HIS:CD2	1:D:24:HIS:C	2.81	0.54
1:F:15:THR:O	1:F:19:ILE:HG12	2.08	0.54
1:F:133:PHE:CD1	1:F:133:PHE:C	2.86	0.54
1:G:89:LEU:O	1:G:90:THR:HG23	2.08	0.54
1:H:101:ALA:HA	1:H:130:TYR:CG	2.43	0.54
1:A:316:LEU:HB2	2:A:348:FAB:O2	2.07	0.54
1:B:138:ILE:HD13	1:B:232:GLY:HA2	1.89	0.54
1:C:24:HIS:O	1:C:24:HIS:CD2	2.61	0.54
1:E:39:PHE:HE2	1:E:161:LEU:CA	2.20	0.54
1:A:15:THR:O	1:A:19:ILE:HG12	2.08	0.53
1:H:256:HIS:HD1	1:H:278:GLU:CD	2.12	0.53
1:D:133:PHE:C	1:D:133:PHE:CD1	2.86	0.53
1:G:24:HIS:O	1:G:24:HIS:CD2	2.61	0.53
1:B:316:LEU:HB2	2:B:348:FAB:O2	2.07	0.53
1:C:21:GLU:HG3	1:C:155:ARG:HH21	1.73	0.53
1:C:133:PHE:CD1	1:C:133:PHE:C	2.86	0.53
1:E:24:HIS:CD2	1:E:24:HIS:O	2.61	0.53
1:G:39:PHE:CE2	1:G:161:LEU:HD13	2.43	0.53
1:H:15:THR:O	1:H:19:ILE:HG12	2.08	0.53
1:A:21:GLU:HG3	1:A:155:ARG:HH21	1.72	0.53
1:A:133:PHE:C	1:A:133:PHE:CD1	2.86	0.53
1:B:133:PHE:CD1	1:B:133:PHE:C	2.86	0.53
1:B:210:LEU:HD11	1:B:270:LEU:HD21	1.91	0.53
1:F:209:TRP:NE1	1:F:210:LEU:HD21	2.24	0.53
1:H:89:LEU:O	1:H:90:THR:HG23	2.08	0.53
1:H:177:VAL:HG22	1:H:304:GLU:HB2	1.89	0.53
1:B:24:HIS:CD2	1:B:24:HIS:O	2.61	0.53
1:B:253:ILE:HA	1:E:42:PHE:CZ	2.44	0.53
1:E:133:PHE:CD1	1:E:133:PHE:C	2.86	0.53
1:F:24:HIS:CD2	1:F:24:HIS:O	2.61	0.53
1:A:269:THR:C	1:A:271:LYS:H	2.15	0.53
1:B:89:LEU:O	1:B:90:THR:HG23	2.08	0.53
1:F:293:ARG:NE	1:F:333:VAL:HG23	2.24	0.53
1:C:89:LEU:O	1:C:90:THR:HG23	2.08	0.53
1:C:168:GLU:O	1:C:171:ALA:N	2.41	0.53
1:E:157:VAL:HG12	1:E:158:LYS:N	2.22	0.53
1:A:24:HIS:O	1:A:24:HIS:CD2	2.61	0.53
1:A:24:HIS:C	1:A:24:HIS:CD2	2.81	0.53
1:B:90:THR:HG21	1:F:209:TRP:HD1	1.74	0.53
1:B:209:TRP:NE1	1:B:210:LEU:HD21	2.24	0.53
1:B:254:GLN:O	1:B:258:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ARG:NE	1:B:333:VAL:HG23	2.24	0.53
1:D:293:ARG:NE	1:D:333:VAL:HG23	2.24	0.53
1:E:293:ARG:NE	1:E:333:VAL:HG23	2.24	0.53
1:F:252:ASN:ND2	1:F:255:ASP:HB2	2.24	0.53
1:A:208:PRO:HB2	1:E:233:LEU:O	2.09	0.53
1:C:1:MET:HE2	1:C:177:VAL:CG2	2.33	0.53
1:D:252:ASN:ND2	1:D:255:ASP:HB2	2.24	0.53
1:A:136:SER:O	1:A:137:LEU:HD23	2.08	0.52
1:A:293:ARG:NE	1:A:333:VAL:HG23	2.24	0.52
1:B:101:ALA:HA	1:B:130:TYR:CD2	2.44	0.52
1:C:293:ARG:NE	1:C:333:VAL:HG23	2.24	0.52
1:A:252:ASN:ND2	1:A:255:ASP:HB2	2.24	0.52
1:C:138:ILE:HD13	1:C:232:GLY:HA2	1.89	0.52
1:E:142:ARG:CG	1:E:142:ARG:NH1	2.69	0.52
1:A:1:MET:HE3	1:A:176:ASP:CB	2.39	0.52
1:D:117:LEU:CD2	1:D:133:PHE:HB2	2.40	0.52
1:F:1:MET:HE1	1:F:177:VAL:CG2	2.37	0.52
1:G:117:LEU:CD2	1:G:133:PHE:HB2	2.40	0.52
1:G:133:PHE:C	1:G:133:PHE:CD1	2.86	0.52
1:H:138:ILE:HD13	1:H:232:GLY:HA2	1.89	0.52
1:H:168:GLU:HG2	1:H:172:ARG:HD2	1.92	0.52
1:A:35:TYR:HD1	1:A:160:PHE:HB2	1.73	0.52
1:A:209:TRP:NE1	1:A:210:LEU:HD21	2.24	0.52
1:C:209:TRP:NE1	1:C:210:LEU:HD21	2.24	0.52
1:D:209:TRP:NE1	1:D:210:LEU:HD21	2.24	0.52
1:E:209:TRP:NE1	1:E:210:LEU:HD21	2.24	0.52
1:G:293:ARG:NE	1:G:333:VAL:HG23	2.24	0.52
1:H:133:PHE:CD1	1:H:133:PHE:C	2.86	0.52
1:H:293:ARG:NE	1:H:333:VAL:HG23	2.24	0.52
1:A:233:LEU:O	1:E:208:PRO:HB2	2.10	0.52
1:B:78:HIS:CG	1:B:87:MET:HE1	2.41	0.52
1:E:61:ASN:OD1	1:E:63:GLN:NE2	2.43	0.52
1:E:252:ASN:ND2	1:E:255:ASP:HB2	2.24	0.52
1:F:117:LEU:CD2	1:F:133:PHE:HB2	2.40	0.52
1:F:184:VAL:HG13	1:F:284:PRO:HA	1.92	0.52
1:G:24:HIS:CD2	1:G:24:HIS:C	2.81	0.52
1:H:209:TRP:NE1	1:H:210:LEU:HD21	2.24	0.52
1:D:14:SER:O	1:D:18:CYS:HB2	2.10	0.52
1:D:267:GLU:OE1	1:D:269:THR:HG23	2.10	0.52
1:E:184:VAL:HG13	1:E:284:PRO:HA	1.92	0.52
1:F:14:SER:O	1:F:18:CYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:SER:OG	1:F:137:LEU:N	2.43	0.52
1:G:136:SER:OG	1:G:137:LEU:N	2.43	0.52
1:G:269:THR:C	1:G:271:LYS:H	2.16	0.52
1:A:136:SER:OG	1:A:137:LEU:N	2.43	0.52
1:A:142:ARG:HG3	1:A:142:ARG:NH1	2.14	0.52
1:B:184:VAL:HG13	1:B:284:PRO:HA	1.92	0.52
1:B:252:ASN:ND2	1:B:255:ASP:HB2	2.24	0.52
1:C:161:LEU:HD11	1:H:253:ILE:HG21	1.92	0.52
1:C:252:ASN:ND2	1:C:255:ASP:HB2	2.24	0.52
1:D:61:ASN:HB2	1:D:63:GLN:HB2	1.92	0.52
1:G:209:TRP:NE1	1:G:210:LEU:HD21	2.24	0.52
1:C:117:LEU:CD2	1:C:133:PHE:HB2	2.40	0.52
1:A:271:LYS:NZ	1:E:83:ASN:OD1	2.42	0.51
1:B:14:SER:O	1:B:18:CYS:HB2	2.10	0.51
1:B:55:TYR:CE2	1:B:314:TYR:HE2	2.29	0.51
1:C:24:HIS:CD2	1:C:24:HIS:C	2.81	0.51
1:D:55:TYR:CE2	1:D:314:TYR:HE2	2.29	0.51
1:E:78:HIS:CG	1:E:87:MET:HE1	2.41	0.51
1:F:55:TYR:CE2	1:F:314:TYR:HE2	2.29	0.51
1:A:208:PRO:HD2	1:A:209:TRP:HE3	1.76	0.51
1:C:14:SER:O	1:C:18:CYS:HB2	2.10	0.51
1:C:55:TYR:CE2	1:C:314:TYR:HE2	2.29	0.51
1:H:252:ASN:ND2	1:H:255:ASP:HB2	2.24	0.51
1:A:125:PHE:N	1:A:125:PHE:CD1	2.76	0.51
1:B:159:PHE:C	1:B:160:PHE:CD1	2.89	0.51
1:B:256:HIS:HD1	1:B:278:GLU:CD	2.12	0.51
1:D:184:VAL:HG13	1:D:284:PRO:HA	1.92	0.51
1:E:117:LEU:CD2	1:E:133:PHE:HB2	2.40	0.51
1:F:142:ARG:CG	1:F:142:ARG:NH1	2.69	0.51
1:G:168:GLU:O	1:G:172:ARG:N	2.27	0.51
1:A:256:HIS:HD1	1:A:278:GLU:CD	2.12	0.51
1:B:117:LEU:CD2	1:B:133:PHE:HB2	2.40	0.51
1:B:208:PRO:HD2	1:B:209:TRP:HE3	1.76	0.51
1:C:78:HIS:CG	1:C:87:MET:HE1	2.41	0.51
1:F:160:PHE:N	1:F:160:PHE:CD2	2.78	0.51
1:H:117:LEU:CD2	1:H:133:PHE:HB2	2.40	0.51
1:A:55:TYR:CE2	1:A:314:TYR:HE2	2.29	0.51
1:C:19:ILE:HD11	1:C:179:ILE:CD1	2.40	0.51
1:C:184:VAL:HG13	1:C:284:PRO:HA	1.92	0.51
1:D:101:ALA:HA	1:D:130:TYR:CG	2.46	0.51
1:E:14:SER:O	1:E:18:CYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:PHE:CE2	1:E:161:LEU:HA	2.44	0.51
1:C:3:VAL:HB	1:C:32:VAL:HG22	1.93	0.51
1:E:21:GLU:HA	1:E:155:ARG:NH1	2.26	0.51
1:F:208:PRO:HD2	1:F:209:TRP:HE3	1.76	0.51
1:G:252:ASN:ND2	1:G:255:ASP:HB2	2.24	0.51
1:G:269:THR:C	1:G:271:LYS:N	2.68	0.51
1:A:1:MET:CE	1:A:177:VAL:HG23	2.41	0.51
1:A:266:LEU:C	1:A:268:PRO:HD3	2.36	0.51
1:E:55:TYR:CE2	1:E:314:TYR:HE2	2.29	0.51
1:G:14:SER:O	1:G:18:CYS:HB2	2.10	0.51
1:A:14:SER:O	1:A:18:CYS:HB2	2.10	0.51
1:A:21:GLU:HA	1:A:155:ARG:NH1	2.26	0.51
1:A:117:LEU:CD2	1:A:133:PHE:HB2	2.40	0.51
1:D:21:GLU:HA	1:D:155:ARG:NH1	2.26	0.51
1:D:124:MET:HE3	1:H:79:ILE:CG2	2.37	0.51
1:F:3:VAL:HB	1:F:32:VAL:HG22	1.93	0.51
1:G:3:VAL:HB	1:G:32:VAL:HG22	1.93	0.51
1:H:14:SER:O	1:H:18:CYS:HB2	2.10	0.51
1:F:21:GLU:HA	1:F:155:ARG:NH1	2.26	0.51
1:A:3:VAL:HB	1:A:32:VAL:HG22	1.93	0.50
1:A:184:VAL:HG13	1:A:284:PRO:HA	1.92	0.50
1:B:93:SER:HG	1:B:135:THR:HB	1.72	0.50
1:H:229:ILE:C	1:H:230:ILE:HG13	2.37	0.50
1:A:21:GLU:CG	1:A:155:ARG:NH2	2.71	0.50
1:A:229:ILE:C	1:A:230:ILE:HG13	2.37	0.50
1:B:21:GLU:HA	1:B:155:ARG:NH1	2.26	0.50
1:C:21:GLU:HA	1:C:155:ARG:NH1	2.26	0.50
1:D:83:ASN:O	1:D:86:ASN:N	2.45	0.50
1:F:229:ILE:C	1:F:230:ILE:HG13	2.37	0.50
1:G:55:TYR:CE2	1:G:314:TYR:HE2	2.29	0.50
1:H:21:GLU:HA	1:H:155:ARG:NH1	2.26	0.50
1:H:24:HIS:CD2	1:H:24:HIS:C	2.81	0.50
1:D:3:VAL:HB	1:D:32:VAL:HG22	1.93	0.50
1:E:3:VAL:HB	1:E:32:VAL:HG22	1.93	0.50
1:H:83:ASN:O	1:H:86:ASN:N	2.45	0.50
1:H:171:ALA:HB1	1:H:298:PHE:CD2	2.46	0.50
1:A:171:ALA:C	1:A:173:GLY:N	2.68	0.50
1:B:36:ALA:O	1:B:161:LEU:HD12	2.12	0.50
1:B:229:ILE:C	1:B:230:ILE:HG13	2.37	0.50
1:D:61:ASN:HB3	1:D:62:PRO:HD2	1.92	0.50
1:E:83:ASN:O	1:E:86:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:GLU:HA	1:G:155:ARG:NH1	2.26	0.50
1:G:256:HIS:HD1	1:G:278:GLU:CD	2.12	0.50
1:A:253:ILE:HG13	1:F:42:PHE:CG	2.43	0.50
1:C:83:ASN:O	1:C:86:ASN:N	2.45	0.50
1:F:83:ASN:O	1:F:86:ASN:N	2.45	0.50
1:H:3:VAL:HB	1:H:32:VAL:HG22	1.93	0.50
1:A:83:ASN:O	1:A:86:ASN:N	2.45	0.50
1:A:89:LEU:HD23	1:A:138:ILE:O	2.12	0.50
1:F:265:ARG:O	1:F:268:PRO:HD3	2.11	0.50
1:H:55:TYR:CE2	1:H:314:TYR:HE2	2.29	0.50
1:H:184:VAL:HG13	1:H:284:PRO:HA	1.92	0.50
1:B:166:SER:HG	1:B:169:GLU:H	1.58	0.50
1:B:178:ILE:HB	1:B:305:VAL:HG22	1.93	0.50
1:C:89:LEU:HD23	1:C:138:ILE:O	2.12	0.50
1:C:162:ARG:HG3	1:C:162:ARG:NH1	2.26	0.50
1:C:229:ILE:C	1:C:230:ILE:HG13	2.36	0.50
1:E:21:GLU:CG	1:E:155:ARG:NH2	2.72	0.50
1:H:142:ARG:CG	1:H:142:ARG:NH1	2.69	0.50
1:H:166:SER:HG	1:H:169:GLU:HB2	1.75	0.50
1:B:21:GLU:HG3	1:B:155:ARG:HH21	1.73	0.50
1:B:89:LEU:HD23	1:B:138:ILE:O	2.12	0.50
1:E:40:THR:OG1	1:E:142:ARG:HD3	2.12	0.50
1:G:34:VAL:N	1:G:158:LYS:O	2.42	0.50
1:B:1:MET:HE3	1:B:176:ASP:HB3	1.93	0.50
1:B:40:THR:OG1	1:B:142:ARG:HD3	2.12	0.50
1:D:95:TYR:N	1:D:95:TYR:CD1	2.80	0.50
1:G:165:GLU:HB2	1:G:169:GLU:OE1	2.12	0.50
1:H:128:TYR:CZ	1:H:216:THR:HB	2.47	0.50
1:B:17:LEU:O	1:B:21:GLU:HB2	2.12	0.49
1:D:17:LEU:O	1:D:21:GLU:HB2	2.12	0.49
1:G:184:VAL:HG13	1:G:284:PRO:HA	1.92	0.49
1:G:208:PRO:HD2	1:G:209:TRP:HE3	1.76	0.49
1:H:89:LEU:HD23	1:H:138:ILE:O	2.12	0.49
1:A:40:THR:OG1	1:A:142:ARG:HD3	2.12	0.49
1:B:3:VAL:HB	1:B:32:VAL:HG22	1.93	0.49
1:C:95:TYR:CD1	1:C:95:TYR:N	2.80	0.49
1:C:246:ASN:C	1:C:246:ASN:OD1	2.56	0.49
1:C:318:ILE:O	1:C:318:ILE:HG12	2.12	0.49
1:D:318:ILE:O	1:D:318:ILE:HG12	2.12	0.49
1:A:17:LEU:O	1:A:21:GLU:HB2	2.12	0.49
1:A:128:TYR:CD2	1:A:128:TYR:N	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASN:C	1:A:246:ASN:OD1	2.56	0.49
1:C:40:THR:OG1	1:C:142:ARG:HD3	2.12	0.49
1:D:167:PHE:N	1:D:167:PHE:CD1	2.80	0.49
1:D:229:ILE:C	1:D:230:ILE:HG13	2.37	0.49
1:F:95:TYR:CD1	1:F:95:TYR:N	2.80	0.49
1:G:89:LEU:HD23	1:G:138:ILE:O	2.12	0.49
1:G:251:ASN:OD1	1:G:280:THR:HG22	2.13	0.49
1:H:40:THR:OG1	1:H:142:ARG:HD3	2.12	0.49
1:C:101:ALA:CB	1:C:130:TYR:CD2	2.96	0.49
1:E:270:LEU:O	1:E:271:LYS:C	2.51	0.49
1:E:318:ILE:O	1:E:318:ILE:HG12	2.12	0.49
1:F:89:LEU:HD23	1:F:138:ILE:O	2.12	0.49
1:G:40:THR:OG1	1:G:142:ARG:HD3	2.12	0.49
1:H:78:HIS:CG	1:H:87:MET:HE1	2.41	0.49
1:B:83:ASN:O	1:B:86:ASN:N	2.45	0.49
1:B:246:ASN:C	1:B:246:ASN:OD1	2.56	0.49
1:C:208:PRO:HD2	1:C:209:TRP:HE3	1.76	0.49
1:E:20:HIS:CE1	1:E:155:ARG:CD	2.96	0.49
1:E:251:ASN:OD1	1:E:280:THR:HG22	2.13	0.49
1:G:17:LEU:O	1:G:21:GLU:HB2	2.12	0.49
1:G:83:ASN:O	1:G:86:ASN:N	2.45	0.49
1:H:177:VAL:HG12	1:H:178:ILE:N	2.28	0.49
1:A:95:TYR:CD1	1:A:95:TYR:N	2.80	0.49
1:B:251:ASN:OD1	1:B:280:THR:HG22	2.13	0.49
1:C:251:ASN:OD1	1:C:280:THR:HG22	2.13	0.49
1:D:20:HIS:CE1	1:D:155:ARG:CD	2.96	0.49
1:F:151:ARG:HH21	1:F:154:GLU:CD	2.21	0.49
1:F:318:ILE:O	1:F:318:ILE:HG12	2.12	0.49
1:H:21:GLU:HG3	1:H:155:ARG:HH21	1.73	0.49
1:C:17:LEU:O	1:C:21:GLU:HB2	2.12	0.49
1:D:35:TYR:CE1	1:D:160:PHE:CD2	3.00	0.49
1:D:269:THR:C	1:D:271:LYS:H	2.21	0.49
1:H:208:PRO:HD2	1:H:209:TRP:HE3	1.76	0.49
1:A:267:GLU:O	1:A:270:LEU:HB2	2.13	0.49
1:B:95:TYR:CD1	1:B:95:TYR:N	2.80	0.49
1:B:318:ILE:O	1:B:318:ILE:HG12	2.12	0.49
1:D:208:PRO:HD2	1:D:209:TRP:HE3	1.76	0.49
1:E:17:LEU:O	1:E:21:GLU:HB2	2.12	0.49
1:E:59:PRO:HB2	1:E:61:ASN:O	2.12	0.49
1:F:246:ASN:C	1:F:246:ASN:OD1	2.56	0.49
1:F:335:GLU:O	1:F:338:ASN:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:TYR:CD1	1:G:160:PHE:HB2	2.47	0.49
1:G:61:ASN:ND2	1:G:63:GLN:N	2.59	0.49
1:H:251:ASN:OD1	1:H:280:THR:HG22	2.13	0.49
1:C:20:HIS:CE1	1:C:155:ARG:CD	2.96	0.49
1:C:268:PRO:HB2	1:G:82:PRO:HA	1.95	0.49
1:D:89:LEU:HD23	1:D:138:ILE:O	2.12	0.49
1:D:251:ASN:OD1	1:D:280:THR:HG22	2.13	0.49
1:F:178:ILE:O	1:F:178:ILE:HG22	2.10	0.49
1:H:93:SER:HG	1:H:135:THR:HB	1.73	0.49
1:H:95:TYR:N	1:H:95:TYR:CD1	2.80	0.49
1:H:318:ILE:O	1:H:318:ILE:HG12	2.12	0.49
1:A:37:ASP:HB3	1:A:163:LYS:HG3	1.95	0.49
1:B:128:TYR:CE2	1:B:216:THR:HB	2.47	0.49
1:C:74:TYR:CE1	1:C:78:HIS:HE1	2.31	0.49
1:C:270:LEU:C	1:C:272:ASP:N	2.64	0.49
1:D:246:ASN:C	1:D:246:ASN:OD1	2.56	0.49
1:E:23:TYR:CE2	1:E:330:PHE:HD2	2.31	0.49
1:F:213:PHE:CD1	1:F:213:PHE:C	2.91	0.49
1:G:23:TYR:CE2	1:G:330:PHE:HD2	2.31	0.49
1:G:246:ASN:C	1:G:246:ASN:OD1	2.56	0.49
1:A:251:ASN:OD1	1:A:280:THR:HG22	2.13	0.48
1:B:74:TYR:CE1	1:B:78:HIS:HE1	2.31	0.48
1:D:213:PHE:CD1	1:D:213:PHE:C	2.91	0.48
1:E:269:THR:C	1:E:271:LYS:N	2.68	0.48
1:F:251:ASN:OD1	1:F:280:THR:HG22	2.13	0.48
1:G:21:GLU:CG	1:G:155:ARG:NH2	2.72	0.48
1:H:190:GLN:O	1:H:190:GLN:HG2	2.13	0.48
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.61	0.48
1:A:142:ARG:CG	1:A:142:ARG:NH1	2.69	0.48
1:A:287:PRO:HB2	1:A:288:GLN:CD	2.38	0.48
1:B:23:TYR:CE2	1:B:330:PHE:HD2	2.31	0.48
1:B:142:ARG:CG	1:B:142:ARG:NH1	2.69	0.48
1:C:253:ILE:HG21	1:H:161:LEU:HD21	1.94	0.48
1:D:21:GLU:CG	1:D:155:ARG:NH2	2.71	0.48
1:D:151:ARG:HH21	1:D:154:GLU:CD	2.21	0.48
1:E:74:TYR:CE1	1:E:78:HIS:HE1	2.31	0.48
1:E:180:ASN:HD22	1:E:307:HIS:HD2	1.60	0.48
1:E:246:ASN:C	1:E:246:ASN:OD1	2.56	0.48
1:A:23:TYR:CE2	1:A:330:PHE:HD2	2.31	0.48
1:A:166:SER:OG	1:A:169:GLU:N	2.41	0.48
1:C:213:PHE:CD1	1:C:213:PHE:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:THR:OG1	1:D:142:ARG:HD3	2.12	0.48
1:E:213:PHE:CD1	1:E:213:PHE:C	2.91	0.48
1:F:17:LEU:O	1:F:21:GLU:HB2	2.13	0.48
1:F:40:THR:OG1	1:F:142:ARG:HD3	2.12	0.48
1:F:74:TYR:CE1	1:F:78:HIS:HE1	2.31	0.48
1:H:23:TYR:CE2	1:H:330:PHE:HD2	2.31	0.48
1:A:318:ILE:HG12	1:A:318:ILE:O	2.12	0.48
1:B:270:LEU:C	1:B:272:ASP:N	2.71	0.48
1:C:23:TYR:CE2	1:C:330:PHE:HD2	2.31	0.48
1:E:190:GLN:O	1:E:190:GLN:HG2	2.13	0.48
1:G:229:ILE:C	1:G:230:ILE:HG13	2.37	0.48
1:H:151:ARG:O	1:H:154:GLU:HG2	2.14	0.48
1:H:213:PHE:CD1	1:H:213:PHE:C	2.91	0.48
1:A:252:ASN:OD1	1:A:254:GLN:HB2	2.14	0.48
1:B:151:ARG:HH21	1:B:154:GLU:CD	2.21	0.48
1:B:238:LEU:N	1:B:238:LEU:CD1	2.74	0.48
1:C:151:ARG:O	1:C:154:GLU:HG2	2.14	0.48
1:E:95:TYR:N	1:E:95:TYR:CD1	2.80	0.48
1:E:229:ILE:C	1:E:230:ILE:HG13	2.37	0.48
1:G:142:ARG:CG	1:G:142:ARG:NH1	2.69	0.48
1:G:318:ILE:O	1:G:318:ILE:HG12	2.12	0.48
1:H:246:ASN:C	1:H:246:ASN:OD1	2.56	0.48
1:A:171:ALA:O	1:A:174:GLY:N	2.43	0.48
1:A:252:ASN:ND2	1:A:255:ASP:OD2	2.44	0.48
1:D:23:TYR:CE2	1:D:330:PHE:HD2	2.31	0.48
1:E:89:LEU:HD23	1:E:138:ILE:O	2.12	0.48
1:C:1:MET:CE	1:C:177:VAL:CG2	2.91	0.48
1:C:190:GLN:HE22	1:C:290:ARG:HH22	1.62	0.48
1:E:6:ILE:HD13	1:E:164:VAL:HG21	1.95	0.48
1:E:151:ARG:O	1:E:154:GLU:HG2	2.14	0.48
1:F:151:ARG:O	1:F:154:GLU:HG2	2.14	0.48
1:G:95:TYR:CD1	1:G:95:TYR:N	2.80	0.48
1:H:180:ASN:ND2	1:H:180:ASN:C	2.72	0.48
1:H:190:GLN:HE22	1:H:290:ARG:HH22	1.62	0.48
1:A:37:ASP:CB	1:A:163:LYS:HG3	2.43	0.48
1:B:20:HIS:CE1	1:B:155:ARG:CD	2.96	0.48
1:B:190:GLN:O	1:B:190:GLN:HG2	2.13	0.48
1:C:107:TRP:HA	1:C:110:MET:HG3	1.96	0.48
1:G:252:ASN:ND2	1:G:255:ASP:OD2	2.44	0.48
1:A:213:PHE:CD1	1:A:213:PHE:C	2.91	0.48
1:C:151:ARG:HH21	1:C:154:GLU:CD	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LEU:HD21	1:E:133:PHE:HB2	1.96	0.48
1:F:125:PHE:N	1:F:125:PHE:CD1	2.81	0.48
1:H:74:TYR:CE1	1:H:78:HIS:HE1	2.32	0.48
1:H:107:TRP:HA	1:H:110:MET:HG3	1.96	0.48
1:A:74:TYR:CE1	1:A:78:HIS:HE1	2.32	0.48
1:A:267:GLU:N	1:A:268:PRO:HD3	2.26	0.48
1:D:107:TRP:HA	1:D:110:MET:HG3	1.96	0.48
1:D:194:LEU:HA	1:D:194:LEU:HD23	1.26	0.48
1:E:335:GLU:O	1:E:338:ASN:N	2.43	0.48
1:F:1:MET:HE3	1:F:176:ASP:CB	2.44	0.48
1:G:107:TRP:HA	1:G:110:MET:HG3	1.96	0.48
1:H:20:HIS:CE1	1:H:155:ARG:CD	2.96	0.48
1:H:40:THR:OG1	1:H:46:ASP:OD1	2.18	0.48
1:B:107:TRP:HA	1:B:110:MET:HG3	1.96	0.47
1:B:168:GLU:O	1:B:169:GLU:C	2.57	0.47
1:B:190:GLN:HE22	1:B:290:ARG:HH22	1.62	0.47
1:C:209:TRP:CD1	1:C:210:LEU:CD2	2.97	0.47
1:D:238:LEU:CD1	1:D:238:LEU:N	2.74	0.47
1:E:21:GLU:HG3	1:E:155:ARG:HH21	1.73	0.47
1:G:267:GLU:O	1:G:269:THR:N	2.47	0.47
1:H:17:LEU:O	1:H:21:GLU:HB2	2.12	0.47
1:H:39:PHE:HE2	1:H:161:LEU:HA	1.79	0.47
1:A:151:ARG:O	1:A:154:GLU:HG2	2.14	0.47
1:A:151:ARG:HH21	1:A:154:GLU:CD	2.21	0.47
1:B:213:PHE:C	1:B:213:PHE:CD1	2.91	0.47
1:C:238:LEU:N	1:C:238:LEU:CD1	2.74	0.47
1:D:101:ALA:HA	1:D:130:TYR:CD1	2.49	0.47
1:D:136:SER:OG	1:D:137:LEU:N	2.43	0.47
1:D:151:ARG:O	1:D:154:GLU:HG2	2.14	0.47
1:E:136:SER:OG	1:E:137:LEU:N	2.43	0.47
1:E:151:ARG:HH21	1:E:154:GLU:CD	2.21	0.47
1:F:107:TRP:HA	1:F:110:MET:HG3	1.96	0.47
1:G:3:VAL:HG13	1:G:179:ILE:HD11	1.96	0.47
1:G:61:ASN:CG	1:G:63:GLN:HB2	2.39	0.47
1:G:327:ALA:O	1:G:330:PHE:HB3	2.14	0.47
1:H:167:PHE:CE2	1:H:189:LEU:CB	2.88	0.47
1:A:190:GLN:O	1:A:190:GLN:HG2	2.13	0.47
1:A:209:TRP:CD1	1:A:210:LEU:CD2	2.97	0.47
1:A:209:TRP:CD1	1:A:210:LEU:HD23	2.49	0.47
1:A:327:ALA:O	1:A:330:PHE:HB3	2.14	0.47
1:B:209:TRP:CD1	1:B:210:LEU:CD2	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASN:ND2	1:B:255:ASP:OD2	2.44	0.47
1:C:327:ALA:O	1:C:330:PHE:HB3	2.14	0.47
1:D:190:GLN:O	1:D:190:GLN:HG2	2.13	0.47
1:D:335:GLU:O	1:D:338:ASN:N	2.43	0.47
1:G:117:LEU:HD21	1:G:133:PHE:HB2	1.96	0.47
1:A:17:LEU:HD12	1:A:17:LEU:HA	1.47	0.47
1:D:21:GLU:HG3	1:D:155:ARG:HH21	1.73	0.47
1:D:209:TRP:CD1	1:D:210:LEU:HD23	2.49	0.47
1:D:209:TRP:CD1	1:D:210:LEU:CD2	2.98	0.47
1:E:265:ARG:O	1:E:266:LEU:C	2.56	0.47
1:E:327:ALA:O	1:E:330:PHE:HB3	2.14	0.47
1:F:190:GLN:O	1:F:190:GLN:HG2	2.13	0.47
1:F:207:ALA:HA	1:F:209:TRP:CZ3	2.50	0.47
1:F:209:TRP:CD1	1:F:210:LEU:HD23	2.49	0.47
1:F:238:LEU:N	1:F:238:LEU:CD1	2.74	0.47
1:H:17:LEU:HD12	1:H:17:LEU:HA	1.47	0.47
1:H:170:VAL:HG12	1:H:175:ALA:CB	2.44	0.47
1:A:207:ALA:HA	1:A:209:TRP:CZ3	2.49	0.47
1:B:128:TYR:HD1	1:B:128:TYR:H	1.59	0.47
1:D:327:ALA:O	1:D:330:PHE:HB3	2.14	0.47
1:E:190:GLN:HE22	1:E:290:ARG:HH22	1.62	0.47
1:F:23:TYR:CE2	1:F:330:PHE:HD2	2.31	0.47
1:G:74:TYR:CE1	1:G:78:HIS:HE1	2.31	0.47
1:G:151:ARG:O	1:G:154:GLU:HG2	2.14	0.47
1:G:250:ILE:HG23	1:G:250:ILE:HD12	1.42	0.47
1:H:265:ARG:O	1:H:265:ARG:HG2	2.15	0.47
1:B:133:PHE:CD1	1:B:134:ASN:N	2.83	0.47
1:B:151:ARG:O	1:B:154:GLU:HG2	2.14	0.47
1:B:157:VAL:HG12	1:B:158:LYS:N	2.23	0.47
1:D:170:VAL:HG12	1:D:178:ILE:CD1	2.44	0.47
1:E:65:ALA:HB2	1:E:106:TYR:CE2	2.50	0.47
1:E:107:TRP:HA	1:E:110:MET:HG3	1.96	0.47
1:F:209:TRP:CD1	1:F:210:LEU:CD2	2.98	0.47
1:G:3:VAL:CG1	1:G:179:ILE:CD1	2.92	0.47
1:G:170:VAL:HB	1:G:178:ILE:HD11	1.96	0.47
1:H:238:LEU:N	1:H:238:LEU:CD1	2.74	0.47
1:A:107:TRP:HA	1:A:110:MET:HG3	1.96	0.47
1:A:115:ARG:NH2	1:A:121:GLU:CD	2.65	0.47
1:A:133:PHE:CD1	1:A:134:ASN:N	2.83	0.47
1:A:209:TRP:HD1	1:E:90:THR:HG21	1.80	0.47
1:B:136:SER:OG	1:B:137:LEU:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:O	1:B:271:LYS:C	2.58	0.47
1:B:327:ALA:O	1:B:330:PHE:HB3	2.14	0.47
1:C:83:ASN:OD1	1:G:271:LYS:NZ	2.45	0.47
1:C:133:PHE:CD1	1:C:134:ASN:N	2.83	0.47
1:C:207:ALA:HA	1:C:209:TRP:CZ3	2.50	0.47
1:D:1:MET:HE3	1:D:176:ASP:HB3	1.96	0.47
1:D:117:LEU:HD21	1:D:133:PHE:HB2	1.96	0.47
1:D:190:GLN:HE22	1:D:290:ARG:HH22	1.62	0.47
1:F:36:ALA:O	1:F:161:LEU:HA	2.15	0.47
1:F:327:ALA:O	1:F:330:PHE:HB3	2.14	0.47
1:G:207:ALA:HA	1:G:209:TRP:CZ3	2.50	0.47
1:H:167:PHE:HE2	1:H:189:LEU:O	1.96	0.47
1:H:209:TRP:CD1	1:H:210:LEU:CD2	2.98	0.47
1:H:327:ALA:O	1:H:330:PHE:HB3	2.14	0.47
1:A:90:THR:HG21	1:E:209:TRP:HD1	1.80	0.47
1:B:207:ALA:HA	1:B:209:TRP:CZ3	2.50	0.47
1:B:267:GLU:C	1:B:267:GLU:OE1	2.58	0.47
1:E:209:TRP:CD1	1:E:210:LEU:HD23	2.49	0.47
1:G:21:GLU:HG3	1:G:155:ARG:HH21	1.73	0.47
1:G:213:PHE:C	1:G:213:PHE:CD1	2.91	0.47
1:G:286:ARG:CG	1:G:287:PRO:CD	2.92	0.47
1:H:207:ALA:HA	1:H:209:TRP:CZ3	2.50	0.47
1:A:166:SER:O	1:A:169:GLU:HB3	2.15	0.47
1:C:171:ALA:CB	1:C:298:PHE:CD2	2.98	0.47
1:C:209:TRP:CD1	1:C:210:LEU:HD23	2.49	0.47
1:G:209:TRP:CD1	1:G:210:LEU:CD2	2.98	0.47
1:H:151:ARG:HH21	1:H:154:GLU:CD	2.21	0.47
1:B:177:VAL:HG22	1:B:304:GLU:HB2	1.97	0.47
1:C:90:THR:HG21	1:G:209:TRP:HD1	1.80	0.47
1:D:74:TYR:CE1	1:D:78:HIS:HE1	2.32	0.47
1:D:207:ALA:HA	1:D:209:TRP:CZ3	2.50	0.47
1:E:207:ALA:HA	1:E:209:TRP:CZ3	2.50	0.47
1:F:190:GLN:HE22	1:F:290:ARG:HH22	1.62	0.47
1:G:39:PHE:HD2	1:G:161:LEU:HD13	1.74	0.47
1:G:151:ARG:HH21	1:G:154:GLU:CD	2.21	0.47
1:G:170:VAL:O	1:G:171:ALA:C	2.57	0.47
1:H:117:LEU:HD21	1:H:133:PHE:HB2	1.96	0.47
1:H:133:PHE:CD1	1:H:134:ASN:N	2.83	0.47
1:E:252:ASN:ND2	1:E:255:ASP:OD2	2.44	0.46
1:G:133:PHE:CD1	1:G:134:ASN:N	2.83	0.46
1:G:209:TRP:CD1	1:G:210:LEU:HD23	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:TRP:CD1	1:B:210:LEU:HD23	2.49	0.46
1:C:233:LEU:O	1:G:208:PRO:HB2	2.14	0.46
1:F:1:MET:HG3	1:F:176:ASP:HB2	1.98	0.46
1:F:101:ALA:HA	1:F:130:TYR:CG	2.50	0.46
1:G:20:HIS:CE1	1:G:155:ARG:CD	2.96	0.46
1:G:267:GLU:N	1:G:268:PRO:HD3	2.29	0.46
1:H:21:GLU:HA	1:H:155:ARG:CZ	2.46	0.46
1:H:21:GLU:CG	1:H:155:ARG:NH2	2.72	0.46
1:A:190:GLN:HE22	1:A:290:ARG:HH22	1.62	0.46
1:E:36:ALA:O	1:E:161:LEU:HA	2.15	0.46
1:E:133:PHE:CD1	1:E:134:ASN:N	2.83	0.46
1:E:209:TRP:CD1	1:E:210:LEU:CD2	2.98	0.46
1:F:59:PRO:HB2	1:F:61:ASN:O	2.15	0.46
1:F:118:THR:O	1:F:121:GLU:HB2	2.16	0.46
1:F:194:LEU:HA	1:F:194:LEU:HD23	1.26	0.46
1:G:21:GLU:HA	1:G:155:ARG:CZ	2.46	0.46
1:H:130:TYR:CD1	1:H:130:TYR:C	2.93	0.46
1:H:267:GLU:HB3	1:H:270:LEU:HG	1.98	0.46
1:A:21:GLU:HA	1:A:155:ARG:CZ	2.46	0.46
1:A:250:ILE:HG23	1:A:250:ILE:HD12	1.43	0.46
1:D:133:PHE:CD1	1:D:134:ASN:N	2.83	0.46
1:D:238:LEU:HD12	1:D:238:LEU:HA	1.50	0.46
1:A:335:GLU:O	1:A:338:ASN:N	2.43	0.46
1:C:117:LEU:HD21	1:C:133:PHE:HB2	1.96	0.46
1:C:250:ILE:HG23	1:C:250:ILE:HD12	1.42	0.46
1:D:263:CYS:O	1:D:267:GLU:N	2.48	0.46
1:E:159:PHE:C	1:E:160:PHE:CD1	2.93	0.46
1:F:145:LEU:HA	1:F:145:LEU:HD23	1.77	0.46
1:G:37:ASP:HB3	1:G:163:LYS:HA	1.96	0.46
1:G:63:GLN:O	1:G:64:GLU:C	2.59	0.46
1:H:209:TRP:CD1	1:H:210:LEU:HD23	2.49	0.46
1:A:40:THR:OG1	1:A:46:ASP:OD1	2.18	0.46
1:B:21:GLU:HA	1:B:155:ARG:CZ	2.46	0.46
1:B:117:LEU:HD21	1:B:133:PHE:HB2	1.96	0.46
1:D:118:THR:O	1:D:121:GLU:HB2	2.16	0.46
1:H:335:GLU:O	1:H:338:ASN:N	2.43	0.46
1:A:20:HIS:CE1	1:A:155:ARG:CD	2.96	0.46
1:A:117:LEU:HD21	1:A:133:PHE:HB2	1.96	0.46
1:A:118:THR:HG23	1:A:118:THR:H	1.36	0.46
1:A:171:ALA:O	1:A:173:GLY:N	2.49	0.46
1:B:21:GLU:CG	1:B:155:ARG:NH2	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:GLU:HA	1:E:155:ARG:CZ	2.46	0.46
1:F:20:HIS:CE1	1:F:155:ARG:CD	2.96	0.46
1:F:58:GLU:CG	1:F:59:PRO:HD2	2.46	0.46
1:G:118:THR:O	1:G:121:GLU:HB2	2.16	0.46
1:G:293:ARG:NH2	1:G:336:GLU:CD	2.74	0.46
1:A:118:THR:O	1:A:121:GLU:HB2	2.16	0.46
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.76	0.46
1:C:190:GLN:O	1:C:190:GLN:HG2	2.13	0.46
1:D:17:LEU:CA	1:D:152:LEU:HD21	2.46	0.46
1:E:208:PRO:HD2	1:E:209:TRP:HE3	1.76	0.46
1:B:23:TYR:O	1:B:24:HIS:C	2.59	0.46
1:C:21:GLU:HA	1:C:155:ARG:NH2	2.31	0.46
1:D:21:GLU:HA	1:D:155:ARG:CZ	2.46	0.46
1:F:133:PHE:CD1	1:F:134:ASN:N	2.83	0.46
1:H:118:THR:O	1:H:121:GLU:HB2	2.16	0.46
1:B:17:LEU:CA	1:B:152:LEU:HD21	2.46	0.46
1:B:61:ASN:HB3	1:B:63:GLN:HG3	1.98	0.46
1:B:159:PHE:C	1:B:160:PHE:CG	2.94	0.46
1:B:250:ILE:HD13	1:E:250:ILE:CD1	2.39	0.46
1:C:118:THR:O	1:C:121:GLU:HB2	2.16	0.46
1:C:180:ASN:ND2	1:C:182:THR:HG23	2.31	0.46
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.77	0.46
1:E:21:GLU:HA	1:E:155:ARG:NH2	2.31	0.46
1:E:76:LEU:HD23	1:E:76:LEU:HA	1.60	0.46
1:E:118:THR:HG23	1:E:118:THR:H	1.36	0.46
1:E:118:THR:O	1:E:121:GLU:HB2	2.16	0.46
1:E:130:TYR:CD1	1:E:131:GLY:N	2.84	0.46
1:G:190:GLN:HE22	1:G:290:ARG:HH22	1.62	0.46
1:B:101:ALA:C	1:B:102:VAL:HG23	2.42	0.45
1:B:238:LEU:HA	1:B:238:LEU:HD12	1.50	0.45
1:E:17:LEU:CA	1:E:152:LEU:HD21	2.46	0.45
1:F:21:GLU:HA	1:F:155:ARG:NH2	2.31	0.45
1:F:21:GLU:HA	1:F:155:ARG:CZ	2.46	0.45
1:G:21:GLU:HA	1:G:155:ARG:NH2	2.31	0.45
1:G:157:VAL:HG12	1:G:158:LYS:N	2.31	0.45
1:H:101:ALA:C	1:H:102:VAL:HG23	2.42	0.45
1:H:286:ARG:CG	1:H:287:PRO:CD	2.92	0.45
1:H:319:HIS:CG	1:H:320:TRP:N	2.85	0.45
1:A:101:ALA:C	1:A:102:VAL:HG23	2.42	0.45
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.61	0.45
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:CA	1:C:152:LEU:HD21	2.46	0.45
1:C:82:PRO:HA	1:G:268:PRO:HB2	1.97	0.45
1:C:142:ARG:HD2	1:C:142:ARG:C	2.42	0.45
1:D:23:TYR:OH	1:D:331:GLY:HA3	2.17	0.45
1:E:286:ARG:HG3	1:E:287:PRO:HD2	1.98	0.45
1:E:319:HIS:CG	1:E:320:TRP:N	2.84	0.45
1:F:101:ALA:C	1:F:102:VAL:HG23	2.42	0.45
1:G:319:HIS:CG	1:G:320:TRP:N	2.85	0.45
1:H:142:ARG:HD2	1:H:142:ARG:C	2.41	0.45
1:A:21:GLU:HA	1:A:155:ARG:NH2	2.31	0.45
1:B:142:ARG:HD2	1:B:142:ARG:C	2.41	0.45
1:C:23:TYR:O	1:C:24:HIS:C	2.59	0.45
1:C:253:ILE:HG13	1:H:42:PHE:CE1	2.51	0.45
1:C:286:ARG:HG3	1:C:287:PRO:HD2	1.98	0.45
1:D:142:ARG:HD2	1:D:142:ARG:C	2.42	0.45
1:F:117:LEU:HD21	1:F:133:PHE:HB2	1.96	0.45
1:G:61:ASN:ND2	1:G:62:PRO:CD	2.78	0.45
1:G:142:ARG:HD2	1:G:142:ARG:C	2.42	0.45
1:H:166:SER:HG	1:H:169:GLU:CB	2.29	0.45
1:H:166:SER:O	1:H:170:VAL:HG23	2.16	0.45
1:H:180:ASN:C	1:H:180:ASN:HD22	2.24	0.45
1:A:17:LEU:CA	1:A:152:LEU:HD21	2.46	0.45
1:A:82:PRO:HA	1:E:268:PRO:HB2	1.99	0.45
1:B:21:GLU:HA	1:B:155:ARG:NH2	2.31	0.45
1:C:21:GLU:HA	1:C:155:ARG:CZ	2.46	0.45
1:C:101:ALA:C	1:C:102:VAL:HG23	2.42	0.45
1:C:142:ARG:CG	1:C:142:ARG:NH1	2.69	0.45
