



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:11 AM UTC

PDB ID : 1C3O / pdb_00001c3o
Title : CRYSTAL STRUCTURE OF THE CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT MUTANT C269S WITH BOUND GLUTAMINE
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 1999-07-28
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

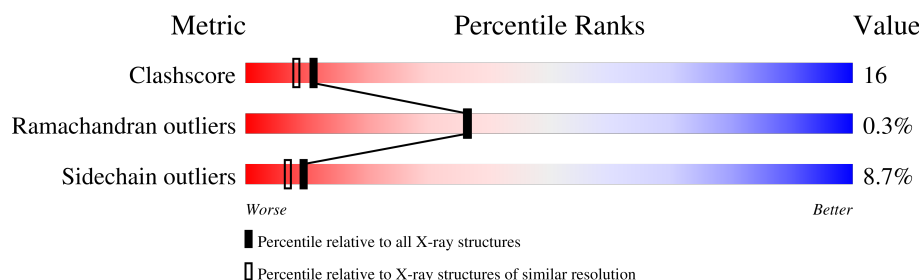
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	67% 27% 5% .
1	C	1073	66% 28% . .
1	E	1073	69% 24% 5% .
1	G	1073	62% 30% 6% .
2	B	382	58% 37% . .
2	D	382	60% 34% 5% .
2	F	382	59% 33% 7% .
2	H	382	53% 40% 6% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	G	4083	-	-	X	-
6	PO4	E	4050	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48477 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 CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	6	0
			8195	5146	1433	1570	46			
1	C	1058	Total	C	N	O	S	0	7	0
			8192	5144	1428	1575	45			
1	E	1058	Total	C	N	O	S	0	10	0
			8211	5155	1431	1580	45			
1	G	1058	Total	C	N	O	S	0	4	0
			8180	5135	1425	1574	46			

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	D	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	F	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	H	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	SER	CYS	engineered mutation	UNP P00907
D	269	SER	CYS	engineered mutation	UNP P00907
F	269	SER	CYS	engineered mutation	UNP P00907
H	269	SER	CYS	engineered mutation	UNP P00907

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mn 3 3	0	0
3	C	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0
3	G	3	Total Mn 3 3	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total K 7 7	0	0
4	B	1	Total K 1 1	0	0
4	C	7	Total K 7 7	0	0
4	D	1	Total K 1 1	0	0
4	E	7	Total K 7 7	0	0
4	F	1	Total K 1 1	0	0
4	G	7	Total K 7 7	0	0
4	H	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

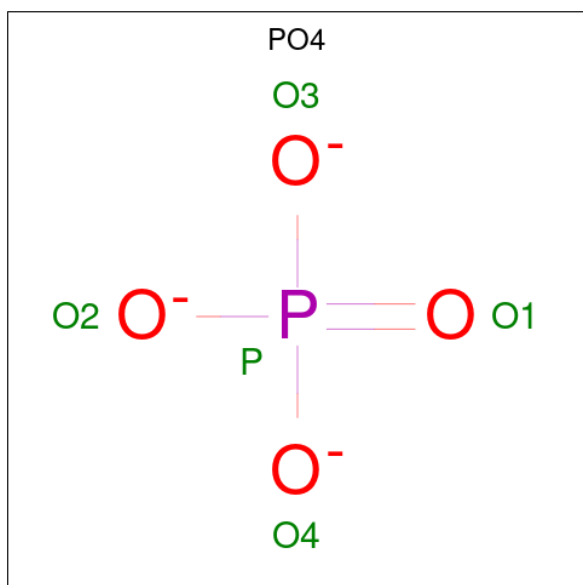
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0
5	D	1	Total Cl 1 1	0	0
5	E	3	Total Cl 3 3	0	0
5	F	1	Total Cl 1 1	0	0

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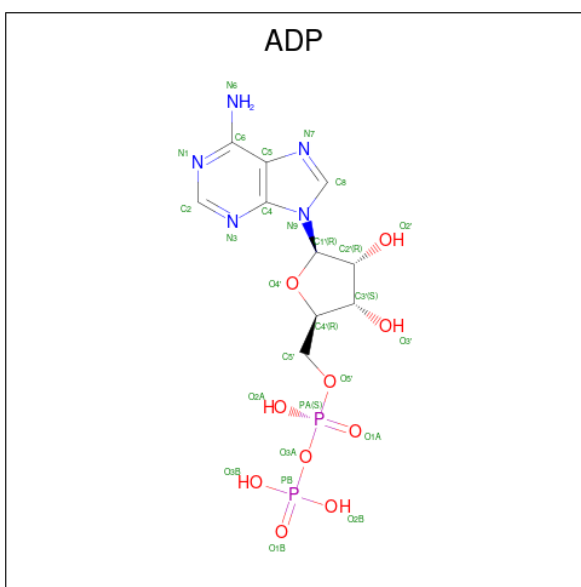
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	3	Total	Cl	0	0
			3	3		
5	H	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



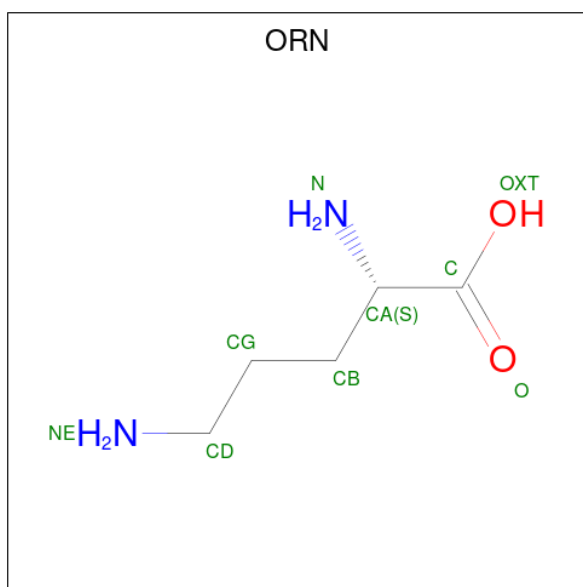
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



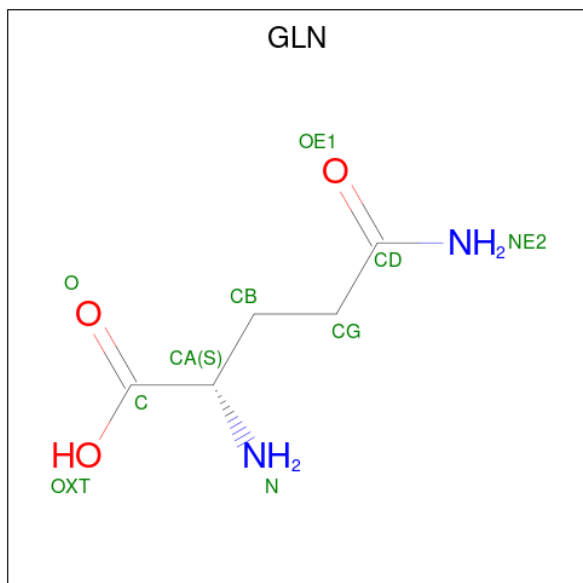
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 8 is L-ornithine (CCD ID: ORN) (formula: $\text{C}_5\text{H}_{12}\text{N}_2\text{O}_2$).



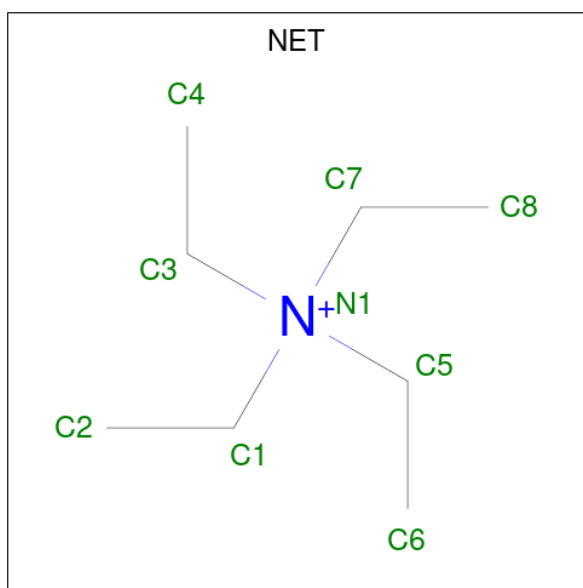
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			10	5	2	3		
9	B	1	Total	C	N	O	0	0
			10	5	2	3		
9	C	1	Total	C	N	O	0	0
			10	5	2	3		
9	D	1	Total	C	N	O	0	0
			10	5	2	3		
9	E	1	Total	C	N	O	0	0
			10	5	2	3		
9	F	1	Total	C	N	O	0	0
			10	5	2	3		
9	G	1	Total	C	N	O	0	0
			10	5	2	3		
9	H	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 10 is TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: $C_8H_{20}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	N	0	0
			9	8	1		
10	C	1	Total	C	N	0	0
			9	8	1		
10	E	1	Total	C	N	0	0
			9	8	1		
10	G	1	Total	C	N	0	0
			9	8	1		

- Molecule 11 is water.

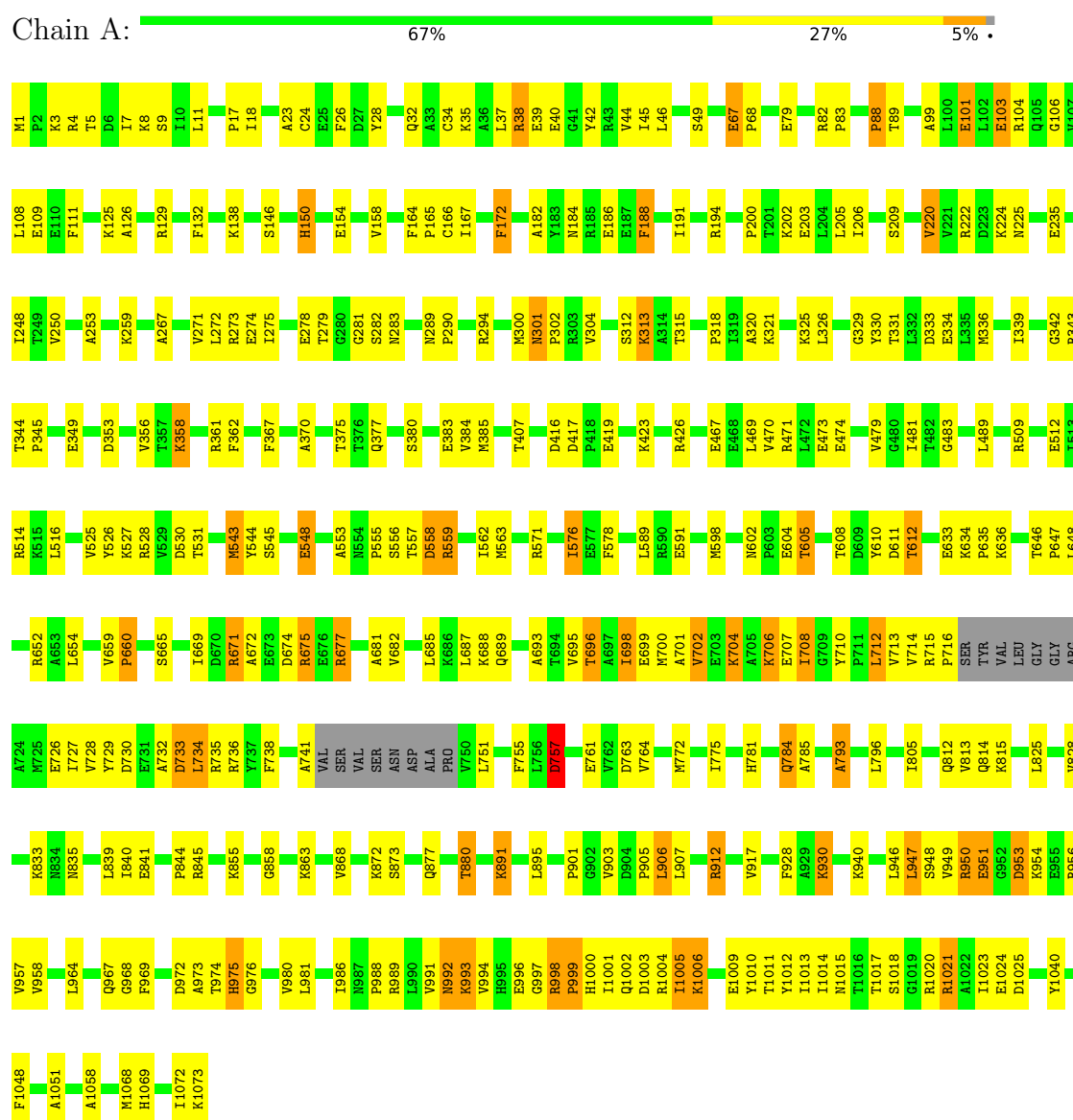
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	699	Total O 699 699	0	0
11	B	231	Total O 231 231	0	0
11	C	706	Total O 706 706	0	0
11	D	250	Total O 250 250	0	0
11	E	754	Total O 754 754	0	0
11	F	231	Total O 231 231	0	0
11	G	622	Total O 622 622	0	0
11	H	173	Total O 173 173	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