1:C:268:PRO:C	1:C:270:LEU:H	2.25	0.45
1:D:23:TYR:O	1:D:26:VAL:HG12	2.17	0.45
1:E:101:ALA:C	1:E:102:VAL:HG23	2.42	0.45
1:F:17:LEU:CA	1:F:152:LEU:HD21	2.46	0.45
1:F:130:TYR:CD1	1:F:131:GLY:N	2.84	0.45
1:F:148:LEU:HA	1:F:148:LEU:HD23	1.76	0.45
1:G:286:ARG:CZ	1:G:290:ARG:HB2	2.47	0.45
1:H:21:GLU:HA	1:H:155:ARG:NH2	2.31	0.45
1:A:286:ARG:CG	1:A:287:PRO:CD	2.92	0.45
1:A:319:HIS:CG	1:A:320:TRP:N	2.84	0.45
1:C:167:PHE:CE2	1:C:189:LEU:HB3	2.52	0.45
1:D:286:ARG:CZ	1:D:290:ARG:HB2	2.47	0.45
1:E:23:TYR:O	1:E:26:VAL:HG12	2.17	0.45
1:E:40:THR:OG1	1:E:46:ASP:OD1	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:VAL:CG1	1:E:178:ILE:HD13	2.46	0.45
1:E:269:THR:C	1:E:271:LYS:H	2.24	0.45
1:F:23:TYR:OH	1:F:331:GLY:HA3	2.17	0.45
1:F:286:ARG:CZ	1:F:290:ARG:HB2	2.47	0.45
1:G:61:ASN:ND2	1:G:62:PRO:HD2	2.32	0.45
1:B:118:THR:O	1:B:121:GLU:HB2	2.16	0.45
1:B:293:ARG:NH2	1:B:336:GLU:CD	2.74	0.45
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.68	0.45
1:C:23:TYR:O	1:C:26:VAL:HG12	2.16	0.45
1:C:23:TYR:OH	1:C:331:GLY:HA3	2.17	0.45
1:C:286:ARG:CZ	1:C:290:ARG:HB2	2.47	0.45
1:C:319:HIS:CG	1:C:320:TRP:N	2.84	0.45
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.61	0.45
1:D:319:HIS:CG	1:D:320:TRP:N	2.84	0.45
1:E:142:ARG:HD2	1:E:142:ARG:C	2.42	0.45
1:E:151:ARG:NH2	1:E:154:GLU:OE1	2.40	0.45
1:E:238:LEU:N	1:E:238:LEU:CD1	2.74	0.45
1:H:17:LEU:CA	1:H:152:LEU:HD21	2.46	0.45
1:H:286:ARG:CZ	1:H:290:ARG:HB2	2.47	0.45
1:B:168:GLU:O	1:B:170:VAL:N	2.49	0.45
1:B:286:ARG:CZ	1:B:290:ARG:HB2	2.47	0.45
1:D:101:ALA:C	1:D:102:VAL:HG23	2.41	0.45
1:G:17:LEU:CA	1:G:152:LEU:HD21	2.46	0.45
1:G:335:GLU:O	1:G:338:ASN:N	2.43	0.45
1:H:107:TRP:O	1:H:108:LYS:C	2.60	0.45
1:A:107:TRP:O	1:A:108:LYS:C	2.60	0.45
1:C:286:ARG:CG	1:C:287:PRO:CD	2.92	0.45
1:E:107:TRP:O	1:E:108:LYS:C	2.60	0.45
1:F:195:LEU:HD12	1:F:195:LEU:HA	1.63	0.45
1:F:252:ASN:ND2	1:F:255:ASP:OD2	2.44	0.45
1:G:293:ARG:HH11	1:G:293:ARG:HD3	1.61	0.45
1:H:252:ASN:ND2	1:H:255:ASP:OD2	2.44	0.45
1:A:23:TYR:OH	1:A:331:GLY:HA3	2.17	0.45
1:C:17:LEU:HD12	1:C:17:LEU:HA	1.47	0.45
1:E:286:ARG:CZ	1:E:290:ARG:HB2	2.47	0.45
1:F:21:GLU:HG3	1:F:155:ARG:HH21	1.73	0.45
1:F:21:GLU:CG	1:F:155:ARG:NH2	2.72	0.45
1:F:23:TYR:O	1:F:26:VAL:HG12	2.16	0.45
1:F:89:LEU:HA	1:F:138:ILE:O	2.17	0.45
1:F:142:ARG:HD2	1:F:142:ARG:C	2.42	0.45
1:G:17:LEU:HD12	1:G:17:LEU:HA	1.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:PRO:HG2	1:G:107:TRP:CG	2.52	0.45
1:G:61:ASN:HD22	1:G:62:PRO:HD2	1.79	0.45
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.50	0.45
1:A:128:TYR:CZ	1:A:216:THR:HB	2.52	0.45
1:A:142:ARG:HD2	1:A:142:ARG:C	2.42	0.45
1:A:238:LEU:N	1:A:238:LEU:CD1	2.74	0.45
1:A:286:ARG:CZ	1:A:290:ARG:HB2	2.47	0.45
1:F:124:MET:HB2	1:F:125:PHE:CE1	2.52	0.45
1:F:286:ARG:CG	1:F:287:PRO:CD	2.92	0.45
1:G:238:LEU:N	1:G:238:LEU:CD1	2.74	0.45
1:H:61:ASN:HB3	1:H:64:GLU:HG3	1.99	0.45
1:H:89:LEU:HA	1:H:138:ILE:O	2.17	0.45
1:B:319:HIS:CG	1:B:320:TRP:N	2.84	0.44
1:D:169:GLU:HG2	1:D:170:VAL:N	2.32	0.44
1:E:23:TYR:OH	1:E:331:GLY:HA3	2.17	0.44
1:F:319:HIS:CG	1:F:320:TRP:N	2.84	0.44
1:G:190:GLN:O	1:G:190:GLN:HG2	2.13	0.44
1:H:23:TYR:O	1:H:26:VAL:HG12	2.17	0.44
1:A:107:TRP:CA	1:A:110:MET:HG3	2.48	0.44
1:B:23:TYR:O	1:B:26:VAL:HG12	2.17	0.44
1:B:23:TYR:OH	1:B:331:GLY:HA3	2.17	0.44
1:C:124:MET:C	1:C:126:PRO:HD3	2.42	0.44
1:C:130:TYR:CD1	1:C:130:TYR:C	2.96	0.44
1:D:21:GLU:HA	1:D:155:ARG:NH2	2.31	0.44
1:F:130:TYR:CD1	1:F:130:TYR:C	2.95	0.44
1:G:107:TRP:O	1:G:108:LYS:C	2.60	0.44
1:G:107:TRP:CA	1:G:110:MET:HG3	2.48	0.44
1:G:145:LEU:HD23	1:G:145:LEU:HA	1.77	0.44
1:G:286:ARG:HG3	1:G:287:PRO:HD2	1.98	0.44
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.26	0.44
1:B:286:ARG:HG3	1:B:287:PRO:HD2	1.98	0.44
1:C:21:GLU:CG	1:C:155:ARG:NH2	2.72	0.44
1:C:252:ASN:ND2	1:C:255:ASP:OD2	2.44	0.44
1:D:190:GLN:HA	1:D:191:PRO:HD3	1.74	0.44
1:D:286:ARG:CG	1:D:287:PRO:CD	2.92	0.44
1:E:39:PHE:CD2	1:E:161:LEU:HD12	2.44	0.44
1:E:107:TRP:CA	1:E:110:MET:HG3	2.48	0.44
1:E:168:GLU:HG3	1:E:298:PHE:CD1	2.51	0.44
1:H:311:HIS:O	1:H:312:GLY:C	2.61	0.44
1:B:89:LEU:HA	1:B:138:ILE:O	2.17	0.44
1:B:266:LEU:HD12	1:B:266:LEU:HA	1.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASN:HD21	1:C:255:ASP:CB	2.31	0.44
1:D:89:LEU:HA	1:D:138:ILE:O	2.17	0.44
1:E:23:TYR:O	1:E:24:HIS:C	2.59	0.44
1:G:23:TYR:O	1:G:24:HIS:C	2.59	0.44
1:G:23:TYR:OH	1:G:331:GLY:HA3	2.17	0.44
1:H:23:TYR:OH	1:H:331:GLY:HA3	2.17	0.44
1:H:293:ARG:NH2	1:H:336:GLU:CD	2.74	0.44
1:A:65:ALA:HB2	1:A:106:TYR:CE2	2.53	0.44
1:B:311:HIS:O	1:B:312:GLY:C	2.61	0.44
1:C:89:LEU:HA	1:C:138:ILE:O	2.17	0.44
1:C:168:GLU:O	1:C:171:ALA:HB3	2.17	0.44
1:C:335:GLU:O	1:C:338:ASN:N	2.43	0.44
2:C:348:FAB:H9	2:C:348:FAB:O2'	2.18	0.44
1:D:107:TRP:CA	1:D:110:MET:HG3	2.48	0.44
1:E:17:LEU:HD12	1:E:17:LEU:HA	1.47	0.44
1:E:157:VAL:CG1	1:E:158:LYS:N	2.80	0.44
1:F:107:TRP:CA	1:F:110:MET:HG3	2.48	0.44
1:G:23:TYR:O	1:G:26:VAL:HG12	2.17	0.44
2:G:348:FAB:O2'	2:G:348:FAB:H9	2.18	0.44
1:H:167:PHE:CE2	1:H:189:LEU:O	2.71	0.44
1:H:190:GLN:HA	1:H:191:PRO:HD3	1.74	0.44
1:A:315:GLY:O	1:A:319:HIS:HB3	2.18	0.44
1:A:331:GLY:O	1:A:334:LEU:HB2	2.17	0.44
1:C:179:ILE:HD13	1:C:326:VAL:HG11	1.99	0.44
1:C:194:LEU:HA	1:C:194:LEU:HD23	1.26	0.44
2:D:348:FAB:H9	2:D:348:FAB:O2'	2.18	0.44
1:E:36:ALA:HA	2:E:348:FAB:N3A	2.33	0.44
1:E:89:LEU:HA	1:E:138:ILE:O	2.17	0.44
1:E:167:PHE:CE1	1:E:189:LEU:HD13	2.53	0.44
1:E:192:ASP:OD1	1:E:194:LEU:HB2	2.18	0.44
1:F:93:SER:HG	1:F:135:THR:HB	1.78	0.44
1:F:107:TRP:O	1:F:108:LYS:C	2.60	0.44
1:F:311:HIS:O	1:F:312:GLY:C	2.61	0.44
1:G:315:GLY:O	1:G:319:HIS:HB3	2.18	0.44
1:A:36:ALA:HA	2:A:348:FAB:N3A	2.33	0.44
1:A:236:VAL:CG1	1:A:237:THR:N	2.81	0.44
1:B:269:THR:O	1:B:271:LYS:N	2.51	0.44
1:B:315:GLY:O	1:B:319:HIS:HB3	2.18	0.44
1:B:331:GLY:O	1:B:334:LEU:HB2	2.18	0.44
1:C:36:ALA:HA	2:C:348:FAB:N3A	2.33	0.44
1:C:209:TRP:NE1	1:C:269:THR:OG1	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:PRO:HG2	1:D:107:TRP:CG	2.52	0.44
1:F:250:ILE:HG23	1:F:250:ILE:HD12	1.42	0.44
2:F:348:FAB:H9	2:F:348:FAB:O2'	2.18	0.44
1:G:101:ALA:C	1:G:102:VAL:HG23	2.42	0.44
1:G:236:VAL:CG1	1:G:237:THR:N	2.81	0.44
1:G:263:CYS:O	1:G:267:GLU:N	2.50	0.44
1:H:36:ALA:HA	2:H:348:FAB:N3A	2.33	0.44
2:H:348:FAB:H9	2:H:348:FAB:O2'	2.18	0.44
1:A:23:TYR:O	1:A:26:VAL:HG12	2.17	0.44
1:A:271:LYS:HE2	1:E:86:ASN:HD21	1.83	0.44
1:B:107:TRP:O	1:B:108:LYS:C	2.60	0.44
1:B:190:GLN:HA	1:B:191:PRO:HD3	1.74	0.44
1:C:107:TRP:O	1:C:108:LYS:C	2.60	0.44
1:C:238:LEU:HD12	1:C:238:LEU:HA	1.50	0.44
1:C:315:GLY:O	1:C:319:HIS:HB3	2.18	0.44
1:D:311:HIS:O	1:D:312:GLY:C	2.61	0.44
1:D:315:GLY:O	1:D:319:HIS:HB3	2.18	0.44
1:E:315:GLY:O	1:E:319:HIS:HB3	2.18	0.44
1:E:331:GLY:O	1:E:334:LEU:HB2	2.18	0.44
2:E:348:FAB:H9	2:E:348:FAB:O2'	2.18	0.44
1:F:252:ASN:HD21	1:F:255:ASP:CB	2.31	0.44
1:G:238:LEU:HD12	1:G:238:LEU:HA	1.50	0.44
1:H:107:TRP:CA	1:H:110:MET:HG3	2.48	0.44
1:H:179:ILE:O	1:H:179:ILE:HG22	2.17	0.44
1:H:192:ASP:OD1	1:H:194:LEU:HB2	2.18	0.44
1:H:250:ILE:HG23	1:H:250:ILE:HD12	1.43	0.44
1:H:278:GLU:C	1:H:279:TYR:CG	2.96	0.44
1:A:89:LEU:HA	1:A:138:ILE:O	2.17	0.44
1:A:97:LEU:HB3	1:A:128:TYR:CG	2.53	0.44
1:B:54:PRO:HG2	1:B:107:TRP:CG	2.52	0.44
1:B:63:GLN:H	1:B:63:GLN:HG2	1.48	0.44
1:C:54:PRO:HG2	1:C:107:TRP:CG	2.52	0.44
1:C:293:ARG:HH11	1:C:293:ARG:HD3	1.61	0.44
1:E:311:HIS:O	1:E:312:GLY:C	2.61	0.44
1:G:36:ALA:HA	2:G:348:FAB:N3A	2.33	0.44
1:H:252:ASN:HD21	1:H:255:ASP:CB	2.31	0.44
1:A:311:HIS:O	1:A:312:GLY:C	2.61	0.43
1:C:128:TYR:CE2	1:C:216:THR:HB	2.53	0.43
1:C:178:ILE:O	1:C:178:ILE:HG22	2.18	0.43
1:C:278:GLU:C	1:C:279:TYR:CG	2.96	0.43
1:E:293:ARG:NH2	1:E:336:GLU:CD	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:GLU:C	1:G:279:TYR:CG	2.96	0.43
1:H:55:TYR:CE2	1:H:314:TYR:CE2	3.06	0.43
1:H:194:LEU:HD23	1:H:194:LEU:HA	1.26	0.43
2:A:348:FAB:H9	2:A:348:FAB:O2'	2.18	0.43
1:C:55:TYR:CE2	1:C:314:TYR:CE2	3.06	0.43
1:D:102:VAL:O	1:D:130:TYR:OH	2.18	0.43
1:D:331:GLY:O	1:D:334:LEU:HB2	2.17	0.43
1:F:36:ALA:HA	2:F:348:FAB:N3A	2.33	0.43
1:A:254:GLN:NE2	1:A:254:GLN:H	2.15	0.43
1:B:236:VAL:CG1	1:B:237:THR:N	2.81	0.43
2:B:348:FAB:O2'	2:B:348:FAB:H9	2.18	0.43
1:C:107:TRP:CA	1:C:110:MET:HG3	2.48	0.43
1:C:268:PRO:C	1:C:270:LEU:N	2.76	0.43
1:D:107:TRP:O	1:D:108:LYS:C	2.60	0.43
1:D:161:LEU:HD13	1:D:161:LEU:HA	1.68	0.43
1:D:192:ASP:OD1	1:D:194:LEU:HB2	2.18	0.43
1:F:76:LEU:HD23	1:F:76:LEU:HA	1.61	0.43
1:F:112:LEU:HA	1:F:112:LEU:HD23	1.82	0.43
1:G:1:MET:HE2	1:G:177:VAL:HG23	1.99	0.43
1:G:331:GLY:O	1:G:334:LEU:HB2	2.17	0.43
1:H:61:ASN:OD1	1:H:63:GLN:HB2	2.18	0.43
1:H:145:LEU:HD23	1:H:145:LEU:HA	1.77	0.43
1:B:36:ALA:HA	2:B:348:FAB:N3A	2.33	0.43
1:B:107:TRP:CA	1:B:110:MET:HG3	2.48	0.43
1:C:331:GLY:O	1:C:334:LEU:HB2	2.17	0.43
1:F:17:LEU:HD12	1:F:17:LEU:HA	1.47	0.43
1:F:55:TYR:CE2	1:F:314:TYR:CE2	3.06	0.43
1:F:192:ASP:OD1	1:F:194:LEU:HB2	2.18	0.43
1:G:39:PHE:HE2	1:G:161:LEU:HA	1.83	0.43
1:G:68:ASN:OD1	1:G:318:ILE:HB	2.19	0.43
1:G:167:PHE:CE1	1:G:189:LEU:CB	2.88	0.43
1:H:315:GLY:O	1:H:319:HIS:HB3	2.18	0.43
1:H:331:GLY:O	1:H:334:LEU:HB2	2.17	0.43
1:A:265:ARG:O	1:A:265:ARG:HG2	2.18	0.43
1:B:252:ASN:HD21	1:B:255:ASP:CB	2.31	0.43
1:C:68:ASN:OD1	1:C:318:ILE:HB	2.19	0.43
1:D:55:TYR:CE2	1:D:314:TYR:CE2	3.06	0.43
1:E:238:LEU:HA	1:E:238:LEU:HD12	1.50	0.43
1:F:331:GLY:O	1:F:334:LEU:HB2	2.17	0.43
1:G:311:HIS:O	1:G:312:GLY:C	2.61	0.43
1:H:115:ARG:NH2	1:H:121:GLU:CD	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:TYR:CE2	1:B:314:TYR:CE2	3.06	0.43
1:B:115:ARG:NH2	1:B:121:GLU:CD	2.65	0.43
1:B:151:ARG:NH2	1:B:154:GLU:OE1	2.40	0.43
1:C:168:GLU:O	1:C:169:GLU:C	2.62	0.43
1:D:36:ALA:HA	2:D:348:FAB:N3A	2.33	0.43
1:D:278:GLU:C	1:D:279:TYR:CG	2.96	0.43
1:E:252:ASN:HD21	1:E:255:ASP:CB	2.31	0.43
1:H:148:LEU:HA	1:H:148:LEU:HD23	1.76	0.43
1:H:166:SER:O	1:H:167:PHE:C	2.54	0.43
1:H:286:ARG:HG3	1:H:287:PRO:HD2	1.98	0.43
1:A:10:VAL:CG1	1:A:11:ILE:N	2.82	0.43
1:B:10:VAL:CG1	1:B:11:ILE:N	2.82	0.43
1:B:170:VAL:CG1	1:B:178:ILE:HD11	2.48	0.43
1:B:335:GLU:O	1:B:338:ASN:N	2.43	0.43
1:C:145:LEU:HA	1:C:145:LEU:HD23	1.77	0.43
1:C:192:ASP:OD1	1:C:194:LEU:HB2	2.18	0.43
1:D:142:ARG:CG	1:D:142:ARG:NH1	2.69	0.43
1:D:167:PHE:HE1	1:D:189:LEU:HB3	1.80	0.43
1:G:89:LEU:HA	1:G:138:ILE:O	2.17	0.43
1:G:252:ASN:HD21	1:G:255:ASP:CB	2.31	0.43
1:H:54:PRO:HG2	1:H:107:TRP:CG	2.52	0.43
1:H:68:ASN:OD1	1:H:318:ILE:HB	2.19	0.43
1:D:10:VAL:CG1	1:D:11:ILE:N	2.82	0.43
1:D:62:PRO:CD	1:D:63:GLN:H	2.30	0.43
1:D:112:LEU:HA	1:D:112:LEU:HD23	1.82	0.43
1:D:236:VAL:CG1	1:D:237:THR:N	2.81	0.43
1:E:148:LEU:HA	1:E:148:LEU:HD23	1.76	0.43
1:E:195:LEU:HD12	1:E:195:LEU:HA	1.63	0.43
1:E:270:LEU:HD23	1:E:270:LEU:HA	1.54	0.43
1:A:101:ALA:CA	1:A:130:TYR:CD2	2.96	0.43
1:A:252:ASN:HD21	1:A:255:ASP:CB	2.31	0.43
1:B:192:ASP:OD1	1:B:194:LEU:HB2	2.18	0.43
1:B:286:ARG:HA	1:B:287:PRO:HD3	1.84	0.43
1:C:151:ARG:NH2	1:C:154:GLU:OE1	2.40	0.43
1:C:257:ASN:O	1:C:258:THR:C	2.61	0.43
1:D:61:ASN:C	1:D:63:GLN:N	2.74	0.43
1:D:293:ARG:HH11	1:D:293:ARG:HD3	1.61	0.43
1:E:278:GLU:C	1:E:279:TYR:CG	2.96	0.43
1:F:286:ARG:HG3	1:F:287:PRO:HD2	1.98	0.43
1:G:179:ILE:N	1:G:179:ILE:CD1	2.77	0.43
1:H:168:GLU:O	1:H:172:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:236:VAL:CG1	1:H:237:THR:N	2.81	0.43
1:A:68:ASN:OD1	1:A:318:ILE:HB	2.19	0.43
1:B:233:LEU:O	1:F:208:PRO:HB2	2.18	0.43
1:B:257:ASN:O	1:B:258:THR:C	2.61	0.43
1:F:10:VAL:CG1	1:F:11:ILE:N	2.82	0.43
1:F:260:TRP:CD1	1:F:260:TRP:C	2.97	0.43
1:G:192:ASP:OD1	1:G:194:LEU:HB2	2.18	0.43
1:H:251:ASN:HA	1:H:280:THR:CG2	2.48	0.43
1:A:54:PRO:HG2	1:A:107:TRP:CG	2.52	0.42
1:A:159:PHE:O	1:A:160:PHE:CD1	2.72	0.42
1:A:192:ASP:OD1	1:A:194:LEU:HB2	2.18	0.42
1:B:145:LEU:HD23	1:B:145:LEU:HA	1.77	0.42
1:B:279:TYR:CD1	1:B:279:TYR:N	2.87	0.42
1:C:170:VAL:O	1:C:175:ALA:HB2	2.18	0.42
1:C:311:HIS:O	1:C:312:GLY:C	2.61	0.42
1:D:286:ARG:HG3	1:D:287:PRO:HD2	1.98	0.42
1:E:54:PRO:HG2	1:E:107:TRP:CG	2.52	0.42
1:H:216:THR:OG1	1:H:226:SER:HB3	2.19	0.42
1:A:278:GLU:C	1:A:279:TYR:CG	2.96	0.42
1:C:216:THR:OG1	1:C:226:SER:HB3	2.20	0.42
1:E:63:GLN:HG2	1:E:63:GLN:H	1.13	0.42
1:E:68:ASN:OD1	1:E:318:ILE:HB	2.19	0.42
1:E:286:ARG:CG	1:E:287:PRO:CD	2.92	0.42
1:F:279:TYR:CD1	1:F:279:TYR:N	2.87	0.42
1:F:315:GLY:O	1:F:319:HIS:HB3	2.18	0.42
1:C:10:VAL:CG1	1:C:11:ILE:N	2.82	0.42
1:D:23:TYR:O	1:D:24:HIS:C	2.59	0.42
1:D:68:ASN:OD1	1:D:318:ILE:HB	2.19	0.42
1:D:250:ILE:HG23	1:D:250:ILE:HD12	1.43	0.42
1:D:324:LEU:HA	1:D:324:LEU:HD23	1.68	0.42
1:E:216:THR:OG1	1:E:226:SER:HB3	2.20	0.42
1:H:23:TYR:O	1:H:24:HIS:C	2.59	0.42
1:A:52:TRP:CE2	1:A:317:THR:HG23	2.55	0.42
1:A:130:TYR:C	1:A:130:TYR:CD1	2.97	0.42
1:A:256:HIS:CD2	1:A:256:HIS:C	2.97	0.42
1:A:269:THR:C	1:A:271:LYS:N	2.77	0.42
1:B:17:LEU:HA	1:B:17:LEU:HD12	1.47	0.42
1:C:251:ASN:HA	1:C:280:THR:CG2	2.48	0.42
1:D:52:TRP:CE2	1:D:317:THR:HG23	2.55	0.42
1:D:124:MET:HB2	1:D:125:PHE:CD1	2.54	0.42
1:F:3:VAL:HG12	1:F:4:VAL:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ASN:OD1	1:F:318:ILE:HB	2.19	0.42
1:F:216:THR:OG1	1:F:226:SER:HB3	2.20	0.42
1:F:278:GLU:C	1:F:279:TYR:CG	2.96	0.42
1:G:61:ASN:HD21	1:G:63:GLN:HG3	1.83	0.42
1:G:216:THR:OG1	1:G:226:SER:HB3	2.20	0.42
1:H:332:LYS:O	1:H:333:VAL:C	2.63	0.42
1:A:128:TYR:OH	1:A:216:THR:HB	2.19	0.42
1:B:52:TRP:CE2	1:B:317:THR:HG23	2.55	0.42
1:B:286:ARG:CG	1:B:287:PRO:CD	2.92	0.42
1:D:88:GLY:HA2	1:D:233:LEU:HD11	2.02	0.42
1:E:3:VAL:HG12	1:E:4:VAL:N	2.35	0.42
1:E:89:LEU:HD23	1:E:89:LEU:HA	1.88	0.42
1:F:332:LYS:O	1:F:333:VAL:C	2.63	0.42
1:G:167:PHE:HE1	1:G:189:LEU:C	2.26	0.42
1:G:279:TYR:CD1	1:G:279:TYR:N	2.87	0.42
1:A:286:ARG:HG3	1:A:287:PRO:HD2	1.98	0.42
1:B:88:GLY:HA2	1:B:233:LEU:HD11	2.02	0.42
1:B:179:ILE:HG23	1:B:179:ILE:HD12	1.55	0.42
1:C:55:TYR:CD1	1:C:223:ILE:HD13	2.55	0.42
1:C:142:ARG:O	1:C:146:GLN:HG3	2.20	0.42
1:C:286:ARG:HD3	1:C:288:GLN:O	2.20	0.42
1:E:257:ASN:O	1:E:258:THR:C	2.61	0.42
1:F:54:PRO:HG2	1:F:107:TRP:CG	2.52	0.42
1:H:52:TRP:CE2	1:H:317:THR:HG23	2.55	0.42
1:A:55:TYR:CE2	1:A:314:TYR:CE2	3.06	0.42
1:A:216:THR:OG1	1:A:226:SER:HB3	2.20	0.42
1:A:279:TYR:CD1	1:A:279:TYR:N	2.87	0.42
1:B:55:TYR:CD1	1:B:223:ILE:HD13	2.55	0.42
1:B:216:THR:OG1	1:B:226:SER:HB3	2.20	0.42
1:B:278:GLU:C	1:B:279:TYR:CG	2.96	0.42
1:D:130:TYR:CD1	1:D:130:TYR:C	2.97	0.42
1:E:52:TRP:CE2	1:E:317:THR:HG23	2.55	0.42
1:E:55:TYR:CE2	1:E:314:TYR:CE2	3.06	0.42
1:E:218:ASP:HB3	1:E:221:ARG:HB2	2.02	0.42
1:F:88:GLY:HA2	1:F:233:LEU:HD11	2.02	0.42
1:F:236:VAL:CG1	1:F:237:THR:N	2.81	0.42
1:G:88:GLY:HA2	1:G:233:LEU:HD11	2.02	0.42
1:G:124:MET:C	1:G:126:PRO:HD3	2.45	0.42
1:H:218:ASP:HB3	1:H:221:ARG:HB2	2.02	0.42
1:H:324:LEU:HA	1:H:324:LEU:HD23	1.68	0.42
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:HG12	1:C:4:VAL:N	2.35	0.42
1:C:332:LYS:O	1:C:333:VAL:C	2.63	0.42
1:D:89:LEU:HD23	1:D:89:LEU:HA	1.88	0.42
1:F:251:ASN:HA	1:F:280:THR:CG2	2.48	0.42
1:G:218:ASP:HB3	1:G:221:ARG:HB2	2.02	0.42
1:H:279:TYR:CD1	1:H:279:TYR:N	2.87	0.42
1:A:178:ILE:HB	1:A:305:VAL:HG22	2.01	0.42
1:A:269:THR:H	1:A:269:THR:HG23	1.45	0.42
1:B:112:LEU:HA	1:B:112:LEU:HD23	1.82	0.42
1:B:218:ASP:HB3	1:B:221:ARG:HB2	2.02	0.42
1:C:97:LEU:HD11	1:C:125:PHE:CD2	2.55	0.42
1:C:129:ARG:HE	1:C:129:ARG:HB3	1.55	0.42
1:C:218:ASP:HB3	1:C:221:ARG:HB2	2.02	0.42
1:D:118:THR:HG23	1:D:118:THR:H	1.36	0.42
1:E:10:VAL:CG1	1:E:11:ILE:N	2.82	0.42
1:F:55:TYR:CD1	1:F:223:ILE:HD13	2.55	0.42
1:G:53:GLN:HA	1:G:54:PRO:HD2	1.94	0.42
1:G:286:ARG:HA	1:G:287:PRO:HD3	1.84	0.42
1:H:142:ARG:O	1:H:146:GLN:HG3	2.20	0.42
1:H:151:ARG:NH2	1:H:154:GLU:OE1	2.40	0.42
1:A:142:ARG:O	1:A:146:GLN:HG3	2.20	0.42
1:A:260:TRP:CD1	1:A:260:TRP:C	2.97	0.42
1:B:167:PHE:O	1:B:168:GLU:C	2.61	0.42
1:B:168:GLU:O	1:B:171:ALA:N	2.53	0.42
1:C:52:TRP:CE2	1:C:317:THR:HG23	2.55	0.42
1:C:115:ARG:NH2	1:C:121:GLU:CD	2.65	0.42
1:C:279:TYR:CD1	1:C:279:TYR:N	2.87	0.42
1:D:195:LEU:HD12	1:D:195:LEU:HA	1.63	0.42
1:D:279:TYR:CD1	1:D:279:TYR:N	2.87	0.42
1:F:52:TRP:CE2	1:F:317:THR:HG23	2.55	0.42
1:F:142:ARG:O	1:F:146:GLN:HG3	2.20	0.42
1:G:55:TYR:CE2	1:G:314:TYR:CE2	3.06	0.42
1:G:142:ARG:O	1:G:146:GLN:HG3	2.20	0.42
1:G:195:LEU:HD12	1:G:195:LEU:HA	1.63	0.42
1:H:10:VAL:CG1	1:H:11:ILE:N	2.82	0.42
1:C:53:GLN:HA	1:C:54:PRO:HD2	1.94	0.41
1:E:55:TYR:CD1	1:E:223:ILE:HD13	2.55	0.41
1:F:190:GLN:HA	1:F:191:PRO:HD3	1.74	0.41
1:G:10:VAL:CG1	1:G:11:ILE:N	2.82	0.41
1:G:52:TRP:CE2	1:G:317:THR:HG23	2.55	0.41
1:A:18:CYS:SG	1:A:324:LEU:HD23	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:CYS:SG	1:B:324:LEU:HD23	2.60	0.41
1:B:68:ASN:OD1	1:B:318:ILE:HB	2.19	0.41
1:D:230:ILE:HA	1:D:231:PRO:HD3	1.83	0.41
1:E:65:ALA:CB	1:E:106:TYR:CE2	3.03	0.41
1:E:98:PHE:O	1:E:128:TYR:HB3	2.20	0.41
1:H:55:TYR:CD1	1:H:223:ILE:HD13	2.55	0.41
1:A:3:VAL:HG12	1:A:4:VAL:N	2.35	0.41
1:A:88:GLY:HA2	1:A:233:LEU:HD11	2.02	0.41
1:B:49:ALA:HB3	2:B:348:FAB:O4	2.21	0.41
1:B:157:VAL:CG1	1:B:158:LYS:N	2.72	0.41
1:B:260:TRP:CD1	1:B:260:TRP:C	2.97	0.41
1:E:18:CYS:SG	1:E:324:LEU:HD23	2.60	0.41
1:G:3:VAL:CG1	1:G:179:ILE:HD11	2.50	0.41
1:G:49:ALA:HB3	2:G:348:FAB:O4	2.21	0.41
1:A:23:TYR:O	1:A:24:HIS:C	2.59	0.41
1:A:49:ALA:HB3	2:A:348:FAB:O4	2.21	0.41
1:A:130:TYR:CD1	1:A:131:GLY:N	2.89	0.41
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.63	0.41
1:B:256:HIS:CD2	1:B:256:HIS:C	2.97	0.41
1:C:293:ARG:NH2	1:C:336:GLU:CD	2.74	0.41
1:E:88:GLY:HA2	1:E:233:LEU:HD11	2.02	0.41
1:E:332:LYS:O	1:E:333:VAL:C	2.63	0.41
1:F:49:ALA:HB3	2:F:348:FAB:O4	2.21	0.41
2:F:348:FAB:HM71	2:F:348:FAB:HM81	1.65	0.41
1:B:97:LEU:HB3	1:B:128:TYR:CD2	2.55	0.41
1:B:138:ILE:HD13	1:B:138:ILE:HG21	1.82	0.41
1:C:236:VAL:CG1	1:C:237:THR:N	2.81	0.41
1:D:142:ARG:O	1:D:146:GLN:HG3	2.20	0.41
1:H:329:LEU:O	1:H:330:PHE:C	2.63	0.41
1:A:337:ARG:O	1:A:338:ASN:HB2	2.21	0.41
1:B:2:ARG:O	1:B:176:ASP:HB2	2.19	0.41
1:B:142:ARG:O	1:B:146:GLN:HG3	2.20	0.41
1:B:159:PHE:N	1:B:159:PHE:CD1	2.88	0.41
1:B:246:ASN:OD1	1:B:247:TRP:N	2.54	0.41
1:C:18:CYS:SG	1:C:324:LEU:HD23	2.60	0.41
1:C:246:ASN:OD1	1:C:247:TRP:N	2.54	0.41
1:D:3:VAL:HG12	1:D:4:VAL:N	2.35	0.41
1:D:252:ASN:HD21	1:D:255:ASP:CB	2.31	0.41
1:E:49:ALA:CB	2:E:348:FAB:H3'	2.48	0.41
1:E:75:LEU:HD23	1:E:75:LEU:HA	1.92	0.41
1:F:7:GLY:HA2	2:F:348:FAB:H1B	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:CYS:SG	1:F:324:LEU:HD23	2.60	0.41
1:F:238:LEU:HD12	1:F:238:LEU:HA	1.49	0.41
1:F:246:ASN:OD1	1:F:247:TRP:N	2.54	0.41
1:G:61:ASN:HD22	1:G:63:GLN:H	1.64	0.41
1:G:150:GLU:O	1:G:151:ARG:C	2.63	0.41
1:H:3:VAL:HG12	1:H:4:VAL:N	2.35	0.41
1:C:86:ASN:HD21	1:G:271:LYS:HE2	1.86	0.41
1:C:195:LEU:HD12	1:C:195:LEU:HA	1.63	0.41
1:D:55:TYR:CD1	1:D:223:ILE:HD13	2.55	0.41
1:D:216:THR:OG1	1:D:226:SER:HB3	2.20	0.41
1:E:142:ARG:O	1:E:146:GLN:HG3	2.20	0.41
1:G:61:ASN:ND2	1:G:63:GLN:CB	2.81	0.41
1:A:286:ARG:HA	1:A:287:PRO:HD3	1.84	0.41
1:B:7:GLY:HA2	2:B:348:FAB:H1B	2.03	0.41
1:B:162:ARG:O	2:B:348:FAB:H2A	2.21	0.41
1:C:88:GLY:HA2	1:C:233:LEU:HD11	2.02	0.41
1:D:269:THR:C	1:D:271:LYS:N	2.74	0.41
1:F:151:ARG:NH2	1:F:154:GLU:OE1	2.40	0.41
1:F:170:VAL:HG23	1:F:170:VAL:H	1.70	0.41
1:G:76:LEU:HA	1:G:76:LEU:HD23	1.61	0.41
1:G:97:LEU:HB3	1:G:128:TYR:CG	2.54	0.41
1:G:337:ARG:O	1:G:338:ASN:HB2	2.21	0.41
1:H:18:CYS:SG	1:H:324:LEU:HD23	2.60	0.41
1:H:150:GLU:O	1:H:151:ARG:C	2.63	0.41
1:A:55:TYR:CD1	1:A:223:ILE:HD13	2.55	0.41
1:A:84:ALA:O	1:A:89:LEU:HB2	2.21	0.41
1:A:207:ALA:HA	1:A:208:PRO:HD3	1.79	0.41
1:A:251:ASN:HA	1:A:280:THR:CG2	2.48	0.41
1:B:3:VAL:HG12	1:B:4:VAL:N	2.35	0.41
1:B:58:GLU:CG	1:B:59:PRO:HD2	2.51	0.41
1:B:167:PHE:CE1	1:B:189:LEU:HD13	2.56	0.41
1:B:194:LEU:HA	1:B:194:LEU:HD23	1.26	0.41
1:B:210:LEU:CD1	1:B:270:LEU:HD21	2.50	0.41
1:C:1:MET:HG3	1:C:176:ASP:HB2	2.01	0.41
1:D:7:GLY:HA2	2:D:348:FAB:H1B	2.03	0.41
1:D:18:CYS:SG	1:D:324:LEU:HD23	2.60	0.41
1:D:61:ASN:N	1:D:61:ASN:ND2	2.63	0.41
1:D:138:ILE:HD13	1:D:138:ILE:HG21	1.81	0.41
1:D:218:ASP:HB3	1:D:221:ARG:HB2	2.02	0.41
1:E:7:GLY:HA2	2:E:348:FAB:H1B	2.03	0.41
1:E:84:ALA:O	1:E:89:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:VAL:HG12	1:E:178:ILE:CD1	2.51	0.41
1:E:256:HIS:CD2	1:E:256:HIS:C	2.97	0.41
1:E:260:TRP:CD1	1:E:260:TRP:C	2.97	0.41
1:E:270:LEU:C	1:E:272:ASP:N	2.76	0.41
1:G:18:CYS:SG	1:G:324:LEU:HD23	2.60	0.41
1:G:55:TYR:CD1	1:G:223:ILE:HD13	2.55	0.41
1:G:61:ASN:HD22	1:G:61:ASN:C	2.28	0.41
1:G:179:ILE:HD12	1:G:179:ILE:H	1.79	0.41
1:G:246:ASN:OD1	1:G:247:TRP:N	2.54	0.41
1:G:251:ASN:HA	1:G:280:THR:CG2	2.48	0.41
1:G:267:GLU:C	1:G:269:THR:N	2.76	0.41
1:H:138:ILE:HD13	1:H:138:ILE:HG21	1.81	0.41
1:H:195:LEU:HD12	1:H:195:LEU:HA	1.63	0.41
1:A:170:VAL:H	1:A:170:VAL:HG23	1.52	0.41
1:A:218:ASP:HB3	1:A:221:ARG:HB2	2.02	0.41
1:A:257:ASN:O	1:A:258:THR:C	2.61	0.41
1:C:84:ALA:O	1:C:89:LEU:HB2	2.21	0.41
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.68	0.41
1:D:1:MET:CE	1:D:177:VAL:HG23	2.51	0.41
1:D:157:VAL:HG12	1:D:158:LYS:N	2.36	0.41
1:D:318:ILE:HG21	1:D:318:ILE:HD13	1.75	0.41
1:E:49:ALA:HB3	2:E:348:FAB:O4	2.21	0.41
1:E:145:LEU:HD23	1:E:145:LEU:HA	1.77	0.41
1:E:236:VAL:CG1	1:E:237:THR:N	2.81	0.41
1:E:246:ASN:OD1	1:E:247:TRP:N	2.54	0.41
1:F:171:ALA:O	1:F:174:GLY:N	2.54	0.41
1:F:255:ASP:O	1:F:256:HIS:C	2.65	0.41
1:G:43:THR:H	1:G:43:THR:HG23	1.66	0.41
1:G:84:ALA:O	1:G:89:LEU:HB2	2.21	0.41
1:H:84:ALA:O	1:H:89:LEU:HB2	2.21	0.41
1:H:337:ARG:O	1:H:338:ASN:HB2	2.21	0.41
1:A:7:GLY:HA2	2:A:348:FAB:H1B	2.03	0.40
1:A:17:LEU:HA	1:A:152:LEU:HD21	2.03	0.40
1:A:293:ARG:NH2	1:A:336:GLU:CD	2.74	0.40
1:B:256:HIS:HB2	1:E:42:PHE:HZ	1.87	0.40
1:C:64:GLU:O	1:C:67:TRP:N	2.54	0.40
1:D:17:LEU:HA	1:D:152:LEU:HD21	2.03	0.40
1:D:49:ALA:HB3	2:D:348:FAB:O4	2.21	0.40
1:E:49:ALA:HB1	1:E:230:ILE:HD12	2.03	0.40
1:E:150:GLU:O	1:E:151:ARG:C	2.63	0.40
1:E:255:ASP:O	1:E:256:HIS:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ALA:O	1:F:89:LEU:HB2	2.21	0.40
1:F:175:ALA:HB1	1:F:177:VAL:O	2.21	0.40
1:F:337:ARG:O	1:F:338:ASN:HB2	2.21	0.40
1:G:3:VAL:HG12	1:G:4:VAL:N	2.35	0.40
1:G:7:GLY:HA2	2:G:348:FAB:H1B	2.03	0.40
1:G:324:LEU:HD23	1:G:324:LEU:HA	1.68	0.40
1:H:49:ALA:CB	2:H:348:FAB:H3'	2.48	0.40
1:H:136:SER:OG	1:H:137:LEU:N	2.43	0.40
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.82	0.40
1:D:49:ALA:HB1	1:D:230:ILE:HD12	2.04	0.40
1:D:84:ALA:O	1:D:89:LEU:HB2	2.21	0.40
1:D:246:ASN:OD1	1:D:247:TRP:N	2.54	0.40
1:D:251:ASN:HA	1:D:280:THR:CG2	2.48	0.40
1:D:260:TRP:CD1	1:D:260:TRP:C	2.97	0.40
1:E:159:PHE:N	1:E:159:PHE:CD1	2.89	0.40
1:G:256:HIS:CD2	1:G:256:HIS:C	2.97	0.40
1:H:255:ASP:O	1:H:256:HIS:C	2.65	0.40
1:H:267:GLU:HA	1:H:268:PRO:HD2	1.69	0.40
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.76	0.40
1:A:166:SER:O	1:A:170:VAL:HG23	2.22	0.40
1:B:329:LEU:O	1:B:330:PHE:C	2.63	0.40
1:C:190:GLN:HA	1:C:191:PRO:HD3	1.74	0.40
1:D:148:LEU:HA	1:D:148:LEU:HD23	1.76	0.40
1:D:293:ARG:NH2	1:D:336:GLU:CD	2.74	0.40
1:E:286:ARG:HA	1:E:287:PRO:HD3	1.84	0.40
1:G:255:ASP:O	1:G:256:HIS:C	2.64	0.40
1:G:260:TRP:CD1	1:G:260:TRP:C	2.97	0.40
1:H:49:ALA:HB1	1:H:230:ILE:HD12	2.04	0.40
1:H:293:ARG:HH11	1:H:293:ARG:HD3	1.61	0.40
1:B:117:LEU:HD23	1:B:133:PHE:HB2	2.04	0.40
1:C:49:ALA:HB3	2:C:348:FAB:O4	2.21	0.40
1:C:150:GLU:O	1:C:151:ARG:C	2.63	0.40
1:D:193:PRO:HG2	1:F:73:ASN:HB3	2.04	0.40
1:D:215:ILE:HG21	1:D:215:ILE:HD13	1.90	0.40
1:E:329:LEU:O	1:E:330:PHE:C	2.63	0.40
1:F:17:LEU:HA	1:F:152:LEU:HD21	2.03	0.40
1:F:49:ALA:HB1	1:F:230:ILE:HD12	2.04	0.40
1:F:207:ALA:HA	1:F:208:PRO:HD3	1.79	0.40
1:F:218:ASP:HB3	1:F:221:ARG:HB2	2.02	0.40
1:F:257:ASN:O	1:F:258:THR:C	2.61	0.40
1:F:329:LEU:O	1:F:330:PHE:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:LEU:HA	1:H:76:LEU:HD23	1.61	0.40
1:A:232:GLY:O	1:E:211:LYS:NZ	2.51	0.40
1:A:329:LEU:O	1:A:330:PHE:C	2.63	0.40
1:C:208:PRO:HB2	1:G:233:LEU:O	2.21	0.40
1:F:138:ILE:HD13	1:F:138:ILE:HG21	1.82	0.40
1:F:324:LEU:HD23	1:F:324:LEU:HA	1.68	0.40
1:H:7:GLY:HA2	2:H:348:FAB:H1B	2.03	0.40
1:H:36:ALA:O	1:H:161:LEU:HA	2.22	0.40
1:H:75:LEU:HD23	1:H:75:LEU:HA	1.92	0.40
1:H:118:THR:HG23	1:H:118:THR:H	1.36	0.40
1:H:286:ARG:HA	1:H:287:PRO:HD3	1.84	0.40

All (5) 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:G:73:ASN:OD1	1:H:2:ARG:NH2[4_565]	1.42	0.78
1:C:2:ARG:NH2	1:D:73:ASN:OD1[3_655]	1.78	0.42
1:C:162:ARG:NH2	1:H:123:ASP:OD1[3_655]	2.01	0.19
1:C:123:ASP:OD1	1:H:162:ARG:NH2[4_565]	2.07	0.13
1:E:247:TRP:NE1	1:F:247:TRP:NE1[7_555]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	337/347 (97%)	311 (92%)	23 (7%)	3 (1%)	14 47
1	B	337/347 (97%)	308 (91%)	26 (8%)	3 (1%)	14 47
1	C	337/347 (97%)	306 (91%)	28 (8%)	3 (1%)	14 47
1	D	337/347 (97%)	310 (92%)	24 (7%)	3 (1%)	14 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	337/347 (97%)	311 (92%)	23 (7%)	3 (1%)	14	47
1	F	337/347 (97%)	312 (93%)	21 (6%)	4 (1%)	10	42
1	G	337/347 (97%)	310 (92%)	24 (7%)	3 (1%)	14	47
1	H	337/347 (97%)	308 (91%)	25 (7%)	4 (1%)	10	42
All	All	2696/2776 (97%)	2476 (92%)	194 (7%)	26 (1%)	12	45