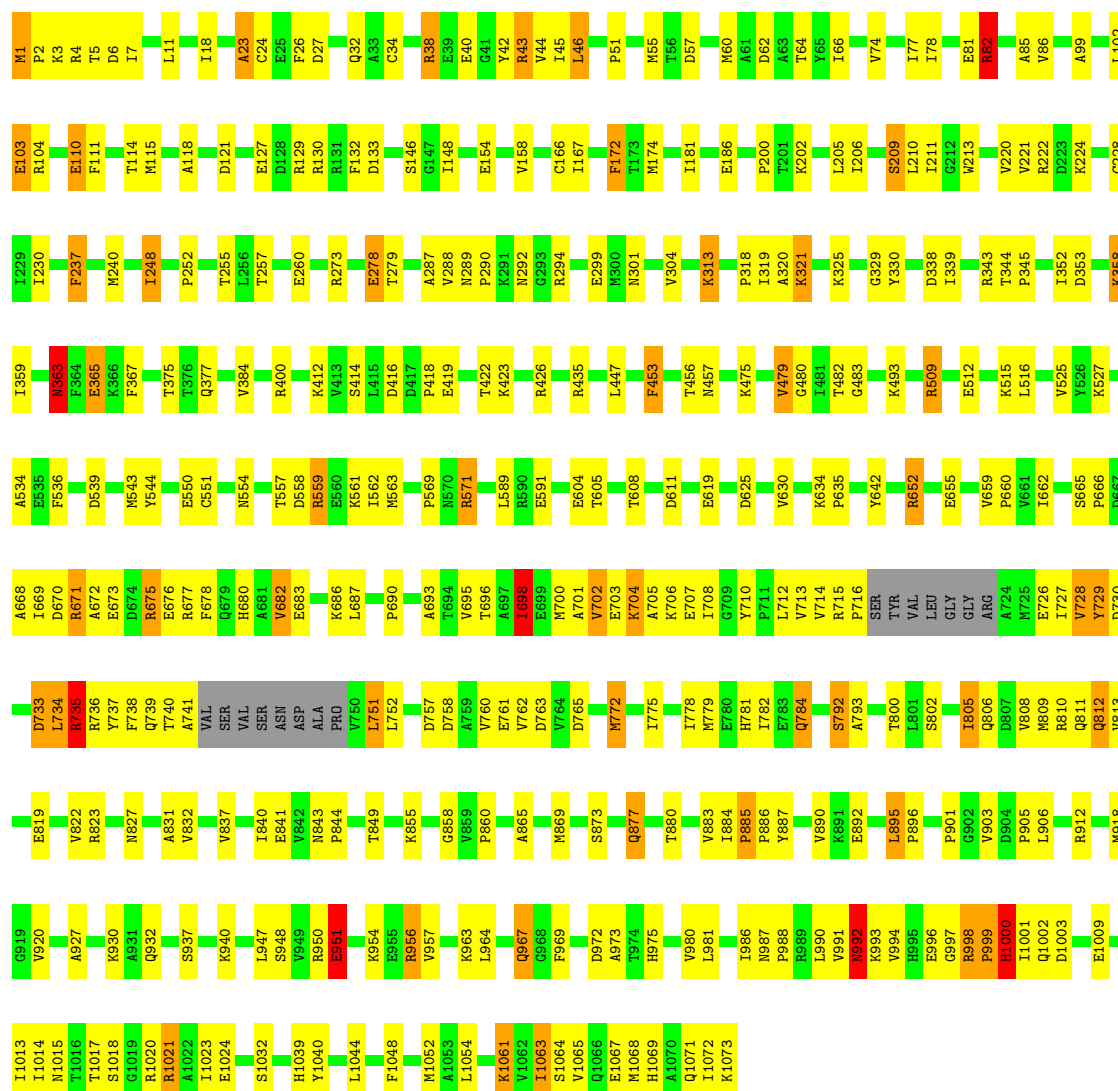
Note EDS was not executed.

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



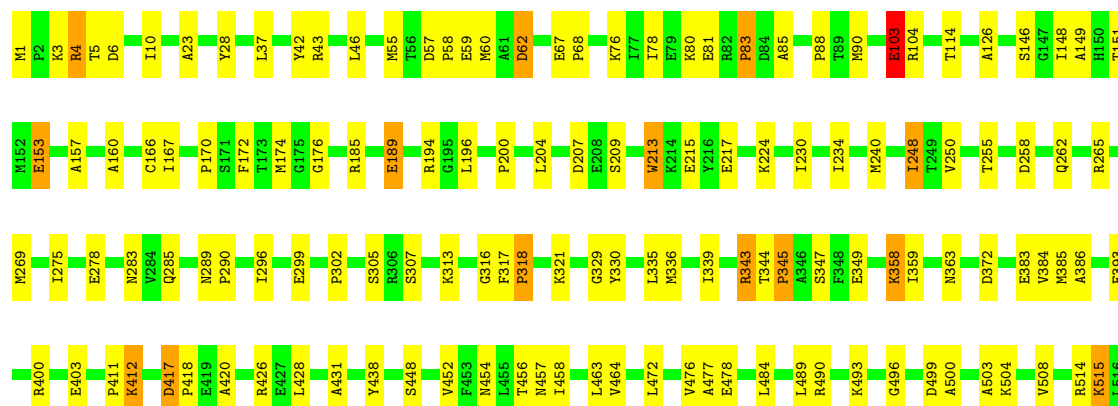
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain C:  66% 28% . .



• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain E:  69% 24% 5% .

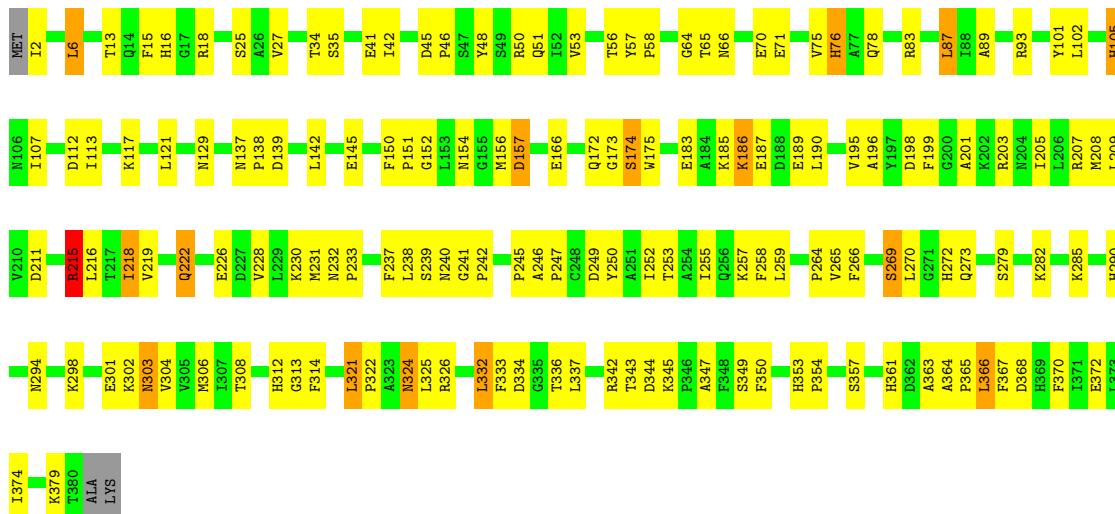






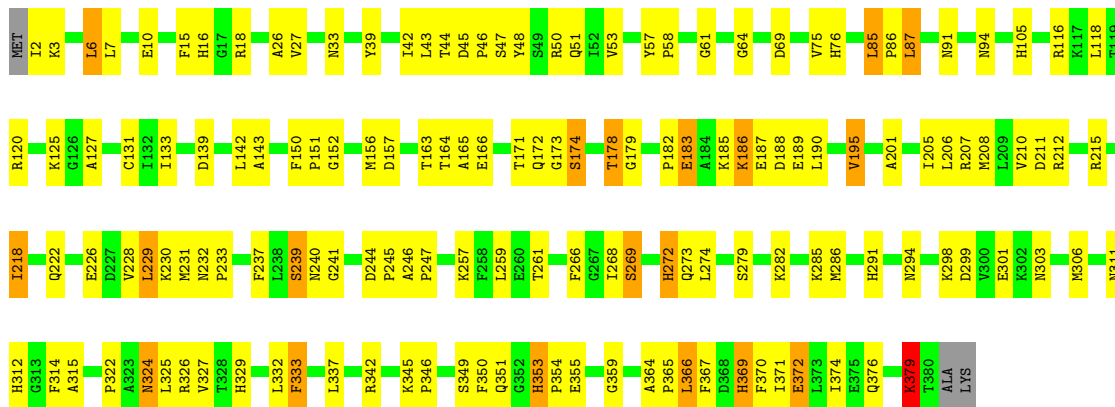
- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain B:  58% 37% .

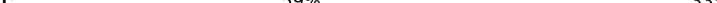


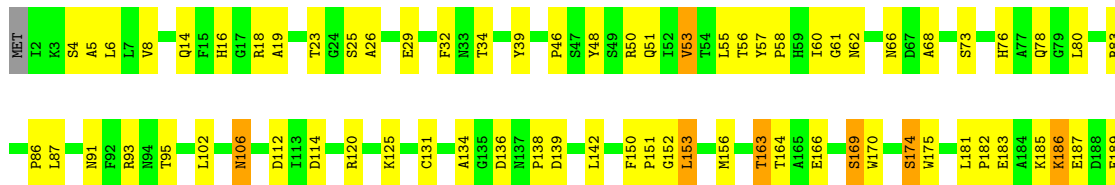
- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

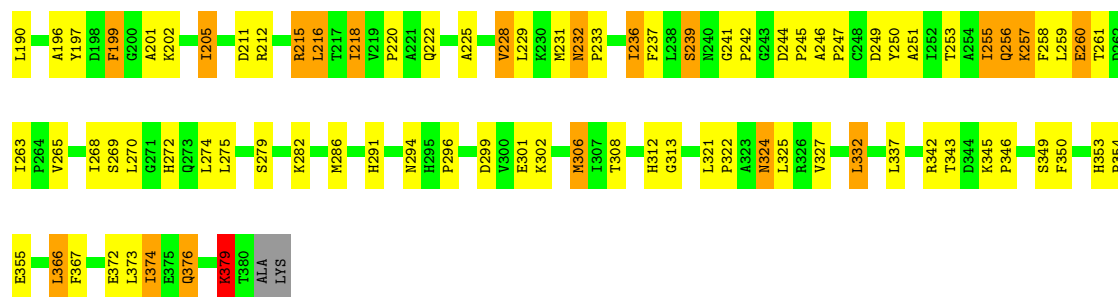
Chain D: 60% 34% 5%



- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

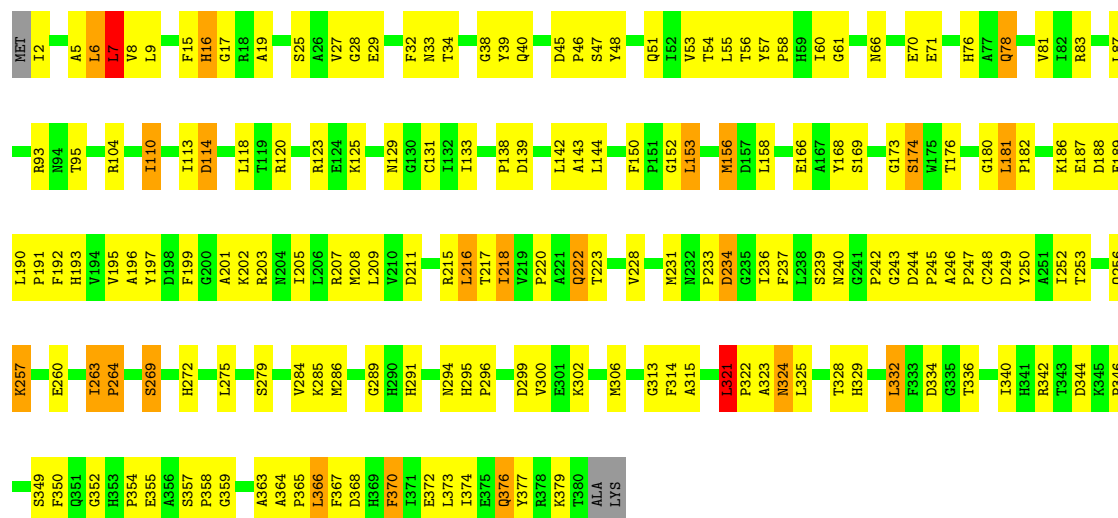
Chain F:  59% 33% 7%





• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 53% 40% 6% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.50Å 164.40Å 332.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	98.4 (30.00-2.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.188 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48477	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NET, K, ORN, PO4, ADP, MN

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	1.14	4/8345 (0.0%)	1.58	54/11276 (0.5%)
1	C	1.13	3/8346 (0.0%)	1.57	69/11281 (0.6%)
1	E	1.17	1/8377 (0.0%)	1.56	66/11320 (0.6%)
1	G	1.09	2/8322 (0.0%)	1.55	61/11249 (0.5%)
2	B	1.05	1/2957 (0.0%)	1.55	22/4016 (0.5%)
2	D	1.11	0/2957	1.60	18/4016 (0.4%)
2	F	1.09	0/2957	1.57	22/4016 (0.5%)
2	H	1.03	0/2957	1.59	23/4016 (0.6%)
All	All	1.12	11/45218 (0.0%)	1.57	335/61190 (0.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	865	ALA	C-O	-6.36	1.16	1.24
1	C	110	GLU	CD-OE1	-5.90	1.14	1.25
1	C	1009	GLU	CD-OE2	5.53	1.35	1.25
1	G	879	VAL	CA-C	-5.28	1.48	1.53
1	A	109	GLU	CD-OE2	5.25	1.35	1.25
2	B	253	THR	CB-OG1	-5.24	1.35	1.43
1	A	1009	GLU	CD-OE2	5.22	1.35	1.25
1	A	186	GLU	CD-OE2	5.12	1.35	1.25
1	A	514	ARG	CZ-NH2	-5.11	1.26	1.33
1	E	76	LYS	CE-NZ	-5.08	1.34	1.49
1	C	1024	GLU	CD-OE2	5.08	1.34	1.25