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	B	30	LEU
1	C	30	LEU
1	D	30	LEU
1	E	30	LEU
1	F	30	LEU
1	G	30	LEU
1	H	30	LEU
1	A	240	GLY
1	B	240	GLY
1	C	240	GLY
1	D	240	GLY
1	E	240	GLY
1	F	240	GLY
1	G	240	GLY
1	H	240	GLY
1	H	173	GLY
1	F	174	GLY
1	C	28	GLN
1	F	28	GLN
1	A	28	GLN
1	B	28	GLN
1	D	28	GLN
1	E	28	GLN
1	G	28	GLN
1	H	28	GLN

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	290/298 (97%)	266 (92%)	24 (8%)	10	38
1	B	290/298 (97%)	261 (90%)	29 (10%)	7	30
1	C	290/298 (97%)	264 (91%)	26 (9%)	9	34
1	D	290/298 (97%)	263 (91%)	27 (9%)	8	33
1	E	290/298 (97%)	267 (92%)	23 (8%)	11	40
1	F	290/298 (97%)	264 (91%)	26 (9%)	9	34
1	G	290/298 (97%)	266 (92%)	24 (8%)	10	38
1	H	290/298 (97%)	266 (92%)	24 (8%)	10	38
All	All	2320/2384 (97%)	2117 (91%)	203 (9%)	9	35

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	76	LEU
1	A	81	SER
1	A	92	VAL
1	A	110	MET
1	A	118	THR
1	A	135	THR
1	A	142	ARG
1	A	146	GLN
1	A	151	ARG
1	A	157	VAL
1	A	159	PHE
1	A	170	VAL
1	A	184	VAL
1	A	205	VAL
1	A	226	SER
1	A	238	LEU
1	A	253	ILE
1	A	254	GLN
1	A	258	THR
1	A	267	GLU
1	A	276	VAL
1	A	280	THR

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Mol	Chain	Res	Type
1	A	291	LEU
1	B	31	ASP
1	B	56	THR
1	B	58	GLU
1	B	62	PRO
1	B	76	LEU
1	B	81	SER
1	B	92	VAL
1	B	110	MET
1	B	118	THR
1	B	129	ARG
1	B	135	THR
1	B	142	ARG
1	B	146	GLN
1	B	151	ARG
1	B	161	LEU
1	B	169	GLU
1	B	170	VAL
1	B	176	ASP
1	B	184	VAL
1	B	205	VAL
1	B	226	SER
1	B	238	LEU
1	B	253	ILE
1	B	258	THR
1	B	265	ARG
1	B	267	GLU
1	B	276	VAL
1	B	280	THR
1	B	291	LEU
1	C	31	ASP
1	C	56	THR
1	C	76	LEU
1	C	81	SER
1	C	92	VAL
1	C	110	MET
1	C	118	THR
1	C	126	PRO
1	C	135	THR
1	C	142	ARG
1	C	146	GLN
1	C	151	ARG

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Mol	Chain	Res	Type
1	C	157	VAL
1	C	161	LEU
1	C	162	ARG
1	C	184	VAL
1	C	205	VAL
1	C	226	SER
1	C	238	LEU
1	C	253	ILE
1	C	258	THR
1	C	269	THR
1	C	276	VAL
1	C	280	THR
1	C	288	GLN
1	C	291	LEU
1	D	31	ASP
1	D	57	SER
1	D	61	ASN
1	D	76	LEU
1	D	81	SER
1	D	92	VAL
1	D	110	MET
1	D	118	THR
1	D	130	TYR
1	D	135	THR
1	D	142	ARG
1	D	146	GLN
1	D	151	ARG
1	D	157	VAL
1	D	161	LEU
1	D	162	ARG
1	D	170	VAL
1	D	184	VAL
1	D	205	VAL
1	D	226	SER
1	D	238	LEU
1	D	253	ILE
1	D	258	THR
1	D	267	GLU
1	D	276	VAL
1	D	280	THR
1	D	291	LEU
1	E	31	ASP

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Mol	Chain	Res	Type
1	E	57	SER
1	E	58	GLU
1	E	63	GLN
1	E	76	LEU
1	E	81	SER
1	E	92	VAL
1	E	110	MET
1	E	118	THR
1	E	135	THR
1	E	142	ARG
1	E	146	GLN
1	E	151	ARG
1	E	177	VAL
1	E	184	VAL
1	E	205	VAL
1	E	226	SER
1	E	238	LEU
1	E	253	ILE
1	E	258	THR
1	E	276	VAL
1	E	280	THR
1	E	291	LEU
1	F	31	ASP
1	F	57	SER
1	F	58	GLU
1	F	76	LEU
1	F	81	SER
1	F	92	VAL
1	F	110	MET
1	F	118	THR
1	F	126	PRO
1	F	135	THR
1	F	142	ARG
1	F	146	GLN
1	F	151	ARG
1	F	178	ILE
1	F	184	VAL
1	F	205	VAL
1	F	226	SER
1	F	238	LEU
1	F	253	ILE
1	F	258	THR

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Mol	Chain	Res	Type
1	F	268	PRO
1	F	269	THR
1	F	276	VAL
1	F	280	THR
1	F	288	GLN
1	F	291	LEU
1	G	31	ASP
1	G	61	ASN
1	G	76	LEU
1	G	81	SER
1	G	92	VAL
1	G	110	MET
1	G	118	THR
1	G	127	ASP
1	G	135	THR
1	G	142	ARG
1	G	146	GLN
1	G	151	ARG
1	G	164	VAL
1	G	170	VAL
1	G	184	VAL
1	G	205	VAL
1	G	226	SER
1	G	238	LEU
1	G	253	ILE
1	G	258	THR
1	G	269	THR
1	G	276	VAL
1	G	280	THR
1	G	291	LEU
1	H	31	ASP
1	H	56	THR
1	H	57	SER
1	H	58	GLU
1	H	76	LEU
1	H	81	SER
1	H	92	VAL
1	H	110	MET
1	H	118	THR
1	H	135	THR
1	H	142	ARG
1	H	146	GLN

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Mol	Chain	Res	Type
1	H	151	ARG
1	H	161	LEU
1	H	184	VAL
1	H	205	VAL
1	H	226	SER
1	H	238	LEU
1	H	253	ILE
1	H	258	THR
1	H	269	THR
1	H	276	VAL
1	H	280	THR
1	H	291	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	53	GLN
1	A	61	ASN
1	A	70	GLN
1	A	78	HIS
1	A	96	ASN
1	A	134	ASN
1	A	146	GLN
1	A	180	ASN
1	A	190	GLN
1	A	212	ASN
1	A	217	HIS
1	A	252	ASN
1	A	254	GLN
1	A	307	HIS
1	B	24	HIS
1	B	63	GLN
1	B	70	GLN
1	B	78	HIS
1	B	134	ASN
1	B	146	GLN
1	B	180	ASN
1	B	190	GLN
1	B	212	ASN
1	B	217	HIS
1	B	254	GLN

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Mol	Chain	Res	Type
1	B	307	HIS
1	C	24	HIS
1	C	53	GLN
1	C	70	GLN
1	C	78	HIS
1	C	96	ASN
1	C	134	ASN
1	C	146	GLN
1	C	180	ASN
1	C	190	GLN
1	C	212	ASN
1	C	217	HIS
1	C	252	ASN
1	C	307	HIS
1	D	24	HIS
1	D	53	GLN
1	D	61	ASN
1	D	63	GLN
1	D	70	GLN
1	D	78	HIS
1	D	96	ASN
1	D	134	ASN
1	D	146	GLN
1	D	190	GLN
1	D	212	ASN
1	D	217	HIS
1	D	252	ASN
1	D	254	GLN
1	D	307	HIS
1	E	24	HIS
1	E	63	GLN
1	E	70	GLN
1	E	78	HIS
1	E	134	ASN
1	E	146	GLN
1	E	190	GLN
1	E	212	ASN
1	E	217	HIS
1	E	252	ASN
1	E	254	GLN
1	E	307	HIS
1	F	24	HIS

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Mol	Chain	Res	Type
1	F	53	GLN
1	F	78	HIS
1	F	96	ASN
1	F	134	ASN
1	F	146	GLN
1	F	180	ASN
1	F	190	GLN
1	F	212	ASN
1	F	217	HIS
1	F	252	ASN
1	F	288	GLN
1	F	307	HIS
1	G	24	HIS
1	G	61	ASN
1	G	63	GLN
1	G	70	GLN
1	G	78	HIS
1	G	134	ASN
1	G	146	GLN
1	G	180	ASN
1	G	190	GLN
1	G	212	ASN
1	G	217	HIS
1	G	307	HIS
1	H	24	HIS
1	H	70	GLN
1	H	78	HIS
1	H	134	ASN
1	H	146	GLN
1	H	180	ASN
1	H	190	GLN
1	H	212	ASN
1	H	217	HIS
1	H	252	ASN
1	H	307	HIS

5.3.3 RNA ⓘ

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](#)

8 ligands are modelled in this entry.