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	757	ASP	CA-CB-CG	11.31	123.91	112.60
1	C	885	PRO	N-CA-CB	11.11	109.00	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	885	PRO	O-C-N	10.08	125.89	121.15
1	A	605	THR	N-CA-C	9.71	123.66	110.55
2	H	264	PRO	N-CA-CB	9.51	112.22	103.19
1	C	605	THR	N-CA-C	9.00	123.84	110.52
1	A	23	ALA	N-CA-C	8.81	121.71	109.29
1	A	715	ARG	CB-CA-C	-8.79	101.47	110.17
1	G	605	THR	N-CA-C	8.56	121.58	110.53
1	G	660	PRO	N-CA-CB	8.40	108.36	102.65
1	A	716	PRO	N-CA-CB	8.20	112.02	103.00
2	B	105	HIS	CA-CB-CG	-8.01	105.79	113.80
2	B	16	HIS	CA-C-N	-7.81	116.15	122.16
2	B	16	HIS	C-N-CA	-7.81	116.15	122.16
1	A	998	ARG	N-CA-C	7.75	118.10	108.11
1	C	557	THR	CA-C-O	7.64	127.30	118.90
1	A	67	GLU	O-C-N	7.63	126.59	121.71
1	A	172	PHE	CA-CB-CG	-7.60	106.20	113.80
1	C	338	ASP	CA-CB-CG	7.60	120.20	112.60
1	C	558	ASP	N-CA-CB	-7.59	97.66	110.49
1	E	23	ALA	N-CA-C	7.58	119.97	109.29
2	D	157	ASP	CA-CB-CG	7.56	120.16	112.60
1	G	44	VAL	N-CA-C	7.55	118.76	107.51
1	C	23	ALA	N-CA-C	7.45	119.80	109.29
1	G	793	ALA	N-CA-C	-7.45	100.92	110.53
1	G	188	PHE	CA-CB-CG	-7.45	106.35	113.80
1	E	477	ALA	CA-C-N	7.43	130.46	120.65
1	E	477	ALA	C-N-CA	7.43	130.46	120.65
1	E	793	ALA	N-CA-C	-7.35	100.63	110.55
2	D	379	LYS	N-CA-C	-7.23	103.09	110.97
2	D	353	HIS	CA-CB-CG	-7.22	106.58	113.80
2	B	353	HIS	CA-CB-CG	-7.18	106.61	113.80
1	E	782	ILE	N-CA-C	-7.16	104.22	110.74
1	C	82	ARG	CA-CB-CG	-7.14	99.82	114.10
2	B	157	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	1025	ASP	CA-CB-CG	7.05	119.65	112.60
1	C	172	PHE	CA-CB-CG	-6.96	106.84	113.80
1	G	295	LEU	N-CA-C	6.95	119.85	108.52
2	F	346	PRO	N-CA-CB	6.87	107.06	102.25
1	E	605	THR	N-CA-C	6.86	121.05	110.42
1	C	625	ASP	CA-CB-CG	-6.79	105.81	112.60
1	C	319	ILE	N-CA-C	6.79	117.49	110.36
1	G	339	ILE	N-CA-C	6.76	123.39	109.34
1	C	339	ILE	N-CA-C	6.75	121.61	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	716	PRO	N-CA-CB	6.74	110.41	103.00
1	G	107	VAL	N-CA-C	6.71	117.47	110.62
1	A	188	PHE	CA-CB-CG	-6.70	107.10	113.80
2	H	16	HIS	CA-CB-CG	-6.70	107.10	113.80
1	G	570	ASN	CA-CB-CG	6.66	119.25	112.60
1	A	928	PHE	CA-CB-CG	-6.60	107.20	113.80
2	H	129	ASN	CA-CB-CG	-6.59	106.01	112.60
1	G	26	PHE	CA-CB-CG	-6.59	107.21	113.80
1	C	1000	HIS	CA-CB-CG	-6.53	107.27	113.80
1	C	735	ARG	O-C-N	6.52	129.06	122.08
1	C	210	LEU	N-CA-C	-6.52	103.94	112.41
1	C	619	GLU	O-C-N	6.51	126.63	121.55
1	G	559	ARG	N-CA-C	6.51	119.34	110.55
1	E	209	SER	N-CA-C	6.50	119.15	109.59
1	G	543	MET	N-CA-C	6.50	120.12	109.85
1	A	367	PHE	CA-CB-CG	-6.49	107.31	113.80
2	D	311	ASN	CA-CB-CG	-6.49	106.11	112.60
2	B	53	VAL	N-CA-C	6.48	118.14	108.23
1	C	716	PRO	N-CA-CB	6.47	110.11	103.00
1	G	557	THR	N-CA-C	-6.45	105.33	113.72
2	D	369	HIS	CA-CB-CG	-6.45	107.35	113.80
1	G	319	ILE	N-CA-C	6.44	117.13	110.36
1	A	34	CYS	CB-CA-C	-6.43	100.79	110.88
1	G	27	ASP	N-CA-C	-6.42	103.57	111.40
1	E	230	ILE	N-CA-CB	6.41	119.75	111.67
1	A	557	THR	N-CA-C	-6.38	105.42	113.72
2	D	10	GLU	CB-CA-C	-6.38	100.60	110.81
2	D	53	VAL	N-CA-C	6.37	117.98	108.23
2	F	232	ASN	CA-CB-CG	-6.37	106.23	112.60
1	A	793	ALA	N-CA-C	-6.37	101.96	110.55
1	G	788	HIS	CA-CB-CG	-6.34	107.46	113.80
1	C	782	ILE	N-CA-C	-6.34	104.97	110.74
1	G	493	LYS	N-CA-CB	6.31	119.17	110.01
1	E	557	THR	CA-C-N	6.29	133.56	121.54
1	E	557	THR	C-N-CA	6.29	133.56	121.54
1	C	543	MET	N-CA-C	6.29	119.43	109.81
1	G	578	PHE	CA-CB-CG	-6.28	107.52	113.80
2	H	370	PHE	N-CA-C	-6.26	104.37	111.07
1	E	189	GLU	CA-CB-CG	-6.26	101.59	114.10
1	E	786	GLY	N-CA-C	-6.25	107.05	114.48
1	C	132	PHE	CA-CB-CG	-6.22	107.58	113.80
1	E	612	THR	N-CA-C	6.21	120.12	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	136	ASP	CA-C-N	-6.21	114.47	122.98
2	F	136	ASP	C-N-CA	-6.21	114.47	122.98
1	E	787	VAL	N-CA-CB	6.20	118.47	111.21
2	F	16	HIS	CA-CB-CG	-6.17	107.63	113.80
1	G	729	TYR	N-CA-C	6.17	121.02	112.45
1	C	536	PHE	CA-CB-CG	-6.15	107.65	113.80
1	C	27	ASP	N-CA-C	-6.14	104.14	111.69
1	C	987	ASN	CB-CA-C	-6.13	104.92	110.44
1	C	634	LYS	CB-CA-C	-6.13	105.67	111.00
2	B	89	ALA	N-CA-C	-6.11	99.76	109.59
1	C	255	THR	N-CA-C	6.10	119.67	112.72
2	F	53	VAL	N-CA-C	6.10	116.90	107.99
2	H	188	ASP	CA-CB-CG	6.09	118.69	112.60
1	E	339	ILE	N-CA-C	6.08	121.34	113.07
2	F	4	SER	N-CA-C	6.08	119.07	110.50
2	F	138	PRO	N-CA-CB	6.06	108.70	103.36
2	B	361	HIS	CA-CB-CG	-6.06	107.74	113.80
1	A	18	ILE	CB-CA-C	-6.04	102.08	111.26
1	A	26	PHE	CA-CB-CG	-6.04	107.76	113.80
1	A	283	ASN	CA-CB-CG	6.04	118.64	112.60
2	H	53	VAL	N-CA-C	6.04	117.47	108.23
1	G	210	LEU	N-CA-C	-6.04	104.09	112.30
1	G	410	ASP	CA-C-N	6.02	125.93	119.85
1	G	410	ASP	C-N-CA	6.02	125.93	119.85
1	A	949	VAL	N-CA-C	6.02	118.53	109.20
2	F	379	LYS	N-CA-C	-6.00	104.74	111.28
1	E	255	THR	N-CA-C	5.97	119.53	112.72
1	C	367	PHE	CA-CB-CG	-5.95	107.85	113.80
2	H	181	LEU	CA-C-O	5.95	124.04	119.46
1	G	850	VAL	CA-C-O	5.90	123.19	118.71
1	G	23	ALA	N-CA-C	5.89	117.60	109.29
1	A	578	PHE	CA-CB-CG	-5.89	107.91	113.80
1	E	559	ARG	N-CA-C	5.89	119.23	110.52
1	C	714	VAL	N-CA-C	5.87	115.80	106.88
1	C	860	PRO	N-CA-CB	5.87	106.51	102.35
1	C	998	ARG	N-CA-C	5.86	118.72	108.82
1	C	237	PHE	N-CA-C	-5.85	104.82	111.14
1	G	424	ILE	CB-CA-C	-5.84	104.39	112.04
1	C	558	ASP	CA-CB-CG	5.83	118.42	112.60
1	E	1072	ILE	N-CA-C	5.83	117.16	108.54
1	A	660	PRO	N-CA-CB	5.82	106.61	102.65
2	D	239	SER	N-CA-C	5.82	117.83	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	GLU	CA-C-N	5.82	128.65	120.28
1	E	103	GLU	C-N-CA	5.82	128.65	120.28
1	E	625	ASP	CA-CB-CG	-5.82	106.78	112.60
1	A	514	ARG	NE-CZ-NH2	-5.81	113.97	119.20
2	D	183	GLU	N-CA-C	-5.80	101.90	110.48
2	D	105	HIS	CA-CB-CG	-5.79	108.00	113.80
1	E	558	ASP	CA-CB-CG	5.79	118.39	112.60
1	E	557	THR	N-CA-C	-5.79	106.08	114.12
1	E	88	PRO	CB-CA-C	-5.78	103.57	109.92
1	C	23	ALA	CA-C-O	5.77	125.45	119.91
1	A	132	PHE	CA-CB-CG	-5.77	108.03	113.80
1	G	75	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	A	1068	MET	CB-CA-C	-5.75	102.10	110.96
2	F	374	ILE	CB-CA-C	-5.75	102.95	112.26
1	A	101	GLU	N-CA-C	-5.73	104.95	111.14
1	G	894	VAL	N-CA-CB	5.73	119.31	111.41
1	G	558	ASP	CA-CB-CG	5.72	118.33	112.60
1	G	1001	ILE	N-CA-C	5.72	117.14	110.62
2	F	174	SER	N-CA-C	5.71	117.91	110.43
1	A	248	ILE	N-CA-C	-5.70	101.37	108.89
1	G	316	GLY	N-CA-C	-5.68	107.27	115.27
1	E	560	GLU	N-CA-C	-5.67	100.75	109.76
1	G	928	PHE	CA-C-O	5.66	126.50	120.10
1	E	575	GLY	O-C-N	5.66	128.82	122.82
1	C	793	ALA	N-CA-C	-5.65	102.92	110.55
1	E	318	PRO	N-CA-CB	5.65	106.49	102.65
2	H	7	LEU	CA-C-N	-5.64	115.27	123.06
2	H	7	LEU	C-N-CA	-5.64	115.27	123.06
1	E	499	ASP	CA-CB-CG	5.63	118.23	112.60
1	E	558	ASP	N-CA-CB	-5.63	100.97	110.49
1	C	998	ARG	O-C-N	5.61	125.86	121.88
1	E	906	LEU	N-CA-CB	-5.61	101.07	110.83
1	C	757	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	279	THR	N-CA-C	5.59	117.20	109.54
2	D	272	HIS	N-CA-C	-5.59	105.10	111.14
1	G	900	PHE	CA-C-N	5.59	125.42	119.28
1	G	900	PHE	C-N-CA	5.59	125.42	119.28
1	C	301	ASN	CB-CA-C	5.58	116.37	110.17
2	F	260	GLU	N-CA-C	-5.58	106.31	113.23
1	G	714	VAL	N-CA-C	5.57	115.67	107.15
1	A	553	ALA	N-CA-C	5.57	117.79	111.11
1	E	543	MET	N-CA-C	5.56	118.64	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	473[A]	GLU	CA-C-N	5.56	127.73	120.28
1	G	473[A]	GLU	C-N-CA	5.56	127.73	120.28
1	G	473[B]	GLU	CA-C-N	5.56	127.73	120.28
1	G	473[B]	GLU	C-N-CA	5.56	127.73	120.28
2	F	216	LEU	N-CA-C	5.56	118.79	109.95
1	C	209	SER	N-CA-C	5.56	118.29	109.96
2	D	299	ASP	CA-CB-CG	5.56	118.16	112.60
2	H	260	GLU	N-CA-C	-5.56	106.67	113.50
2	H	114	ASP	CA-CB-CG	5.55	118.15	112.60
2	F	353	HIS	CA-CB-CG	-5.55	108.25	113.80
1	G	881	LYS	N-CA-CB	5.54	119.21	110.23
1	E	213	TRP	CD2-CE2-CZ2	-5.53	116.87	122.40
2	H	220	PRO	N-CA-CB	5.53	107.96	103.32
1	C	453	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	150	HIS	O-C-N	5.51	128.24	122.23
1	E	942	HIS	CA-CB-CG	-5.51	108.29	113.80
1	G	953	ASP	CA-CB-CG	5.50	118.11	112.60
2	F	237	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	39	GLU	CB-CA-C	-5.49	100.12	110.67
1	E	62	ASP	CA-CB-CG	-5.49	107.11	112.60
1	E	877	GLN	CB-CG-CD	-5.49	103.27	112.60
2	F	16	HIS	CA-C-N	-5.49	117.94	122.16
2	F	16	HIS	C-N-CA	-5.49	117.94	122.16
1	C	248	ILE	N-CA-C	-5.45	101.69	108.89
2	H	257	LYS	N-CA-C	-5.45	105.03	110.97
1	A	44	VAL	N-CA-C	5.44	115.79	108.17
1	A	1005	ILE	CB-CA-C	-5.44	104.91	111.88
1	C	702	VAL	O-C-N	5.43	127.14	121.87
1	A	146	SER	N-CA-C	5.43	115.40	108.24
1	G	879	VAL	O-C-N	5.42	127.72	122.30
2	B	76	HIS	CA-CB-CG	-5.41	108.39	113.80
2	B	45	ASP	CA-C-O	5.41	123.32	119.32
1	A	612	THR	N-CA-C	5.40	119.13	112.54
2	B	308	THR	N-CA-C	5.40	117.61	109.41
2	H	372	GLU	N-CA-CB	-5.39	102.19	110.12
1	E	707	GLU	CA-C-N	5.39	127.35	120.56
1	E	707	GLU	C-N-CA	5.39	127.35	120.56
1	G	690	PRO	N-CA-CB	5.39	108.34	103.33
2	H	156	MET	N-CA-C	5.38	117.08	108.41
1	C	129	ARG	N-CA-C	5.38	117.90	111.71
1	E	316	GLY	N-CA-C	-5.38	107.69	115.27
1	A	712	LEU	N-CA-C	5.38	118.22	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	738	PHE	CA-CB-CG	-5.38	108.42	113.80
1	C	557	THR	CA-C-N	5.37	131.80	121.54
1	C	557	THR	C-N-CA	5.37	131.80	121.54
1	A	88	PRO	CB-CA-C	-5.37	104.01	109.92
1	G	885	PRO	N-CA-CB	5.37	108.29	103.08
1	A	209	SER	N-CA-C	5.37	118.68	110.20
1	A	825	LEU	N-CA-C	5.37	117.79	110.55
1	A	999	PRO	N-CA-CB	5.36	108.50	102.60
1	C	682	VAL	O-C-N	5.36	127.30	121.94
1	E	248	ILE	N-CA-C	-5.35	101.83	108.89
1	A	339	ILE	N-CA-C	5.34	119.94	113.00
1	G	364	PHE	N-CA-C	5.34	118.58	111.75
1	C	760	VAL	CB-CA-C	-5.33	104.51	110.96
1	E	305	SER	N-CA-C	5.33	115.17	108.45
1	G	569	PRO	CB-CA-C	-5.33	104.12	111.21
1	E	906	LEU	N-CA-C	5.33	118.08	109.40
1	E	431	ALA	CA-C-N	5.32	128.52	122.67
1	E	431	ALA	C-N-CA	5.32	128.52	122.67
1	G	3	LYS	N-CA-C	5.31	118.14	110.28
1	C	278	GLU	CB-CA-C	-5.31	100.63	109.55
1	G	970	GLU	N-CA-C	-5.30	101.63	110.17
1	G	557	THR	CA-C-N	5.30	131.67	121.54
1	G	557	THR	C-N-CA	5.30	131.67	121.54
1	E	716	PRO	N-CA-CB	5.30	108.83	103.00
1	G	209	SER	N-CA-C	5.29	117.90	110.23
1	C	895	LEU	CA-C-N	5.29	127.14	121.00
1	C	895	LEU	C-N-CA	5.29	127.14	121.00
1	G	712	LEU	N-CA-C	5.29	117.86	109.50
1	E	417	ASP	CA-C-O	5.27	123.52	119.46
1	A	968	GLY	CA-C-O	5.27	123.72	118.77
1	E	680	HIS	N-CA-CB	-5.27	102.37	110.16
1	G	557	THR	CA-C-O	5.26	124.84	119.05
1	E	1000	HIS	CA-CB-CG	-5.26	108.54	113.80
1	C	877	GLN	OE1-CD-NE2	5.26	127.86	122.60
1	C	82	ARG	CG-CD-NE	-5.25	100.45	112.00
1	C	554	ASN	CB-CA-C	-5.25	105.78	110.71
2	B	137	ASN	CB-CA-C	-5.25	103.56	111.27
1	E	520	TYR	N-CA-C	-5.25	106.66	113.16
1	E	737	TYR	CB-CA-C	-5.24	102.88	110.96
1	A	543	MET	N-CA-C	5.24	118.13	109.85
2	B	368	ASP	CA-CB-CG	-5.24	107.36	112.60
2	D	195	VAL	N-CA-CB	5.24	117.33	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	690	PRO	N-CA-CB	5.23	107.72	103.32
2	H	321	LEU	N-CA-C	5.23	117.01	109.48
1	E	555	PRO	N-CA-CB	5.23	107.90	103.35
2	D	69	ASP	CA-CB-CG	5.23	117.83	112.60
1	E	83	PRO	CB-CA-C	-5.22	104.26	111.21
2	B	216	LEU	N-CA-C	5.22	118.25	109.95
1	E	317	PHE	CA-C-O	5.22	122.68	119.29
2	B	215	ARG	CB-CA-C	5.22	118.36	109.75
1	G	370	ALA	N-CA-C	5.21	117.85	110.50
1	E	726	GLU	CB-CG-CD	5.21	121.45	112.60
1	G	453	PHE	CA-CB-CG	-5.21	108.59	113.80
2	F	163	THR	N-CA-C	5.20	117.24	110.43
2	B	201	ALA	N-CA-C	5.20	117.77	110.23
1	C	758	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	993[A]	LYS	N-CA-C	-5.20	104.02	110.41
1	A	993[B]	LYS	N-CA-C	-5.20	104.02	110.41
1	A	301	ASN	CB-CA-C	5.19	115.93	110.17
1	G	850	VAL	N-CA-C	5.18	119.15	112.67
1	A	530	ASP	O-C-N	5.18	127.19	121.85
1	A	407	THR	N-CA-C	-5.17	105.86	113.61
1	A	555	PRO	N-CA-CB	5.16	107.84	103.35
1	C	304	VAL	N-CA-C	-5.16	104.43	110.05
1	C	1039	HIS	CA-CB-CG	-5.16	108.64	113.80
1	G	1001	ILE	CA-CB-CG1	5.16	119.17	110.40
1	A	785	ALA	N-CA-C	-5.15	103.35	110.35
1	E	345	PRO	CB-CA-C	-5.15	103.50	110.60
2	B	174	SER	N-CA-C	5.14	117.50	110.55
1	C	62	ASP	CA-CB-CG	-5.14	107.46	112.60
1	C	26	PHE	CA-CB-CG	-5.13	108.67	113.80
2	D	359	GLY	O-C-N	5.12	126.89	121.77
2	B	303	ASN	CA-CB-CG	-5.12	107.48	112.60
2	B	112	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	90	MET	N-CA-C	5.12	119.21	112.92
2	B	129	ASN	CA-C-N	-5.11	115.49	122.03
2	B	129	ASN	C-N-CA	-5.11	115.49	122.03
1	E	659	VAL	CA-C-O	5.11	124.26	119.76
1	A	953	ASP	CA-CB-CG	5.11	117.71	112.60
2	D	359	GLY	CA-C-N	5.11	125.02	119.76
2	D	359	GLY	C-N-CA	5.11	125.02	119.76
1	G	478	GLU	N-CA-C	5.10	116.65	111.14
1	E	936	ASN	CA-CB-CG	5.10	117.70	112.60
2	F	308	THR	N-CA-C	5.10	117.16	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	THR	CA-C-N	5.09	131.27	121.54
1	A	557	THR	C-N-CA	5.09	131.27	121.54
1	A	994	VAL	N-CA-C	5.09	116.43	110.62
1	C	792	SER	N-CA-C	5.09	118.36	110.17
1	C	121	ASP	N-CA-CB	5.09	117.69	110.16
1	C	230	ILE	N-CA-CB	5.08	117.77	111.41
1	C	435	ARG	N-CA-C	5.08	117.48	111.33
1	G	420	ALA	N-CA-C	5.08	117.47	111.33
2	H	295	HIS	CA-C-O	5.08	123.37	119.46
2	H	295	HIS	N-CA-C	5.07	116.93	109.42
1	G	265	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	E	372	ASP	N-CA-C	5.07	118.50	112.72
1	E	431	ALA	N-CA-C	5.07	117.66	110.10
1	E	464	VAL	N-CA-CB	5.07	116.81	110.47
2	D	85	LEU	CB-CA-C	5.05	115.17	110.17
2	F	256	GLN	O-C-N	5.05	127.47	122.12
1	C	44	VAL	N-CA-C	5.05	115.36	107.99
1	C	642	TYR	N-CA-CB	-5.05	103.23	110.65
1	E	729	TYR	N-CA-C	5.05	119.57	113.41
2	H	359	GLY	CA-C-N	5.05	125.33	119.93
2	H	359	GLY	C-N-CA	5.05	125.33	119.93
2	H	346	PRO	N-CA-CB	5.04	106.12	102.79
2	B	264	PRO	N-CA-CB	5.04	107.79	103.36
2	F	199	PHE	N-CA-C	-5.04	106.44	112.59
1	C	999	PRO	N-CA-CB	5.03	108.14	102.60
1	C	729	TYR	N-CA-C	5.03	119.41	113.12
1	E	454	ASN	O-C-N	5.02	127.44	122.12
1	G	207	ASP	CA-CB-CG	5.02	117.62	112.60
1	E	80	LYS	N-CA-C	5.02	116.75	111.28
2	F	95	THR	N-CA-CB	5.02	117.80	110.88
2	H	174	SER	N-CA-C	5.01	117.32	110.55
1	A	370	ALA	N-CA-C	5.01	117.57	110.50
1	C	832	VAL	N-CA-C	5.01	113.96	106.85
1	E	955	GLU	CA-C-O	5.01	126.11	120.00
1	C	363	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	843	ASN	O-C-N	5.01	125.95	121.04
1	C	992	ASN	N-CA-C	5.00	117.77	109.46
1	E	713	VAL	CB-CA-C	-5.00	105.79	111.59
2	H	234	ASP	CA-C-O	5.00	125.69	119.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8195	0	8247	251	0
1	C	8192	0	8230	257	0
1	E	8211	0	8245	233	0
1	G	8180	0	8214	300	0
2	B	2895	0	2861	96	0
2	D	2895	0	2861	101	0
2	F	2895	0	2861	111	0
2	H	2895	0	2861	135	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	1	0
5	B	1	0	0	0	0
5	C	3	0	0	2	0
5	D	1	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
5	G	3	0	0	3	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	0	0
7	C	54	0	24	1	0
7	E	54	0	24	5	0
7	G	54	0	24	2	0
8	A	9	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	9	0	11	1	0
8	E	9	0	11	0	0
8	G	9	0	11	0	0
9	A	10	0	7	0	0
9	B	10	0	7	3	0
9	C	10	0	7	0	0
9	D	10	0	7	2	0
9	E	10	0	7	0	0
9	F	10	0	7	4	0
9	G	10	0	7	0	0
9	H	10	0	7	2	0
10	A	9	0	20	0	0
10	C	9	0	20	1	0
10	E	9	0	20	2	0
10	G	9	0	20	0	0
11	A	699	0	0	15	0
11	B	231	0	0	4	0
11	C	706	0	0	19	0
11	D	250	0	0	5	0
11	E	754	0	0	23	0
11	F	231	0	0	4	0
11	G	622	0	0	20	0
11	H	173	0	0	4	0
All	All	48477	0	44656	1462	0