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$
2	FAB	E	348	-	59,63,63	1.27	4 (6%)	82,97,97	1.82	17 (20%)
2	FAB	G	348	-	59,63,63	1.28	4 (6%)	82,97,97	1.82	17 (20%)
2	FAB	B	348	-	59,63,63	1.28	4 (6%)	82,97,97	1.82	17 (20%)
2	FAB	A	348	-	59,63,63	1.28	4 (6%)	82,97,97	1.82	17 (20%)
2	FAB	D	348	-	59,63,63	1.28	4 (6%)	82,97,97	1.82	16 (19%)
2	FAB	C	348	-	59,63,63	1.29	4 (6%)	82,97,97	1.81	18 (21%)
2	FAB	F	348	-	59,63,63	1.28	4 (6%)	82,97,97	1.81	16 (19%)
2	FAB	H	348	-	59,63,63	1.29	4 (6%)	82,97,97	1.82	17 (20%)

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
2	FAB	E	348	-	-	5/40/58/58	0/6/6/6
2	FAB	G	348	-	-	5/40/58/58	0/6/6/6
2	FAB	B	348	-	-	5/40/58/58	0/6/6/6
2	FAB	A	348	-	-	5/40/58/58	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAB	D	348	-	-	5/40/58/58	0/6/6/6
2	FAB	C	348	-	-	5/40/58/58	0/6/6/6
2	FAB	F	348	-	-	5/40/58/58	0/6/6/6
2	FAB	H	348	-	-	5/40/58/58	0/6/6/6

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	348	FAB	C3'-C2'	7.14	1.63	1.52
2	D	348	FAB	C3'-C2'	7.10	1.63	1.52
2	A	348	FAB	C3'-C2'	7.09	1.63	1.52
2	H	348	FAB	C3'-C2'	7.07	1.63	1.52
2	F	348	FAB	C3'-C2'	7.07	1.63	1.52
2	G	348	FAB	C3'-C2'	7.06	1.63	1.52
2	B	348	FAB	C3'-C2'	7.02	1.63	1.52
2	E	348	FAB	C3'-C2'	7.01	1.63	1.52
2	H	348	FAB	P-O3P	4.08	1.63	1.59
2	E	348	FAB	P-O3P	4.03	1.63	1.59
2	F	348	FAB	P-O3P	3.99	1.63	1.59
2	C	348	FAB	P-O3P	3.98	1.63	1.59
2	B	348	FAB	P-O3P	3.98	1.63	1.59
2	G	348	FAB	P-O3P	3.96	1.63	1.59
2	D	348	FAB	P-O3P	3.96	1.63	1.59
2	A	348	FAB	P-O3P	3.93	1.63	1.59
2	D	348	FAB	PA-O3P	3.17	1.62	1.59
2	A	348	FAB	PA-O3P	3.16	1.62	1.59
2	G	348	FAB	PA-O3P	3.15	1.62	1.59
2	C	348	FAB	PA-O3P	3.15	1.62	1.59
2	B	348	FAB	PA-O3P	3.14	1.62	1.59
2	H	348	FAB	PA-O3P	3.13	1.62	1.59
2	F	348	FAB	PA-O3P	3.13	1.62	1.59
2	E	348	FAB	PA-O3P	3.08	1.62	1.59
2	B	348	FAB	C9A-N10	-2.14	1.37	1.41
2	H	348	FAB	C9A-N10	-2.12	1.37	1.41
2	G	348	FAB	C9A-N10	-2.11	1.37	1.41
2	F	348	FAB	C9A-N10	-2.09	1.37	1.41
2	E	348	FAB	C9A-N10	-2.08	1.37	1.41
2	A	348	FAB	C9A-N10	-2.08	1.37	1.41
2	C	348	FAB	C9A-N10	-2.07	1.37	1.41
2	D	348	FAB	C9A-N10	-2.06	1.37	1.41

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	348	FAB	C4'-C3'-C2'	5.32	118.13	109.45
2	D	348	FAB	C4'-C3'-C2'	5.31	118.12	109.45
2	A	348	FAB	C4'-C3'-C2'	5.31	118.12	109.45
2	H	348	FAB	C4'-C3'-C2'	5.31	118.12	109.45
2	B	348	FAB	C4'-C3'-C2'	5.30	118.11	109.45
2	G	348	FAB	C4'-C3'-C2'	5.30	118.11	109.45
2	C	348	FAB	C4'-C3'-C2'	5.29	118.08	109.45
2	F	348	FAB	C4'-C3'-C2'	5.28	118.08	109.45
2	D	348	FAB	C7M-C7-C8	-5.25	110.04	120.76
2	C	348	FAB	C7M-C7-C8	-5.25	110.04	120.76
2	A	348	FAB	C7M-C7-C8	-5.24	110.05	120.76
2	G	348	FAB	C7M-C7-C8	-5.24	110.06	120.76
2	H	348	FAB	C7M-C7-C8	-5.24	110.06	120.76
2	B	348	FAB	C7M-C7-C8	-5.24	110.07	120.76
2	E	348	FAB	C7M-C7-C8	-5.23	110.08	120.76
2	F	348	FAB	C7M-C7-C8	-5.22	110.09	120.76
2	E	348	FAB	C9-C9A-N10	-4.86	115.32	121.85
2	H	348	FAB	C9-C9A-N10	-4.85	115.33	121.85
2	C	348	FAB	C9-C9A-N10	-4.85	115.33	121.85
2	B	348	FAB	C9-C9A-N10	-4.84	115.34	121.85
2	A	348	FAB	C9-C9A-N10	-4.83	115.36	121.85
2	F	348	FAB	C9-C9A-N10	-4.81	115.39	121.85
2	D	348	FAB	C9-C9A-N10	-4.81	115.39	121.85
2	G	348	FAB	C9-C9A-N10	-4.80	115.40	121.85
2	D	348	FAB	C7M-C7-C6	4.55	127.59	119.57
2	G	348	FAB	C7M-C7-C6	4.54	127.57	119.57
2	B	348	FAB	C7M-C7-C6	4.53	127.56	119.57
2	H	348	FAB	C7M-C7-C6	4.52	127.53	119.57
2	A	348	FAB	C7M-C7-C6	4.52	127.53	119.57
2	E	348	FAB	C7M-C7-C6	4.52	127.53	119.57
2	C	348	FAB	C7M-C7-C6	4.51	127.52	119.57
2	F	348	FAB	C7M-C7-C6	4.49	127.49	119.57
2	D	348	FAB	O4-C4-C4X	-4.18	118.67	128.01
2	F	348	FAB	O4-C4-C4X	-4.17	118.71	128.01
2	A	348	FAB	O4-C4-C4X	-4.16	118.72	128.01
2	H	348	FAB	O4-C4-C4X	-4.16	118.73	128.01
2	G	348	FAB	O4-C4-C4X	-4.15	118.74	128.01
2	C	348	FAB	O4-C4-C4X	-4.15	118.75	128.01
2	E	348	FAB	O4-C4-C4X	-4.14	118.76	128.01
2	B	348	FAB	O4-C4-C4X	-4.14	118.76	128.01
2	D	348	FAB	O4-C4-N3	3.98	127.60	120.11
2	H	348	FAB	O4-C4-N3	3.96	127.56	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	348	FAB	O4-C4-N3	3.96	127.56	120.11
2	F	348	FAB	O4-C4-N3	3.96	127.56	120.11
2	A	348	FAB	O4-C4-N3	3.95	127.55	120.11
2	E	348	FAB	O4-C4-N3	3.95	127.54	120.11
2	B	348	FAB	O4-C4-N3	3.94	127.53	120.11
2	C	348	FAB	O4-C4-N3	3.93	127.50	120.11
2	B	348	FAB	C5X-C9A-N10	3.25	122.88	119.04
2	E	348	FAB	C5X-C9A-N10	3.23	122.86	119.04
2	H	348	FAB	C5X-C9A-N10	3.22	122.84	119.04
2	A	348	FAB	C5X-C9A-N10	3.21	122.84	119.04
2	G	348	FAB	C5X-C9A-N10	3.19	122.81	119.04
2	C	348	FAB	C5X-C9A-N10	3.18	122.80	119.04
2	F	348	FAB	C5X-C9A-N10	3.17	122.79	119.04
2	D	348	FAB	C5X-C9A-N10	3.17	122.79	119.04
2	E	348	FAB	C3B-C2B-C1B	-3.16	95.48	101.46
2	G	348	FAB	C3B-C2B-C1B	-3.16	95.49	101.46
2	A	348	FAB	C3B-C2B-C1B	-3.15	95.51	101.46
2	F	348	FAB	C3B-C2B-C1B	-3.14	95.51	101.46
2	C	348	FAB	C3B-C2B-C1B	-3.14	95.52	101.46
2	H	348	FAB	C3B-C2B-C1B	-3.14	95.52	101.46
2	B	348	FAB	C3B-C2B-C1B	-3.14	95.52	101.46
2	D	348	FAB	C3B-C2B-C1B	-3.14	95.52	101.46
2	A	348	FAB	O2-C2-N3	2.98	124.31	118.58
2	H	348	FAB	O2-C2-N3	2.98	124.31	118.58
2	F	348	FAB	O2-C2-N3	2.97	124.29	118.58
2	G	348	FAB	O2-C2-N3	2.97	124.28	118.58
2	E	348	FAB	O2-C2-N3	2.97	124.28	118.58
2	D	348	FAB	O2-C2-N3	2.97	124.28	118.58
2	B	348	FAB	O2-C2-N3	2.96	124.27	118.58
2	C	348	FAB	O2-C2-N3	2.95	124.24	118.58
2	D	348	FAB	C8M-C8-C9	2.69	124.31	119.57
2	C	348	FAB	C8M-C8-C9	2.69	124.30	119.57
2	G	348	FAB	C8M-C8-C9	2.68	124.30	119.57
2	A	348	FAB	C8M-C8-C9	2.68	124.29	119.57
2	F	348	FAB	C8M-C8-C9	2.68	124.29	119.57
2	B	348	FAB	C8M-C8-C9	2.67	124.28	119.57
2	E	348	FAB	C8M-C8-C9	2.67	124.28	119.57
2	F	348	FAB	C5'-C3'-C4'	-2.66	101.09	111.60
2	H	348	FAB	C8M-C8-C9	2.66	124.25	119.57
2	E	348	FAB	C5'-C3'-C4'	-2.65	101.10	111.60
2	A	348	FAB	C5'-C3'-C4'	-2.65	101.12	111.60
2	B	348	FAB	C5'-C3'-C4'	-2.65	101.12	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	348	FAB	C5'-C3'-C4'	-2.65	101.13	111.60
2	C	348	FAB	C5'-C3'-C4'	-2.64	101.14	111.60
2	H	348	FAB	C5'-C3'-C4'	-2.64	101.16	111.60
2	G	348	FAB	C5'-C3'-C4'	-2.64	101.17	111.60
2	D	348	FAB	N3-C2-N1	-2.22	114.78	119.50
2	A	348	FAB	N3-C2-N1	-2.22	114.78	119.50
2	H	348	FAB	N3-C2-N1	-2.22	114.78	119.50
2	G	348	FAB	N3-C2-N1	-2.21	114.81	119.50
2	E	348	FAB	N3-C2-N1	-2.21	114.81	119.50
2	F	348	FAB	N3-C2-N1	-2.20	114.83	119.50
2	C	348	FAB	N3-C2-N1	-2.19	114.84	119.50
2	B	348	FAB	N3-C2-N1	-2.19	114.85	119.50
2	B	348	FAB	C1'-C2D-C3D	2.14	115.45	109.66
2	E	348	FAB	C8M-C8-C7	-2.13	116.41	120.76
2	C	348	FAB	C1'-C2D-C3D	2.13	115.43	109.66
2	B	348	FAB	C8M-C8-C7	-2.13	116.42	120.76
2	D	348	FAB	C8M-C8-C7	-2.13	116.42	120.76
2	E	348	FAB	C1'-C2D-C3D	2.13	115.42	109.66
2	A	348	FAB	C1'-C2D-C3D	2.12	115.42	109.66
2	G	348	FAB	C8M-C8-C7	-2.12	116.42	120.76
2	F	348	FAB	C8M-C8-C7	-2.12	116.43	120.76
2	G	348	FAB	C1'-C2D-C3D	2.12	115.40	109.66
2	D	348	FAB	C1'-C2D-C3D	2.11	115.39	109.66
2	F	348	FAB	C1'-C2D-C3D	2.11	115.39	109.66
2	A	348	FAB	C8M-C8-C7	-2.11	116.45	120.76
2	C	348	FAB	C8M-C8-C7	-2.10	116.46	120.76
2	H	348	FAB	C1'-C2D-C3D	2.10	115.36	109.66
2	H	348	FAB	C8M-C8-C7	-2.10	116.48	120.76
2	E	348	FAB	O2A-PA-O3P	2.09	112.92	107.27
2	G	348	FAB	O2A-PA-O3P	2.08	112.89	107.27
2	C	348	FAB	O2A-PA-O3P	2.08	112.89	107.27
2	D	348	FAB	O2A-PA-O3P	2.08	112.88	107.27
2	B	348	FAB	O2A-PA-O3P	2.07	112.88	107.27
2	A	348	FAB	O2A-PA-O3P	2.07	112.87	107.27
2	F	348	FAB	O2A-PA-O3P	2.07	112.87	107.27
2	H	348	FAB	O2A-PA-O3P	2.06	112.83	107.27
2	F	348	FAB	O3B-C3B-C2B	-2.05	105.24	111.82
2	B	348	FAB	O3B-C3B-C2B	-2.04	105.28	111.82
2	A	348	FAB	O3B-C3B-C2B	-2.04	105.29	111.82
2	H	348	FAB	O3B-C3B-C2B	-2.03	105.30	111.82
2	G	348	FAB	O3B-C3B-C2B	-2.03	105.30	111.82
2	C	348	FAB	O3B-C3B-C2B	-2.03	105.31	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	348	FAB	O3D-C3D-C2D	-2.03	104.32	108.93
2	E	348	FAB	O3B-C3B-C2B	-2.03	105.31	111.82
2	D	348	FAB	O3B-C3B-C2B	-2.02	105.34	111.82
2	H	348	FAB	O3D-C3D-C2D	-2.02	104.35	108.93
2	G	348	FAB	O3D-C3D-C2D	-2.01	104.36	108.93
2	E	348	FAB	O3D-C3D-C2D	-2.01	104.36	108.93
2	A	348	FAB	O3D-C3D-C2D	-2.01	104.37	108.93
2	C	348	FAB	O3D-C3D-C2D	-2.00	104.38	108.93
2	C	348	FAB	O2B-C2B-C3B	-2.00	105.40	111.82

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	348	FAB	O3'-C2'-N5-C5X
2	B	348	FAB	O3'-C2'-N5-C5X
2	C	348	FAB	O3'-C2'-N5-C5X
2	D	348	FAB	O3'-C2'-N5-C5X
2	E	348	FAB	O3'-C2'-N5-C5X
2	F	348	FAB	O3'-C2'-N5-C5X
2	G	348	FAB	O3'-C2'-N5-C5X
2	H	348	FAB	O3'-C2'-N5-C5X
2	A	348	FAB	O4B-C4B-C5B-O5B
2	B	348	FAB	O4B-C4B-C5B-O5B
2	C	348	FAB	O4B-C4B-C5B-O5B
2	D	348	FAB	O4B-C4B-C5B-O5B
2	E	348	FAB	O4B-C4B-C5B-O5B
2	F	348	FAB	O4B-C4B-C5B-O5B
2	G	348	FAB	O4B-C4B-C5B-O5B
2	H	348	FAB	O4B-C4B-C5B-O5B
2	A	348	FAB	C3'-C2'-N5-C5X
2	B	348	FAB	C3'-C2'-N5-C5X
2	C	348	FAB	C3'-C2'-N5-C5X
2	D	348	FAB	C3'-C2'-N5-C5X
2	E	348	FAB	C3'-C2'-N5-C5X
2	F	348	FAB	C3'-C2'-N5-C5X
2	G	348	FAB	C3'-C2'-N5-C5X
2	H	348	FAB	C3'-C2'-N5-C5X
2	A	348	FAB	C3B-C4B-C5B-O5B
2	B	348	FAB	C3B-C4B-C5B-O5B
2	C	348	FAB	C3B-C4B-C5B-O5B
2	D	348	FAB	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	E	348	FAB	C3B-C4B-C5B-O5B
2	F	348	FAB	C3B-C4B-C5B-O5B
2	G	348	FAB	C3B-C4B-C5B-O5B
2	H	348	FAB	C3B-C4B-C5B-O5B
2	A	348	FAB	P-O3P-PA-O5B
2	B	348	FAB	P-O3P-PA-O5B
2	C	348	FAB	P-O3P-PA-O5B
2	D	348	FAB	P-O3P-PA-O5B
2	E	348	FAB	P-O3P-PA-O5B
2	F	348	FAB	P-O3P-PA-O5B
2	G	348	FAB	P-O3P-PA-O5B
2	H	348	FAB	P-O3P-PA-O5B

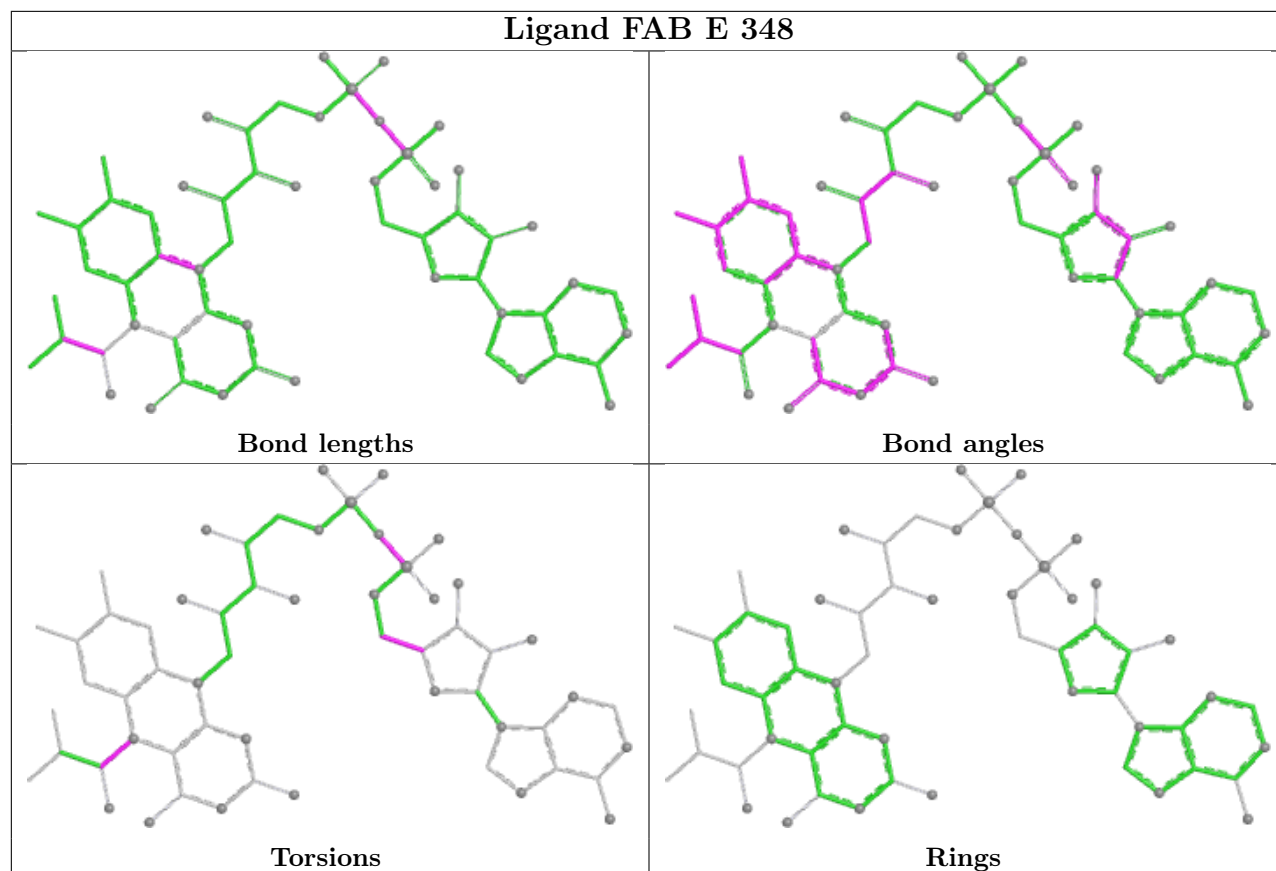
There are no ring outliers.