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 16.

All (1462) 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:808:VAL:HA	1:E:811[B]:GLN:HE21	1.12	1.11
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.34	1.10
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.28	1.10
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.36	1.08
2:D:228:VAL:HA	2:D:231:MET:HE2	1.27	1.06
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.38	1.04
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.35	1.03
2:D:286:MET:HE1	2:D:312:HIS:ND1	1.75	1.00
1:E:696:THR:H	1:E:700:MET:HE3	1.27	1.00
1:G:784:GLN:H	1:G:784:GLN:NE2	1.57	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.44	0.99
1:C:1063:ILE:HD13	1:C:1068:MET:HG3	1.41	0.99
2:H:228:VAL:HA	2:H:231:MET:HE3	1.44	0.98
1:E:1002:GLN:HE22	1:E:1006[B]:LYS:NZ	1.60	0.97
1:A:784:GLN:HE21	1:A:784:GLN:H	0.98	0.96
2:H:286:MET:HE2	2:H:289:GLY:HA2	1.48	0.96
1:A:784:GLN:H	1:A:784:GLN:NE2	1.64	0.95
1:A:956[B]:ARG:HG2	1:A:956[B]:ARG:HH11	1.31	0.94
1:G:784:GLN:HE21	1:G:784:GLN:N	1.64	0.94
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.47	0.93
1:E:1002:GLN:HE22	1:E:1006[B]:LYS:HZ3	1.07	0.93
1:A:38[A]:ARG:HG3	1:A:38[A]:ARG:HH11	1.34	0.93
1:C:38:ARG:HG3	1:C:38:ARG:HH11	1.35	0.91
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.84	0.91
1:G:939:MET:HE2	1:G:1050:THR:CG2	2.03	0.89
2:D:286:MET:HE2	2:D:315:ALA:HB2	1.52	0.89
1:G:1021:ARG:HG2	1:G:1021:ARG:HH11	1.38	0.89
1:C:1001:ILE:HD12	1:C:1002:GLN:N	1.88	0.88
2:B:324:ASN:HD22	2:B:324:ASN:N	1.70	0.88
1:E:808:VAL:HA	1:E:811[B]:GLN:NE2	1.89	0.88
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.56	0.87
2:B:324:ASN:HD22	2:B:324:ASN:H	1.18	0.87
1:C:994:VAL:HG13	1:C:1000:HIS:ND1	1.89	0.87
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.04	0.87
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.03	0.87
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.57	0.86
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.56	0.86
1:E:698:ILE:HG13	1:E:738:PHE:CD1	2.11	0.86
1:E:784:GLN:H	1:E:784:GLN:NE2	1.73	0.86
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.05	0.85
1:G:563:MET:CE	1:G:635:PRO:HG3	2.08	0.84
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.92	0.84
1:A:1001:ILE:HD12	1:A:1002:GLN:N	1.90	0.84
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.12	0.84
1:E:784:GLN:H	1:E:784:GLN:HE21	1.23	0.84
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.93	0.83
1:G:1063:ILE:HD13	1:G:1068:MET:HG3	1.59	0.83
1:C:670:ASP:HB3	1:C:677:ARG:HH21	1.43	0.83
2:F:228:VAL:HA	2:F:231:MET:CE	2.09	0.83
1:C:563:MET:CE	1:C:635:PRO:HG3	2.09	0.83
2:D:286:MET:HE1	2:D:312:HIS:CE1	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.14	0.82
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.61	0.82
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.59	0.82
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.94	0.82
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.62	0.82
1:G:663:GLY:HA3	1:G:869:MET:HE2	1.62	0.81
2:D:241:GLY:O	9:D:4034:GLN:HG3	1.80	0.81
2:H:187:GLU:HG2	2:H:215:ARG:CD	2.10	0.81
2:F:201:ALA:HB2	2:F:239:SER:CB	2.10	0.81
1:C:670:ASP:HB3	1:C:677:ARG:NH2	1.97	0.80
1:A:734:LEU:HD12	1:A:734:LEU:O	1.82	0.80
1:C:1001:ILE:HD12	1:C:1002:GLN:H	1.44	0.80
1:A:38[B]:ARG:HG2	1:A:38[B]:ARG:HH11	1.43	0.80
1:E:1002:GLN:NE2	1:E:1006[B]:LYS:HZ3	1.79	0.80
1:A:313:LYS:HE2	1:A:608:THR:O	1.82	0.80
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.45	0.80
1:E:1002:GLN:NE2	1:E:1006[B]:LYS:NZ	2.31	0.79
1:C:74:VAL:HG11	1:C:102:LEU:HD11	1.64	0.79
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.64	0.79
2:F:241:GLY:O	9:F:4056:GLN:HG3	1.82	0.79
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.65	0.79
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.65	0.79
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.62	0.79
2:F:228:VAL:HA	2:F:231:MET:HE2	1.64	0.78
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.11	0.78
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.18	0.78
1:E:1:MET:HB2	1:E:224:LYS:NZ	1.97	0.78
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.46	0.78
1:A:695:VAL:CG1	1:A:700:MET:HB3	2.14	0.77
1:E:151:THR:HB	1:E:153[B]:GLU:OE2	1.85	0.77
1:C:1:MET:HB2	1:C:224:LYS:NZ	1.99	0.77
1:G:181:ILE:HD11	1:G:376:THR:HG23	1.65	0.77
1:E:1:MET:HB2	1:E:224:LYS:HZ2	1.47	0.77
1:G:64:THR:O	1:G:1065:VAL:HG23	1.85	0.77
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.66	0.77
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.20	0.77
2:B:324:ASN:H	2:B:324:ASN:ND2	1.80	0.77
1:G:704:LYS:O	1:G:708:ILE:HD12	1.85	0.77
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.65	0.76
1:E:808:VAL:CA	1:E:811[B]:GLN:HE21	1.94	0.76
1:G:903:VAL:HG13	11:G:3404:HOH:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.67	0.76
2:H:299:ASP:OD1	2:H:302:LYS:HD3	1.85	0.76
2:B:226:GLU:O	2:B:230:LYS:HG3	1.86	0.76
2:D:324:ASN:H	2:D:324:ASN:HD22	1.31	0.76
1:E:696:THR:N	1:E:700:MET:HE3	2.00	0.76
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.50	0.76
1:C:363:ASN:HA	1:C:365:GLU:OE2	1.86	0.76
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.20	0.76
1:A:784:GLN:HE21	1:A:784:GLN:N	1.80	0.76
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.68	0.75
1:C:973:ALA:O	1:C:991[A]:VAL:HG12	1.85	0.75
1:G:385:MET:HG2	1:G:618:PHE:CE1	2.21	0.75
2:H:324:ASN:HD22	2:H:324:ASN:H	1.35	0.75
1:G:998:ARG:HA	1:G:999:PRO:C	2.12	0.75
1:C:967:GLN:HG3	1:C:1054:LEU:HD13	1.69	0.75
1:E:153[A]:GLU:HG2	11:E:4283:HOH:O	1.85	0.75
1:E:698:ILE:O	1:E:702:VAL:HG23	1.86	0.74
1:C:509:ARG:HD3	11:C:4652:HOH:O	1.87	0.74
1:G:865:ALA:O	1:G:869:MET:HG3	1.86	0.74
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.17	0.74
1:C:1:MET:HB2	1:C:224:LYS:HZ2	1.51	0.74
1:G:548:GLU:HG2	2:H:114:ASP:CG	2.12	0.74
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.68	0.74
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.70	0.74
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.67	0.74
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.18	0.74
2:H:54:THR:HG21	2:H:118:LEU:HD23	1.70	0.74
2:F:150:PHE:CD2	2:F:151:PRO:HD2	2.23	0.73
2:H:71:GLU:O	2:H:203:ARG:HG3	1.87	0.73
1:A:681:ALA:O	1:A:685:LEU:HG	1.88	0.73
2:B:71:GLU:O	2:B:203:ARG:HG3	1.87	0.73
1:C:38:ARG:HG3	1:C:38:ARG:NH1	2.02	0.73
1:G:954:LYS:O	1:G:957:VAL:HG12	1.88	0.73
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.70	0.73
1:A:772:MET:SD	1:A:880:THR:HG22	2.29	0.73
1:E:166:CYS:C	1:E:167:ILE:HD12	2.13	0.73
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.89	0.73
1:C:802:SER:O	1:C:806:GLN:HG3	1.89	0.73
2:H:324:ASN:HD22	2:H:324:ASN:N	1.87	0.73
1:A:973:ALA:O	1:A:991:VAL:HG12	1.88	0.73
1:A:930:LYS:HE3	11:A:4162:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LYS:HE3	11:C:4153:HOH:O	1.89	0.72
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.71	0.72
1:C:400:ARG:HD3	11:C:4391:HOH:O	1.88	0.72
1:G:873:SER:O	1:G:877:GLN:HG3	1.89	0.72
1:A:698:ILE:HD12	1:A:698:ILE:H	1.54	0.72
1:E:863:LYS:O	1:E:867:ARG:HG3	1.89	0.72
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.54	0.72
1:G:181:ILE:CD1	1:G:376:THR:HG23	2.20	0.72
2:F:251:ALA:O	2:F:255:ILE:HD12	1.88	0.72
1:G:57:ASP:HB3	1:G:59:GLU:OE2	1.89	0.72
1:A:318:PRO:HG3	1:A:610:TYR:OH	1.88	0.72
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.72	0.72
1:E:1004:ARG:HD3	1:E:1009[B]:GLU:OE2	1.90	0.71
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.72	0.71
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.20	0.71
2:H:228:VAL:HA	2:H:231:MET:CE	2.18	0.71
1:A:997:GLY:O	1:A:998:ARG:HG3	1.90	0.71
1:E:59:GLU:HG2	1:E:60:MET:HE2	1.72	0.71
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.73	0.71
1:G:663:GLY:HA3	1:G:869:MET:CE	2.21	0.71
1:G:734:LEU:HD12	1:G:734:LEU:O	1.89	0.71
2:B:117:LYS:HE3	11:B:4071:HOH:O	1.89	0.71
1:G:58:PRO:HD2	1:G:59:GLU:OE2	1.90	0.71
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.54	0.71
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.73	0.71
2:F:324:ASN:O	2:F:342:ARG:HD2	1.91	0.70
1:G:166:CYS:C	1:G:167:ILE:HD12	2.15	0.70
2:H:286:MET:HE2	2:H:289:GLY:CA	2.20	0.70
2:D:246:ALA:HB3	2:D:247:PRO:HD3	1.73	0.70
2:D:259:LEU:HD13	2:D:342:ARG:NH1	2.06	0.70
1:A:873:SER:O	1:A:877:GLN:HG3	1.92	0.70
1:E:213:TRP:CZ3	1:E:296:ILE:HD12	2.27	0.70
1:A:38[A]:ARG:HG3	1:A:38[A]:ARG:NH1	2.02	0.70
2:H:133:ILE:CD1	2:H:143:ALA:HB2	2.16	0.70
1:C:726:GLU:HG3	1:C:727:ILE:H	1.55	0.70
2:H:218:ILE:N	2:H:218:ILE:HD13	2.07	0.69
1:E:126:ALA:HB3	1:E:302:PRO:HG3	1.73	0.69
1:C:998:ARG:HG2	1:C:999:PRO:HA	1.73	0.69
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.27	0.69
2:D:228:VAL:HA	2:D:231:MET:CE	2.14	0.69
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:324:ASN:H	2:F:324:ASN:HD22	1.40	0.69
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.57	0.69
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.74	0.69
1:E:1001:ILE:HD12	1:E:1002:GLN:N	2.07	0.69
1:G:648:LEU:HD22	1:G:845:ARG:HD3	1.75	0.69
1:A:974:THR:HG21	1:A:993[B]:LYS:HD3	1.74	0.69
1:E:1:MET:N	1:E:224:LYS:HE3	2.07	0.69
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.73	0.69
2:H:6:LEU:HD12	2:H:7:LEU:N	2.08	0.69
2:H:34:THR:HA	2:H:56:THR:OG1	1.92	0.68
1:G:784:GLN:H	1:G:784:GLN:HE21	0.79	0.68
1:G:79:GLU:HG2	1:G:111:PHE:CE2	2.29	0.68
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.23	0.68
1:E:103:GLU:HG3	1:E:104:ARG:N	2.06	0.68
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.74	0.68
1:C:726:GLU:HG3	1:C:727:ILE:N	2.08	0.68
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.29	0.68
1:C:883:VAL:O	1:C:884:ILE:HD13	1.94	0.68
1:E:224:LYS:HE2	1:E:329:GLY:O	1.94	0.68
1:E:43:ARG:NH2	1:E:81:GLU:OE2	2.27	0.68
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.08	0.68
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.74	0.68
2:B:324:ASN:O	2:B:342:ARG:HD2	1.94	0.67
1:C:1063:ILE:CD1	1:C:1068:MET:HG3	2.22	0.67
1:G:939:MET:HE2	1:G:1050:THR:HG21	1.76	0.67
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.60	0.67
1:A:563:MET:CE	1:A:635:PRO:HG3	2.24	0.67
1:E:1:MET:N	11:E:4680:HOH:O	2.25	0.67
1:E:1021:ARG:HG2	1:E:1021:ARG:HH11	1.57	0.67
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.29	0.67
2:B:187:GLU:HG2	2:B:215:ARG:CD	2.22	0.67
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.74	0.67
2:H:286:MET:CE	2:H:289:GLY:HA2	2.23	0.67
1:G:273:ARG:HD2	11:G:3191:HOH:O	1.95	0.67
2:F:139:ASP:OD2	2:F:142:LEU:HB2	1.94	0.67
2:H:6:LEU:HD11	2:H:8:VAL:HG22	1.77	0.67
1:G:4:ARG:HD3	1:G:7:ILE:HD12	1.76	0.67
1:G:475:LYS:O	1:G:479:VAL:HG13	1.95	0.67
1:A:698:ILE:O	1:A:701:ALA:HB3	1.95	0.66
2:H:55:LEU:HD13	2:H:60:ILE:HD12	1.77	0.66
1:C:698:ILE:HD12	1:C:698:ILE:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LYS:HE2	1:C:329:GLY:O	1.95	0.66
1:A:772:MET:CE	1:A:880:THR:HG22	2.26	0.66
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.76	0.66
1:G:1:MET:HB2	1:G:224:LYS:NZ	2.11	0.66
1:A:636:LYS:NZ	11:A:4475:HOH:O	2.29	0.65
1:C:32:GLN:OE1	1:C:320:ALA:HB3	1.95	0.65
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.77	0.65
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.77	0.65
1:G:936:ASN:HB2	11:G:2917:HOH:O	1.97	0.65
1:G:1030:ARG:NH1	1:G:1030:ARG:HG3	2.10	0.65
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.27	0.65
2:B:218:ILE:HD13	2:B:218:ILE:N	2.12	0.65
2:D:64:GLY:HA3	2:D:94:ASN:OD1	1.97	0.65
1:G:695:VAL:CG1	1:G:700:MET:HB3	2.21	0.65
2:B:279:SER:O	2:B:322:PRO:HG3	1.95	0.65
1:E:954:LYS:O	1:E:980:VAL:HG11	1.96	0.65
2:H:205:ILE:HG13	2:H:355:GLU:HG3	1.79	0.65
1:A:726:GLU:HG3	1:A:727:ILE:H	1.62	0.65
1:C:708:ILE:HG21	1:C:712:LEU:HD11	1.79	0.65
2:D:152:GLY:O	2:D:156:MET:HE3	1.96	0.65
2:F:8:VAL:HG22	2:F:14:GLN:HG2	1.78	0.65
2:F:232:ASN:N	2:F:233:PRO:HD3	2.11	0.65
2:H:324:ASN:O	2:H:342:ARG:HD2	1.97	0.65
1:C:652:ARG:NH1	1:C:670:ASP:OD2	2.30	0.64
2:D:205:ILE:HG13	2:D:355:GLU:HG3	1.79	0.64
1:G:772:MET:SD	1:G:880:THR:HG22	2.37	0.64
1:C:154:GLU:OE1	11:C:4246:HOH:O	2.15	0.64
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.43	0.64
1:E:515:LYS:O	1:E:515:LYS:HD3	1.98	0.64
1:E:343:ARG:NH2	11:E:4720:HOH:O	2.30	0.64
2:F:218:ILE:HD13	2:F:218:ILE:N	2.12	0.64
1:A:358:LYS:HE3	11:A:4129:HOH:O	1.97	0.64
1:C:734:LEU:O	1:C:734:LEU:HD12	1.97	0.64
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.79	0.64
2:B:249:ASP:OD2	2:B:250:TYR:N	2.31	0.64
1:C:994:VAL:HG13	1:C:1000:HIS:CE1	2.31	0.64
2:B:272:HIS:ND1	2:B:349:SER:OG	2.30	0.64
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.28	0.64
1:A:698:ILE:H	1:A:698:ILE:CD1	2.11	0.64
2:F:186:LYS:O	2:F:189:GLU:HB2	1.97	0.64
1:E:646:THR:HB	1:E:647:PRO:HD3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1030:ARG:HG3	1:G:1030:ARG:HH11	1.63	0.64
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.44	0.63
1:E:998:ARG:HG2	1:E:999:PRO:HA	1.80	0.63
1:G:901:PRO:HD2	5:G:4084:CL:CL	2.36	0.63
1:E:6:ASP:OD2	1:E:6:ASP:N	2.29	0.63
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.34	0.63
1:A:648:LEU:HD22	1:A:845:ARG:HD3	1.79	0.63
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.79	0.63
1:A:38[B]:ARG:HG2	1:A:38[B]:ARG:NH1	2.04	0.63
1:C:695:VAL:CG1	1:C:701:ALA:HB2	2.24	0.63
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.80	0.63
1:A:956[B]:ARG:HG2	1:A:956[B]:ARG:NH1	2.03	0.63
1:A:976:GLY:O	1:A:980:VAL:HG23	1.99	0.63
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.98	0.63
2:B:152:GLY:O	2:B:156:MET:HE3	1.99	0.63
1:G:698:ILE:HD12	1:G:698:ILE:H	1.62	0.63
2:H:363:ALA:C	2:H:365:PRO:HD2	2.23	0.63
1:A:636:LYS:NZ	11:A:4560:HOH:O	2.30	0.63
2:D:212:ARG:HG3	2:D:212:ARG:HH11	1.63	0.63
1:E:151:THR:OG1	1:E:153[B]:GLU:HG2	1.99	0.63
1:G:817:ALA:HB2	1:G:826:MET:SD	2.39	0.63
2:H:269:SER:HB3	9:H:4079:GLN:OE1	1.99	0.63
1:A:150:HIS:N	1:A:154:GLU:OE2	2.32	0.62
1:C:890:VAL:HG23	1:C:927:ALA:HB1	1.79	0.62
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.07	0.62
2:F:225:ALA:O	2:F:229:LEU:HG	1.99	0.62
1:A:905:PRO:HB2	1:A:1040:TYR:OH	2.00	0.62
1:C:734:LEU:HD11	1:C:738:PHE:CE2	2.34	0.62
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.18	0.62
1:A:166:CYS:C	1:A:167:ILE:HD12	2.25	0.62
1:A:659:VAL:HG13	1:A:660:PRO:HD2	1.81	0.62
1:A:698:ILE:HD12	1:A:698:ILE:N	2.13	0.62
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.64	0.62
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.82	0.62
1:C:947:LEU:N	1:C:947:LEU:HD12	2.13	0.62
1:G:167:ILE:HD12	1:G:167:ILE:N	2.15	0.62
1:A:4:ARG:HD3	1:A:7:ILE:HD12	1.82	0.62
1:A:726:GLU:HG3	1:A:727:ILE:N	2.15	0.62
1:A:992:ASN:ND2	1:G:975:HIS:NE2	2.48	0.62
2:H:202:LYS:NZ	2:H:355:GLU:OE1	2.30	0.62
1:A:772:MET:HE1	1:A:880:THR:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:LEU:HD11	1:C:812:GLN:HG2	1.80	0.61
1:E:4:ARG:HA	11:E:4160:HOH:O	1.99	0.61
1:E:734:LEU:HD12	1:E:734:LEU:O	2.00	0.61
1:G:757[B]:ASP:OD1	1:G:833:LYS:NZ	2.33	0.61
2:H:328:THR:HG21	11:H:3665:HOH:O	1.99	0.61
2:H:5:ALA:HB3	2:H:110:ILE:HG13	1.81	0.61
2:H:187:GLU:CG	2:H:215:ARG:HD2	2.21	0.61
1:A:907:LEU:HD11	8:A:4011:ORN:HD3	1.82	0.61
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.35	0.61
1:C:784:GLN:H	1:C:784:GLN:HE21	1.49	0.61
1:C:698:ILE:HD12	1:C:698:ILE:N	2.16	0.61
1:E:167:ILE:HD12	1:E:167:ILE:N	2.15	0.61
1:E:1021:ARG:HH11	1:E:1021:ARG:CG	2.14	0.61
2:H:244:ASP:OD2	2:H:245:PRO:HD2	2.00	0.61
1:A:1021:ARG:HH11	1:A:1021:ARG:CG	2.13	0.61
1:G:805:ILE:HD12	1:G:832:VAL:HG11	1.83	0.61
1:A:973:ALA:C	1:A:991:VAL:HG12	2.26	0.61
1:C:416:ASP:O	1:C:418:PRO:HD3	2.01	0.61
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.83	0.61
2:H:284:VAL:O	2:H:315:ALA:N	2.33	0.61
1:C:812:GLN:NE2	11:C:4684:HOH:O	2.06	0.60
1:E:998:ARG:HA	1:E:999:PRO:C	2.25	0.60
1:A:375:THR:HG23	1:A:377:GLN:H	1.66	0.60
1:C:675:ARG:H	1:C:675:ARG:CD	2.11	0.60
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.82	0.60
1:G:1063:ILE:HD13	1:G:1068:MET:CG	2.30	0.60
2:B:298:LYS:HE2	2:B:303:ASN:OD1	2.01	0.60
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.83	0.60
1:C:1017:THR:HG21	1:C:1023:ILE:HA	1.84	0.60
1:G:10:ILE:HD12	1:G:42:TYR:HB3	1.83	0.60
1:A:956[A]:ARG:HD3	11:A:4668:HOH:O	2.01	0.60
1:C:698:ILE:H	1:C:698:ILE:CD1	2.15	0.60
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.82	0.60
1:G:475:LYS:NZ	11:G:3293:HOH:O	2.33	0.60
1:G:1001:ILE:CD1	1:G:1002:GLN:N	2.65	0.60
1:A:757:ASP:O	1:A:833:LYS:NZ	2.32	0.60
1:E:702:VAL:HG11	1:E:735:ARG:NH2	2.15	0.60
1:E:956[A]:ARG:HB3	1:E:1044:LEU:CD2	2.31	0.60
1:C:822:VAL:O	1:C:823:ARG:HD3	2.01	0.60
1:C:1021:ARG:HH11	1:C:1021:ARG:HG3	1.65	0.60
2:F:324:ASN:HD22	2:F:324:ASN:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:LEU:CB	2:H:242:PRO:HB2	2.31	0.60
1:A:1020:ARG:NH2	1:A:1023:ILE:HG21	2.17	0.60
1:G:641:GLN:OE1	1:G:869:MET:HE1	2.02	0.60
1:C:890:VAL:HG23	1:C:927:ALA:CB	2.31	0.60
1:E:812:GLN:NE2	11:E:4800:HOH:O	2.35	0.60
2:H:33:ASN:HA	2:H:291:HIS:O	2.02	0.60
2:H:344:ASP:OD2	2:H:344:ASP:N	2.34	0.60
2:B:186:LYS:O	2:B:189:GLU:HB2	2.02	0.59
2:B:370:PHE:O	2:B:374:ILE:HG13	2.02	0.59
1:G:676:GLU:O	1:G:680:HIS:ND1	2.35	0.59
1:C:784:GLN:H	1:C:784:GLN:NE2	1.99	0.59
1:E:563:MET:CE	1:E:635:PRO:HG3	2.32	0.59
1:C:708:ILE:CG2	1:C:712:LEU:HD11	2.31	0.59
1:G:282:SER:N	11:G:3572:HOH:O	2.35	0.59
1:G:343:ARG:NH1	11:G:3545:HOH:O	2.34	0.59
1:A:646:THR:HB	1:A:647:PRO:HD3	1.83	0.59
1:A:954:LYS:O	1:A:957:VAL:HG12	2.02	0.59
1:C:313:LYS:HE2	1:C:608:THR:O	2.02	0.59
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.50	0.59
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.85	0.59
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.83	0.59
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.50	0.59
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.83	0.59
1:C:563:MET:HE1	1:C:635:PRO:HG3	1.85	0.59
2:F:286:MET:HE1	2:F:312:HIS:ND1	2.17	0.59
1:G:509:ARG:HH11	1:G:509:ARG:HB2	1.66	0.59
2:H:55:LEU:CD1	2:H:60:ILE:HD12	2.32	0.59
2:D:174:SER:O	2:D:182:PRO:HD3	2.03	0.59
1:A:675:ARG:CD	1:A:675:ARG:H	2.15	0.59
1:A:906:LEU:O	1:A:912:ARG:NH2	2.30	0.59
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.17	0.59
2:D:26:ALA:O	2:D:131:CYS:HA	2.03	0.59
1:A:772:MET:HE1	1:A:880:THR:HG22	1.85	0.59
1:C:509:ARG:NH1	1:C:512:GLU:OE1	2.35	0.59
1:C:954:LYS:O	1:C:957:VAL:HG12	2.02	0.59
1:E:1020:ARG:O	1:E:1024:GLU:HG3	2.03	0.59
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.84	0.59
2:B:187:GLU:CG	2:B:215:ARG:HD2	2.26	0.58
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.85	0.58
1:A:315:THR:O	1:A:531:THR:HG22	2.03	0.58
1:C:975:HIS:HE2	1:E:992:ASN:ND2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:195:VAL:HG21	2:D:231:MET:HE3	1.84	0.58
2:H:46:PRO:O	2:H:242:PRO:HG3	2.03	0.58
1:C:133:ASP:OD2	11:C:4117:HOH:O	2.17	0.58
2:H:324:ASN:ND2	2:H:324:ASN:H	2.00	0.58
1:E:318:PRO:HG3	1:E:610:TYR:OH	2.03	0.58
1:G:698:ILE:HD12	1:G:698:ILE:N	2.18	0.58
2:B:46:PRO:HA	2:B:76:HIS:CG	2.37	0.58
1:C:447:LEU:HD23	1:G:446:GLY:O	2.02	0.58
1:C:998:ARG:CG	1:C:999:PRO:HA	2.33	0.58
2:D:118:LEU:O	2:D:118:LEU:HD12	2.04	0.58
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.33	0.58
2:B:285:LYS:HG3	2:B:314:PHE:CD1	2.39	0.58
1:E:734:LEU:HD12	1:E:734:LEU:C	2.27	0.58
1:G:165:PRO:HA	1:G:182:ALA:O	2.04	0.58
1:C:980:VAL:HG13	11:C:4704:HOH:O	2.03	0.58
1:C:1052:MET:HG2	11:C:4681:HOH:O	2.04	0.58
2:F:269:SER:HB3	9:F:4056:GLN:OE1	2.04	0.58
2:F:379:LYS:HZ3	2:F:379:LYS:HB2	1.68	0.58
1:G:1021:ARG:HH11	1:G:1021:ARG:CG	2.12	0.58
1:C:728:VAL:CG1	1:C:733:ASP:HB3	2.33	0.58
1:A:272:LEU:HD11	1:A:282:SER:HB2	1.85	0.58
2:B:350:PHE:HB2	2:B:366:LEU:HD22	1.86	0.58
1:C:1063:ILE:HD13	1:C:1068:MET:CG	2.26	0.58
1:A:863:LYS:HE2	11:A:4575:HOH:O	2.03	0.57
2:D:350:PHE:HB2	2:D:366:LEU:HD22	1.86	0.57