8 monomers are involved in 50 short contacts:

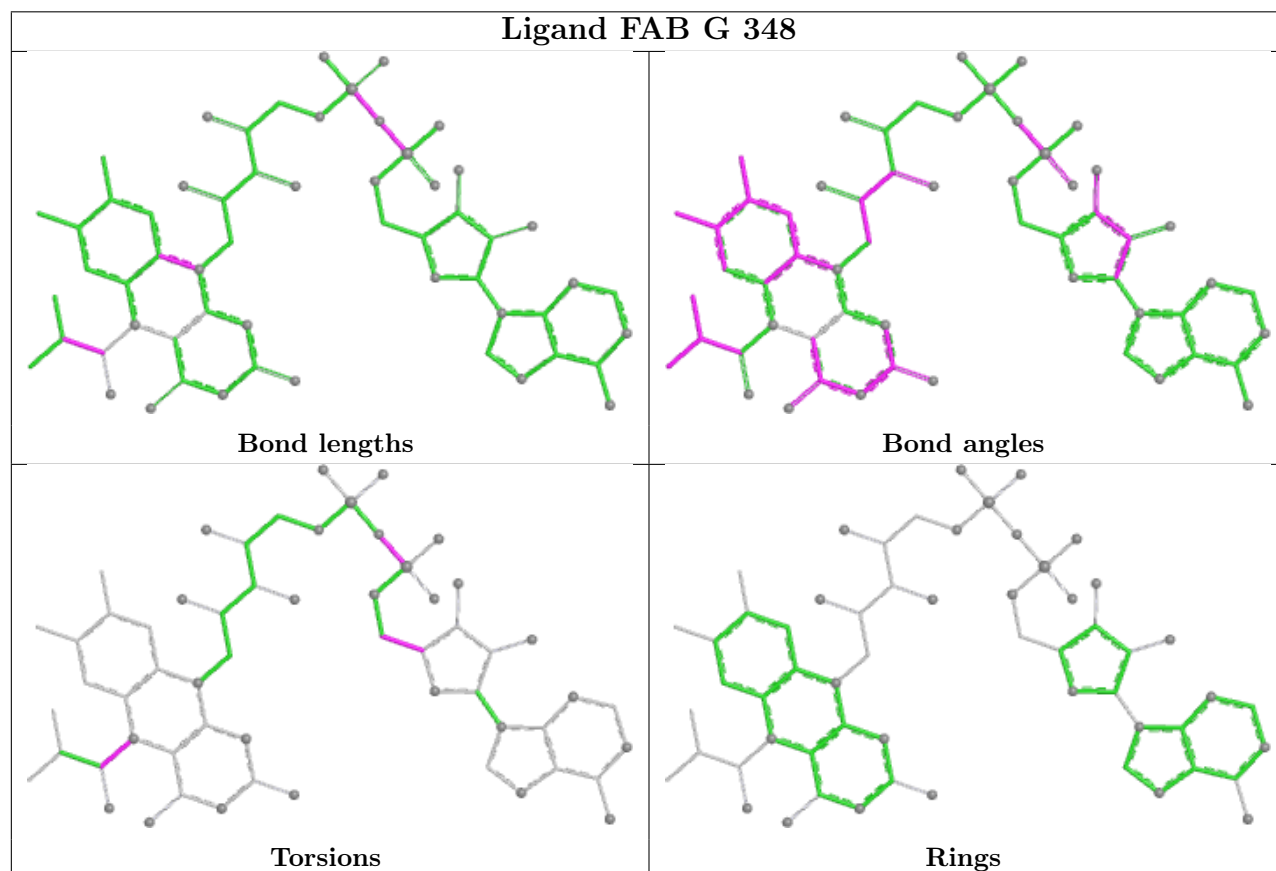
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	348	FAB	7	0
2	G	348	FAB	6	0
2	B	348	FAB	7	0
2	A	348	FAB	6	0
2	D	348	FAB	6	0
2	C	348	FAB	5	0
2	F	348	FAB	7	0
2	H	348	FAB	6	0

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.

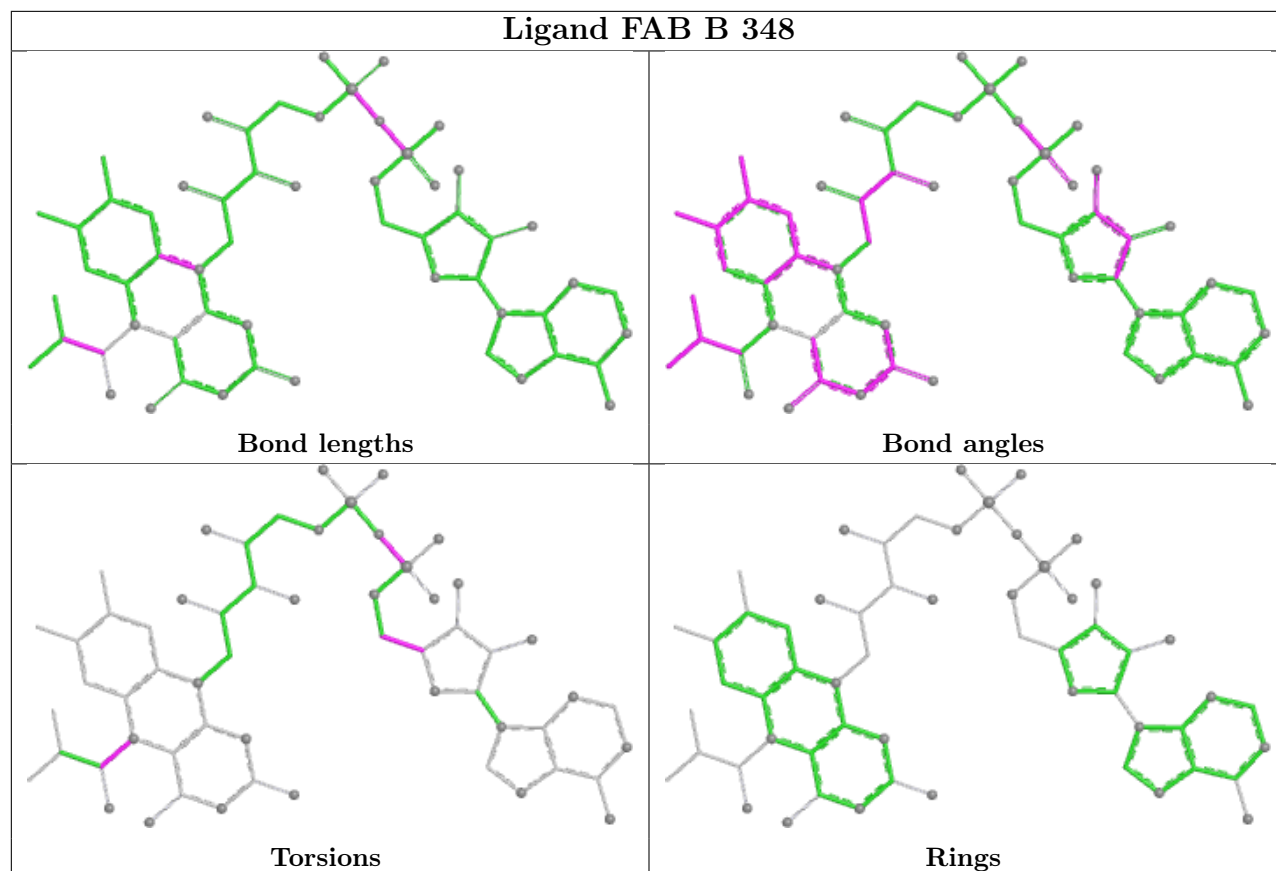
Ligand FAB E 348



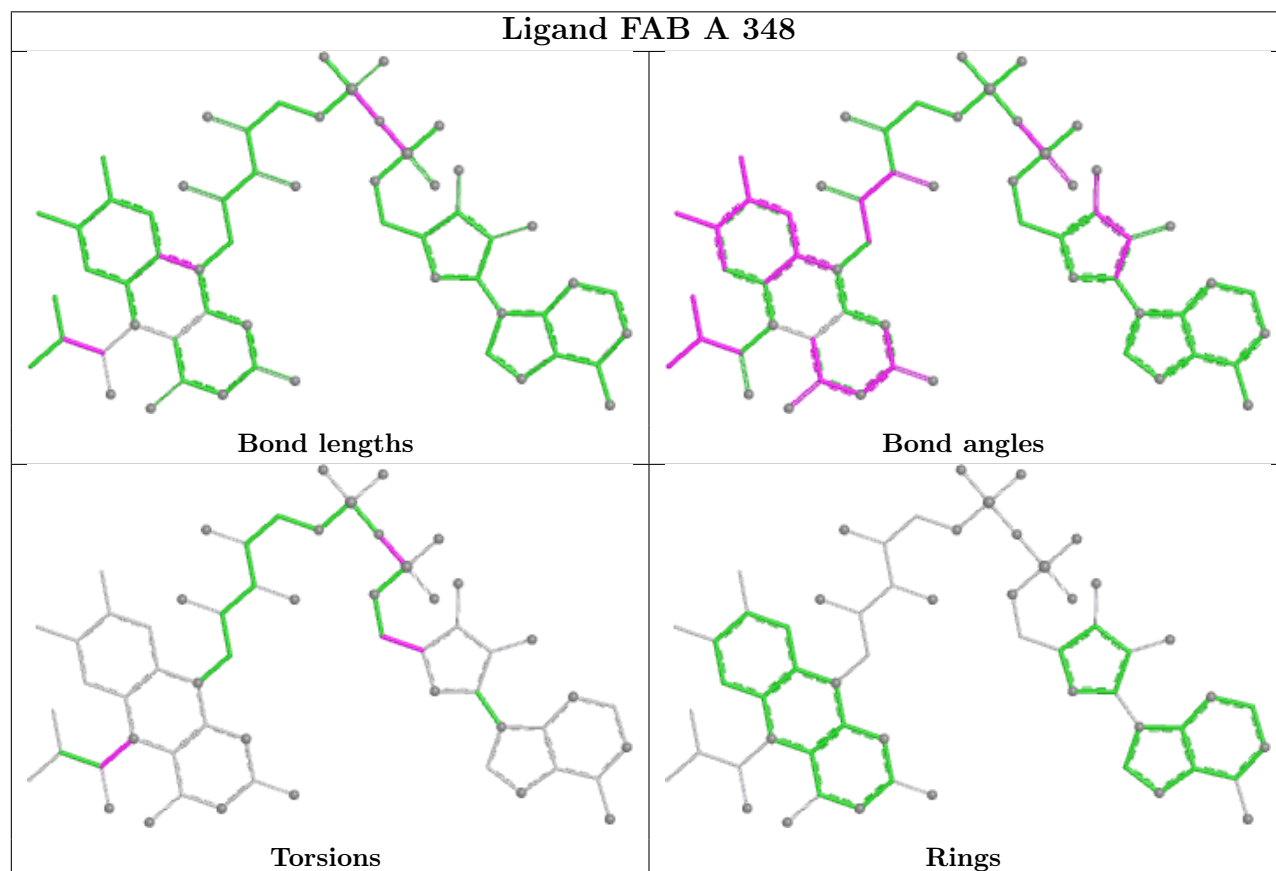
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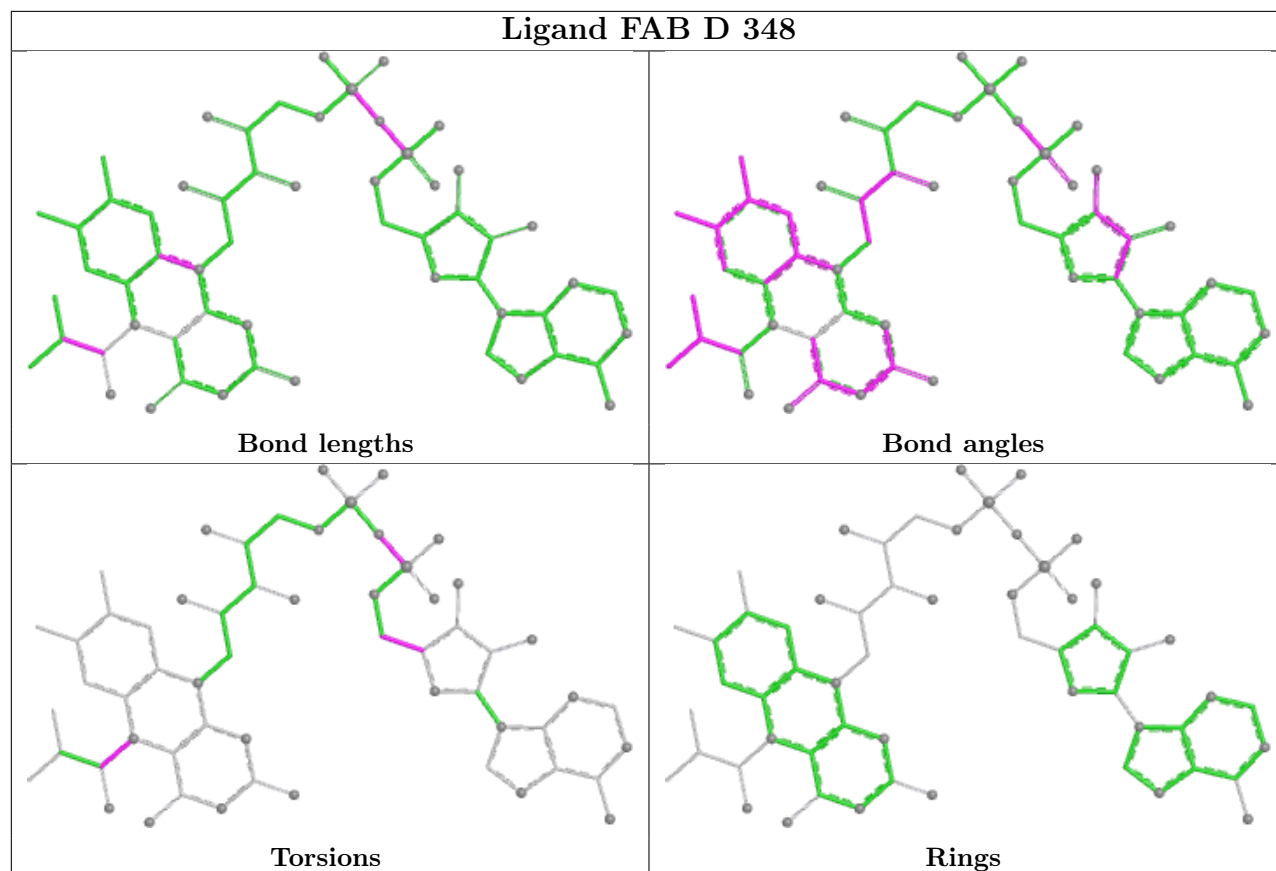
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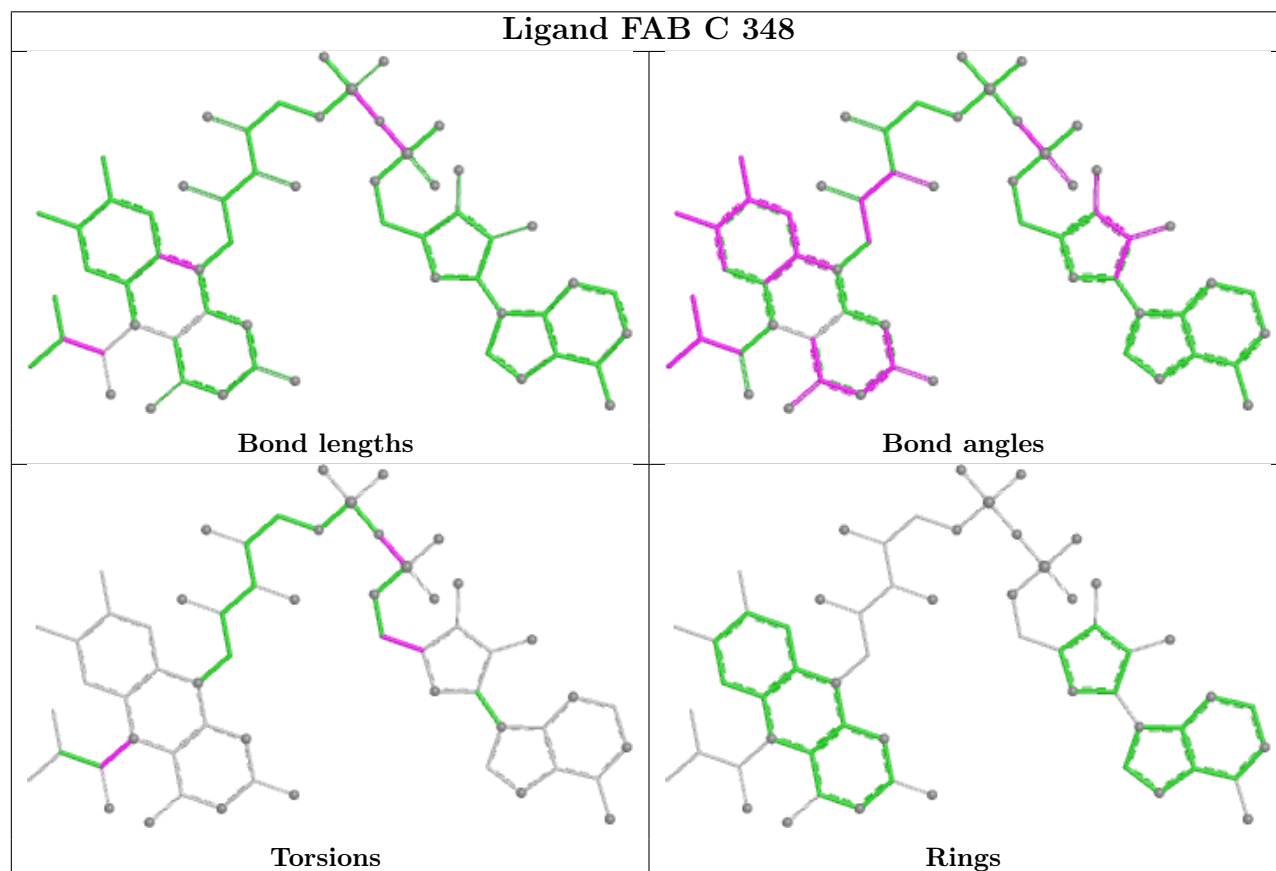
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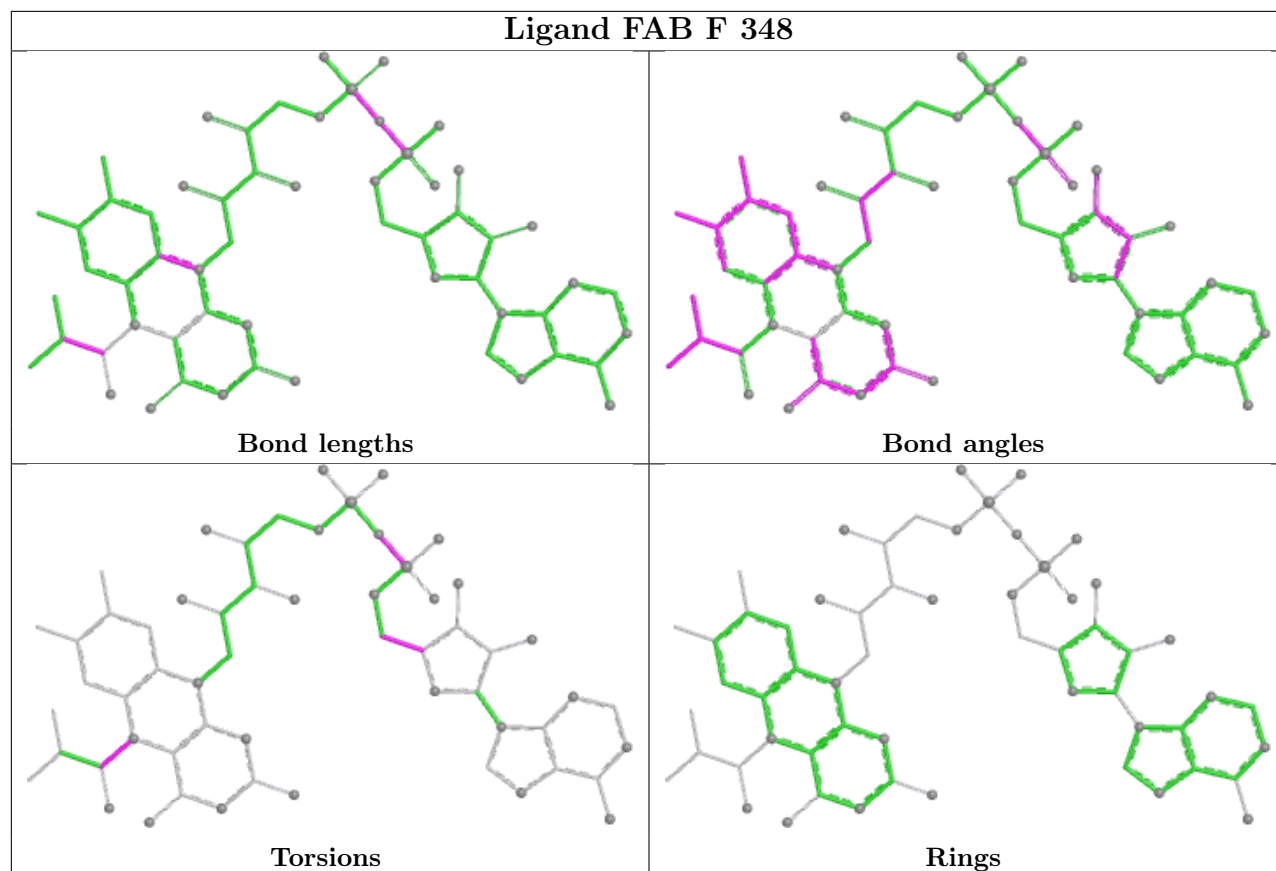
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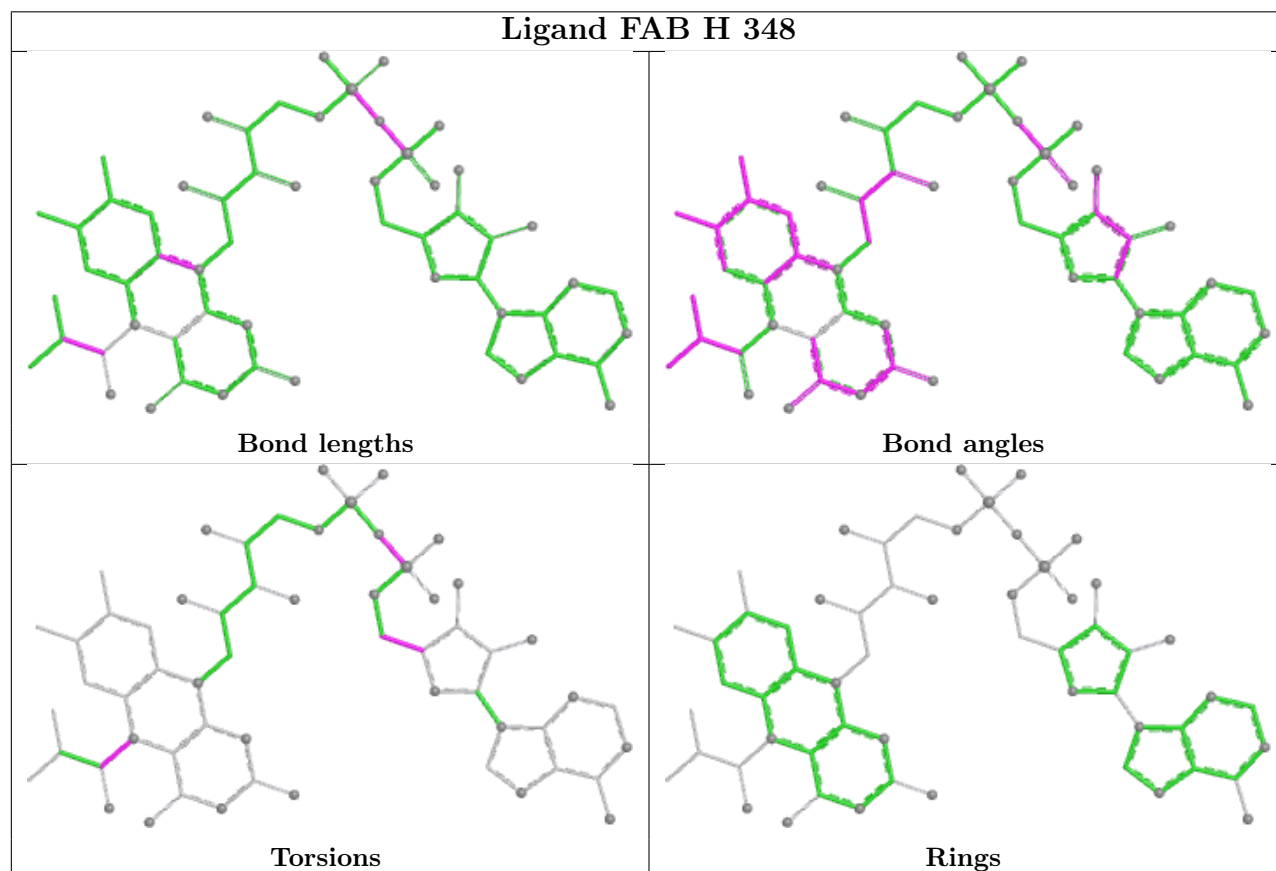
Ligand FAB C 348



Ligand FAB F 348



Ligand FAB H 348



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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	338/347 (97%)	0.41	18 (5%)	32	20	2, 15, 55, 99	24 (7%)
1	B	338/347 (97%)	0.43	18 (5%)	32	20	1, 16, 62, 99	26 (7%)
1	C	338/347 (97%)	0.41	19 (5%)	30	19	2, 15, 59, 99	27 (7%)
1	D	338/347 (97%)	0.40	27 (7%)	18	12	2, 15, 56, 99	24 (7%)
1	E	338/347 (97%)	0.40	21 (6%)	26	17	2, 15, 57, 99	26 (7%)
1	F	338/347 (97%)	0.44	23 (6%)	23	15	2, 14, 56, 99	27 (7%)
1	G	338/347 (97%)	0.48	17 (5%)	34	22	2, 16, 60, 99	28 (8%)
1	H	338/347 (97%)	0.40	22 (6%)	25	16	2, 15, 60, 99	27 (7%)
All	All	2704/2776 (97%)	0.42	165 (6%)	27	17	1, 15, 59, 99	209 (7%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	28	GLN	10.5
1	C	28	GLN	8.4
1	G	28	GLN	7.8
1	F	28	GLN	7.6
1	A	28	GLN	7.2
1	D	28	GLN	7.1
1	E	28	GLN	6.9
1	F	26	VAL	6.8
1	B	301	SER	6.6
1	C	339	LEU	6.6
1	C	26	VAL	6.5
1	D	302	ASN	6.2
1	A	339	LEU	6.2
1	G	300	SER	6.1
1	C	300	SER	5.7
1	G	339	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	27	LEU	5.5
1	H	339	LEU	5.4
1	E	301	SER	5.3
1	D	339	LEU	5.3
1	D	301	SER	5.2
1	F	301	SER	5.2
1	H	26	VAL	5.1
1	G	301	SER	5.0
1	B	302	ASN	5.0
1	B	27	LEU	5.0
1	E	27	LEU	5.0
1	H	299	GLY	5.0
1	B	26	VAL	4.8
1	D	26	VAL	4.6
1	F	300	SER	4.5
1	H	27	LEU	4.5
1	B	300	SER	4.4
1	C	27	LEU	4.4
1	E	26	VAL	4.4
1	B	339	LEU	4.4
1	D	27	LEU	4.2
1	B	28	GLN	4.2
1	G	27	LEU	4.1
1	E	220	GLU	4.1
1	H	298	PHE	3.9
1	D	338	ASN	3.8
1	F	299	GLY	3.8
1	E	24	HIS	3.7
1	A	27	LEU	3.7
1	E	298	PHE	3.7
1	F	339	LEU	3.6
1	C	338	ASN	3.6
1	H	25	SER	3.6
1	C	25	SER	3.6
1	E	339	LEU	3.6
1	D	25	SER	3.6
1	F	302	ASN	3.5
1	D	298	PHE	3.5
1	G	26	VAL	3.4
1	B	173	GLY	3.4
1	C	30	LEU	3.3
1	D	299	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	218	ASP	3.3
1	H	302	ASN	3.3
1	A	297	ARG	3.2
1	F	221	ARG	3.2
1	G	62	PRO	3.2
1	A	249	GLU	3.2
1	G	299	GLY	3.2
1	D	300	SER	3.2
1	H	234	GLN	3.2
1	D	31	ASP	3.2
1	A	26	VAL	3.1
1	A	25	SER	3.1
1	E	25	SER	3.1
1	F	338	ASN	3.1
1	E	60	SER	3.0
1	D	24	HIS	3.0
1	A	304	GLU	3.0
1	E	299	GLY	3.0
1	E	302	ASN	3.0
1	F	24	HIS	3.0
1	G	30	LEU	2.9
1	F	30	LEU	2.9
1	C	302	ASN	2.9
1	B	337	ARG	2.9
1	C	298	PHE	2.9
1	E	30	LEU	2.9
1	E	300	SER	2.8
1	G	25	SER	2.8
1	B	338	ASN	2.8
1	E	338	ASN	2.8
1	D	295	GLN	2.8
1	A	335	GLU	2.8
1	A	338	ASN	2.8
1	A	337	ARG	2.8
1	F	25	SER	2.8
1	C	24	HIS	2.7
1	G	302	ASN	2.7
1	D	303	THR	2.7
1	H	301	SER	2.7
1	A	299	GLY	2.7
1	F	303	THR	2.7
1	C	337	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	225	ASN	2.6
1	E	225	ASN	2.6
1	H	338	ASN	2.6
1	B	298	PHE	2.6
1	F	60	SER	2.6
1	F	252	ASN	2.6
1	F	220	GLU	2.6
1	E	31	ASP	2.5
1	D	220	GLU	2.5
1	H	30	LEU	2.5
1	F	234	GLN	2.5
1	G	298	PHE	2.5
1	A	300	SER	2.5
1	H	220	GLU	2.4
1	H	261	GLU	2.4
1	H	225	ASN	2.4
1	C	299	GLY	2.4
1	G	174	GLY	2.4
1	A	301	SER	2.4
1	D	337	ARG	2.4
1	C	66	ASN	2.4
1	C	301	SER	2.4
1	D	57	SER	2.4
1	A	66	ASN	2.3
1	A	298	PHE	2.3
1	G	334	LEU	2.3
1	D	297	ARG	2.3
1	D	63	GLN	2.3
1	H	80	GLY	2.3
1	B	30	LEU	2.3
1	D	218	ASP	2.3
1	H	300	SER	2.3
1	D	99	ARG	2.3
1	A	30	LEU	2.2
1	G	338	ASN	2.2
1	B	31	ASP	2.2
1	C	60	SER	2.2
1	D	225	ASN	2.2
1	F	73	ASN	2.2
1	H	64	GLU	2.2
1	B	297	ARG	2.1
1	D	61	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	176	ASP	2.1
1	G	218	ASP	2.1
1	H	176	ASP	2.1
1	E	279	TYR	2.1
1	C	99	ARG	2.1
1	E	249	GLU	2.1
1	F	225	ASN	2.1
1	H	99	ARG	2.1
1	B	64	GLU	2.1
1	C	59	PRO	2.1
1	D	30	LEU	2.1
1	B	222	GLY	2.1
1	F	298	PHE	2.1
1	H	61	ASN	2.1
1	E	218	ASP	2.1
1	G	304	GLU	2.1
1	B	252	ASN	2.0
1	E	66	ASN	2.0
1	F	31	ASP	2.0
1	B	166	SER	2.0
1	D	60	SER	2.0
1	F	66	ASN	2.0
1	D	234	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

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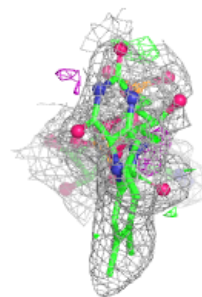
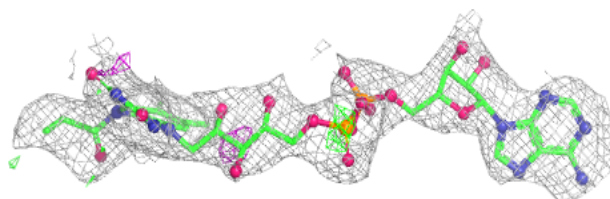
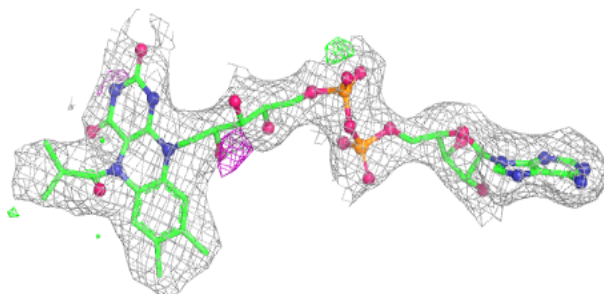
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAB	E	348	58/58	0.95	0.10	1,6,21,24	0
2	FAB	H	348	58/58	0.95	0.10	1,6,21,24	0
2	FAB	C	348	58/58	0.96	0.09	1,6,21,24	0
2	FAB	D	348	58/58	0.96	0.10	1,6,21,24	0
2	FAB	A	348	58/58	0.96	0.10	1,6,21,24	0
2	FAB	G	348	58/58	0.96	0.10	1,6,21,24	0
2	FAB	B	348	58/58	0.96	0.10	1,6,21,24	0
2	FAB	F	348	58/58	0.97	0.09	1,6,21,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

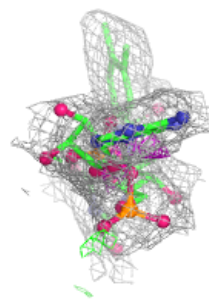
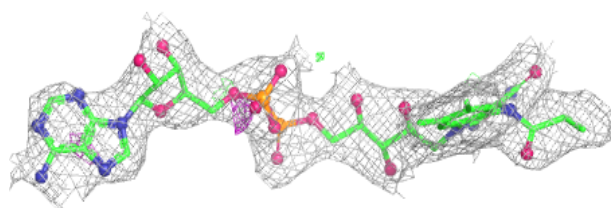
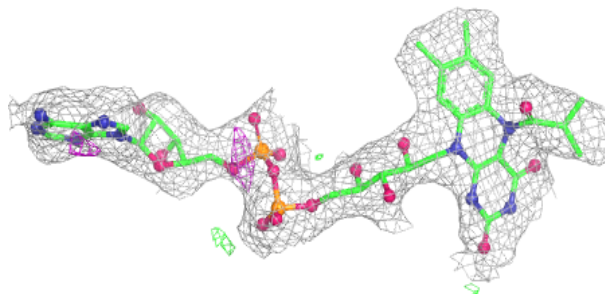
Electron density around FAB E 348:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

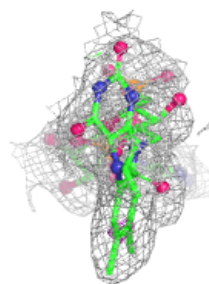
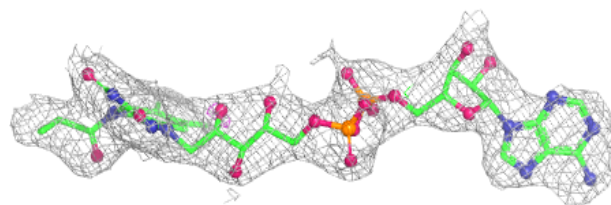
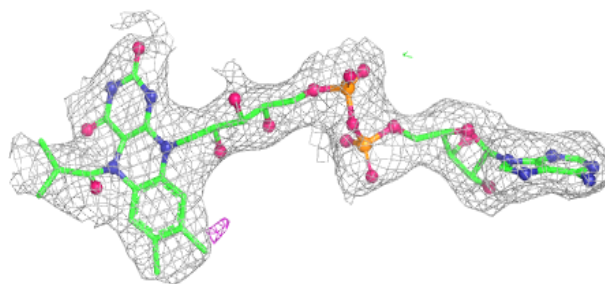


Electron density around FAB H 348:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

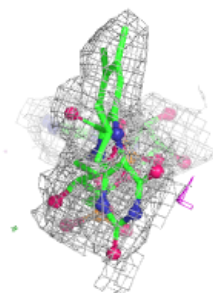
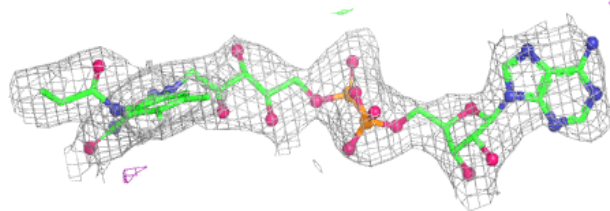
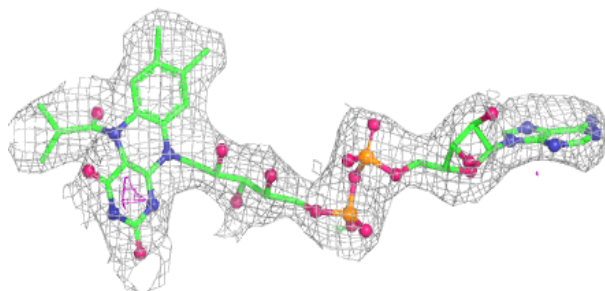
**Electron density around FAB C 348:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

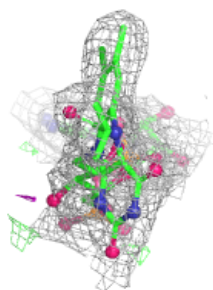
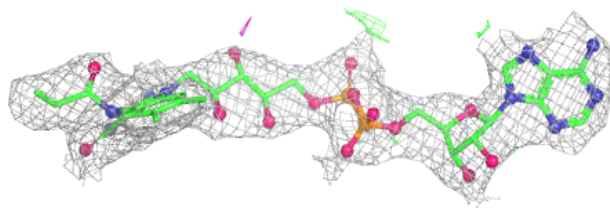
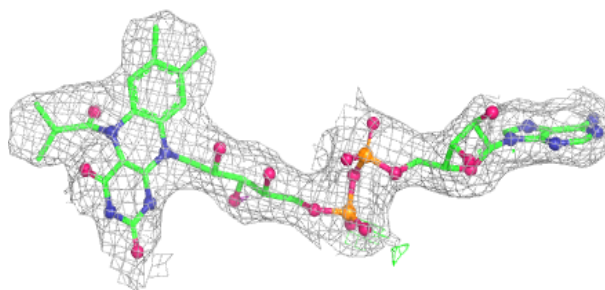


Electron density around FAB D 348:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

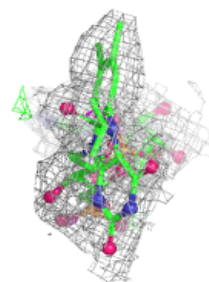
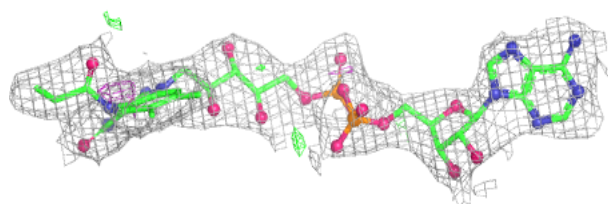
**Electron density around FAB A 348:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

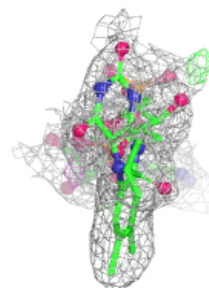
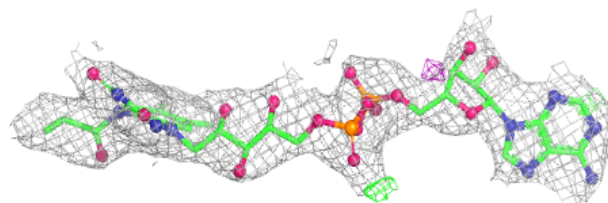
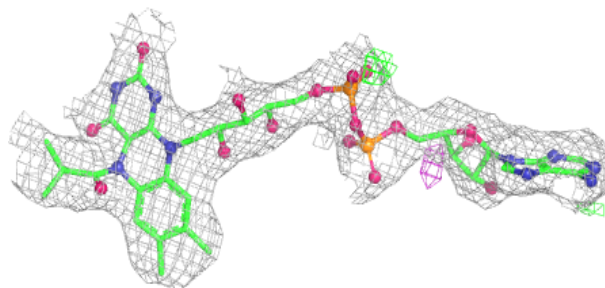


Electron density around FAB G 348:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

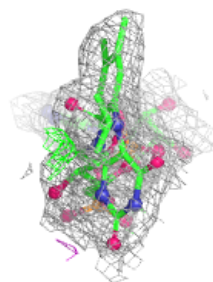
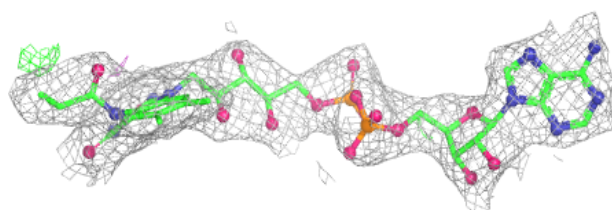
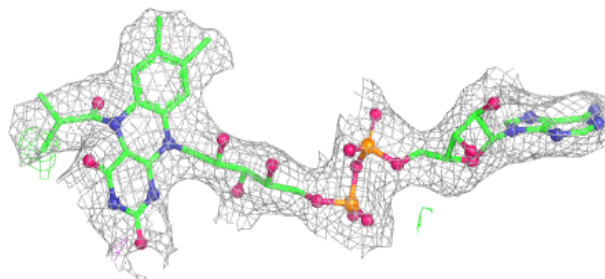
**Electron density around FAB B 348:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FAB F 348:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.