1:E:59:GLU:CG	1:E:60:MET:HE2	2.34	0.57
1:G:809:MET:O	1:G:813:VAL:HG23	2.03	0.57
1:A:964:LEU:O	1:A:969:PHE:HB2	2.03	0.57
2:B:313:GLY:HA3	11:B:4020:HOH:O	2.04	0.57
1:C:103:GLU:HG3	1:C:104:ARG:N	2.15	0.57
1:C:695:VAL:CG1	1:C:700:MET:HB3	2.34	0.57
2:D:6:LEU:HD13	2:D:16:HIS:CE1	2.39	0.57
1:C:479:VAL:CG2	1:C:483:GLY:HA3	2.34	0.57
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.52	0.57
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.69	0.57
2:H:246:ALA:HB3	2:H:247:PRO:HD3	1.85	0.57
1:A:734:LEU:HD12	1:A:734:LEU:C	2.25	0.57
1:E:194:ARG:HD3	11:E:4114:HOH:O	2.04	0.57
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.40	0.57
2:H:133:ILE:HG22	2:H:138:PRO:HB3	1.85	0.57
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:THR:HG23	11:A:4539:HOH:O	2.04	0.57
1:E:213:TRP:CE2	1:E:289:ASN:HB2	2.39	0.57
1:G:1:MET:H3	1:G:224:LYS:HE3	1.70	0.57
1:G:729:TYR:CE1	1:G:1019:GLY:HA2	2.39	0.57
1:G:560:GLU:OE1	1:G:636:LYS:HE3	2.05	0.57
2:H:78:GLN:HA	2:H:78:GLN:NE2	2.19	0.57
1:E:1017:THR:HG22	1:E:1023:ILE:HG13	1.87	0.57
1:A:194:ARG:NH2	11:A:4602:HOH:O	2.28	0.57
1:E:691:ALA:HB3	1:E:708:ILE:HG23	1.86	0.57
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.86	0.57
1:C:419[B]:GLU:OE1	1:G:422:THR:HG21	2.05	0.57
1:C:559:ARG:HG3	1:C:559:ARG:HH11	1.69	0.57
1:E:265:ARG:NH2	1:E:269:MET:HE1	2.20	0.57
1:E:344:THR:HB	1:E:345:PRO:HD2	1.87	0.57
1:E:693:ALA:HB3	1:E:708:ILE:HD11	1.86	0.57
2:B:139:ASP:OD2	2:B:142:LEU:HB2	2.05	0.56
1:C:901:PRO:HD2	5:C:4039:CL:CL	2.42	0.56
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.87	0.56
1:A:321:LYS:NZ	1:A:611:ASP:OD1	2.36	0.56
1:A:562:ILE:HG21	1:A:589:LEU:CD1	2.35	0.56
2:F:253:THR:O	2:F:256:GLN:HB2	2.05	0.56
1:A:344:THR:HB	1:A:345:PRO:HD2	1.86	0.56
1:A:772:MET:HE1	1:A:880:THR:CA	2.35	0.56
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.40	0.56
1:C:40:GLU:OE1	1:C:325:LYS:HE2	2.04	0.56
1:C:375:THR:HG23	1:C:377:GLN:H	1.69	0.56
1:C:672:ALA:HB3	1:C:844:PRO:HG3	1.86	0.56
1:C:693:ALA:HB1	1:C:704:LYS:HG2	1.86	0.56
2:F:350:PHE:HB2	2:F:366:LEU:HD22	1.87	0.56
1:G:534:ALA:O	2:H:123:ARG:HD3	2.05	0.56
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.87	0.56
1:A:998:ARG:CB	1:A:999:PRO:HA	2.34	0.56
1:E:196:LEU:HG	1:E:204:LEU:HD11	1.86	0.56
1:E:698:ILE:HG13	1:E:738:PHE:CG	2.39	0.56
1:G:349:GLU:O	2:H:294:ASN:HB2	2.04	0.56
1:G:954:LYS:O	1:G:980:VAL:HG11	2.06	0.56
1:E:726:GLU:HG3	1:E:1020:ARG:NH2	2.21	0.56
1:E:1019:GLY:O	1:E:1023:ILE:HD12	2.05	0.56
1:A:489:LEU:HD22	1:A:516:LEU:HD23	1.86	0.56
1:C:695:VAL:HG21	1:C:752:LEU:HD22	1.88	0.56
1:G:569:PRO:O	1:G:571:ARG:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:796:LEU:C	1:G:796:LEU:HD23	2.31	0.56
1:C:3:LYS:HG2	11:C:4580:HOH:O	2.04	0.56
2:D:306:MET:HE1	2:D:366:LEU:HD11	1.86	0.56
2:F:272:HIS:HA	2:F:349:SER:HB2	1.88	0.56
2:H:248:CYS:O	2:H:252:ILE:HG13	2.06	0.56
2:D:44:THR:O	2:D:46:PRO:HD3	2.06	0.56
1:G:1001:ILE:HD12	1:G:1002:GLN:N	2.20	0.56
1:G:1036:TYR:C	1:G:1037:LYS:HG2	2.28	0.56
2:H:139:ASP:OD2	2:H:142:LEU:HB2	2.06	0.56
1:A:682:VAL:HG11	1:A:689:GLN:HE21	1.71	0.56
1:E:757:ASP:O	1:E:833:LYS:NZ	2.27	0.56
1:G:964:LEU:O	1:G:969:PHE:HB2	2.06	0.56
1:G:679:GLN:HG2	1:G:689:GLN:HE22	1.71	0.55
2:H:169:SER:HA	2:H:216:LEU:O	2.07	0.55
1:A:700:MET:O	1:A:704:LYS:HB2	2.06	0.55
1:A:1020:ARG:HH21	1:A:1023:ILE:HG21	1.70	0.55
2:B:172:GLN:O	2:B:207:ARG:HA	2.06	0.55
2:B:259:LEU:O	2:B:345:LYS:HE3	2.07	0.55
1:C:1048:PHE:O	1:C:1052:MET:HG3	2.07	0.55
1:G:548:GLU:HG2	2:H:114:ASP:OD1	2.05	0.55
1:C:858:GLY:HA2	1:C:1069:HIS:NE2	2.21	0.55
1:C:1068:MET:O	1:C:1071:GLN:HB2	2.07	0.55
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.36	0.55
1:A:103:GLU:HG2	1:A:108:LEU:HD12	1.89	0.55
1:A:948:SER:O	1:A:1015:ASN:HA	2.06	0.55
2:B:46:PRO:HA	2:B:76:HIS:CB	2.37	0.55
1:C:735:ARG:O	1:C:738:PHE:HB2	2.07	0.55
2:D:178:THR:HB	11:D:1596:HOH:O	2.06	0.55
1:G:668:ALA:O	1:G:671:ARG:HB2	2.07	0.55
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.41	0.55
1:E:950:ARG:HD3	11:E:4812:HOH:O	2.06	0.55
1:A:88:PRO:HB3	1:A:99:ALA:HB2	1.88	0.55
1:A:695:VAL:HG11	1:A:701:ALA:CA	2.37	0.55
1:A:696:THR:OG1	1:A:700:MET:HE1	2.06	0.55
1:A:947:LEU:N	1:A:947:LEU:HD12	2.21	0.55
1:C:222:ARG:NH1	1:C:273:ARG:HA	2.21	0.55
1:C:735:ARG:O	1:C:738:PHE:N	2.39	0.55
2:D:206:LEU:O	2:D:210:VAL:HG23	2.07	0.55
1:E:1:MET:H2	1:E:224:LYS:HE3	1.70	0.55
1:G:556:SER:HB2	1:G:558:ASP:HB2	1.88	0.55
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ALA:N	2:B:365:PRO:HD2	2.22	0.55
2:D:240:ASN:HB2	9:D:4034:GLN:OE1	2.06	0.55
1:A:167:ILE:HD12	1:A:167:ILE:N	2.22	0.54
2:D:46:PRO:HA	2:D:76:HIS:CG	2.41	0.54
1:E:652:ARG:NH2	1:E:667:ASP:OD2	2.40	0.54
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.88	0.54
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.22	0.54
2:B:46:PRO:O	2:B:242:PRO:HG3	2.06	0.54
2:D:285:LYS:HG3	2:D:314:PHE:CE1	2.42	0.54
1:A:28:TYR:O	1:A:32:GLN:HG3	2.07	0.54
1:C:992:ASN:ND2	1:C:996:GLU:HB3	2.23	0.54
1:E:897:PHE:HB3	11:E:4620:HOH:O	2.08	0.54
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.88	0.54
2:H:173:GLY:O	2:H:207:ARG:HG2	2.08	0.54
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.21	0.54
1:G:701:ALA:O	1:G:705:ALA:N	2.30	0.54
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.87	0.54
1:E:185:ARG:HG2	1:E:189:GLU:OE2	2.07	0.54
2:F:78:GLN:NE2	11:F:2502:HOH:O	2.33	0.54
1:G:540:THR:HG22	1:G:541:ALA:N	2.23	0.54
1:A:79:GLU:HB2	1:A:111:PHE:CZ	2.42	0.54
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.90	0.54
1:C:353:ASP:OD1	2:D:116:ARG:HD2	2.08	0.54
1:E:196:LEU:HG	1:E:204:LEU:CD1	2.37	0.54
1:E:703:GLU:O	1:E:706:LYS:HB2	2.07	0.54
1:E:726:GLU:HG3	1:E:1020:ARG:HH21	1.72	0.54
1:G:181:ILE:HD11	1:G:376:THR:CG2	2.35	0.54
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.89	0.54
1:E:730:ASP:O	1:E:733:ASP:HB2	2.07	0.54
1:E:956[B]:ARG:HB3	1:E:1044:LEU:CD2	2.37	0.54
1:G:671:ARG:NH2	1:G:819:GLU:O	2.40	0.54
1:C:257:THR:HG23	2:D:91:ASN:ND2	2.23	0.54
1:C:670:ASP:CB	1:C:677:ARG:HH21	2.18	0.54
2:H:186:LYS:O	2:H:189:GLU:HB2	2.08	0.54
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.38	0.54
1:A:998:ARG:HG2	1:A:999:PRO:HA	1.90	0.54
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.08	0.54
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.08	0.54
1:E:710:TYR:HB3	1:E:729:TYR:O	2.08	0.54
1:E:802:SER:OG	1:E:805:ILE:HB	2.08	0.54
1:E:808:VAL:HA	1:E:811[B]:GLN:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:ILE:HG22	1:G:149:ALA:N	2.22	0.54
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.23	0.53
1:G:922:ARG:NH2	1:G:1060:GLU:OE2	2.41	0.53
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.42	0.53
1:C:237:PHE:HB3	1:C:248:ILE:O	2.07	0.53
1:G:475:LYS:HD3	1:G:488:PHE:CZ	2.43	0.53
2:D:355:GLU:OE2	2:D:355:GLU:N	2.37	0.53
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.90	0.53
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.07	0.53
1:A:362:PHE:CE1	1:A:380:SER:HB3	2.43	0.53
1:E:682:VAL:CG1	1:E:687:LEU:HB2	2.38	0.53
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.09	0.53
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.89	0.53
2:H:193:HIS:O	2:H:234:ASP:HB2	2.08	0.53
2:H:352:GLY:O	2:H:354:PRO:HD3	2.08	0.53
2:H:365:PRO:HA	2:H:368:ASP:OD1	2.08	0.53
2:F:272:HIS:HA	2:F:349:SER:CB	2.39	0.53
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.25	0.53
1:A:481:ILE:HG22	11:A:4626:HOH:O	2.08	0.53
1:A:695:VAL:HG11	1:A:701:ALA:N	2.23	0.53
2:B:105:HIS:ND1	11:B:4218:HOH:O	2.34	0.53
1:C:252:PRO:HD3	1:C:352:ILE:HD11	1.90	0.53
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.38	0.53
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.89	0.53
1:E:930:LYS:HE3	11:E:4218:HOH:O	2.09	0.53
1:A:4:ARG:CD	1:A:7:ILE:HD12	2.39	0.53
1:A:687:LEU:HD22	1:A:812:GLN:HG2	1.91	0.53
1:A:713:VAL:HG12	1:A:713:VAL:O	2.08	0.53
2:B:228:VAL:HA	2:B:231:MET:HE2	1.91	0.53
1:E:947:LEU:HD12	1:E:947:LEU:N	2.24	0.53
1:E:1:MET:H3	1:E:224:LYS:HE3	1.73	0.53
1:G:340:THR:O	1:G:343:ARG:HB2	2.09	0.53
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.31	0.53
2:H:46:PRO:HA	2:H:76:HIS:CG	2.43	0.53
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.24	0.53
1:C:695:VAL:HG11	1:C:701:ALA:N	2.23	0.53
1:C:695:VAL:HG11	1:C:701:ALA:CA	2.38	0.53
1:A:331:THR:O	1:A:334:GLU:HB2	2.09	0.53
2:B:354:PRO:HB2	2:B:367:PHE:CE2	2.44	0.53
1:C:676:GLU:O	1:C:680:HIS:ND1	2.42	0.53
2:H:156:MET:HG2	2:H:158:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:734:LEU:HD12	1:G:734:LEU:C	2.30	0.52
1:G:1001:ILE:O	1:G:1005:ILE:HG13	2.08	0.52
2:H:133:ILE:HD12	2:H:143:ALA:CB	2.19	0.52
2:B:41:GLU:OE2	2:B:41:GLU:N	2.36	0.52
1:C:762:VAL:HG13	1:C:779:MET:O	2.08	0.52
1:E:103:GLU:HG2	11:E:4778:HOH:O	2.09	0.52
1:E:701:ALA:O	1:E:705:ALA:N	2.28	0.52
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.44	0.52
1:G:40:GLU:CG	1:G:325:LYS:HE2	2.39	0.52
1:G:761:GLU:HG2	1:G:781:HIS:CE1	2.44	0.52
1:E:213:TRP:HZ3	1:E:296:ILE:HD12	1.74	0.52
1:G:151:THR:HG21	11:G:3075:HOH:O	2.09	0.52
1:A:659:VAL:CG1	1:A:660:PRO:HD2	2.39	0.52
1:C:973:ALA:C	1:C:991[A]:VAL:HG12	2.33	0.52
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.90	0.52
1:C:805:ILE:HD13	1:C:837:VAL:CG2	2.40	0.52
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.44	0.52
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.75	0.52
2:F:324:ASN:HA	2:F:343:THR:OG1	2.10	0.52
1:G:993:LYS:NZ	11:G:3612:HOH:O	2.29	0.52
1:A:419:GLU:HG3	11:E:4704:HOH:O	2.10	0.52
1:C:110:GLU:HG2	1:C:111:PHE:CE1	2.44	0.52
2:D:156:MET:HA	11:D:1820:HOH:O	2.10	0.52
2:F:197:TYR:O	2:F:239:SER:HB3	2.10	0.52
1:G:158:VAL:O	1:G:161:ASP:HB3	2.10	0.52
1:G:361:ARG:CZ	1:G:571:ARG:HG2	2.40	0.52
2:H:193:HIS:NE2	2:H:217:THR:OG1	2.27	0.52
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.22	0.52
2:F:205:ILE:HG12	2:F:355:GLU:CG	2.40	0.52
1:G:489:LEU:HD13	1:G:522:LEU:HD23	1.92	0.52
1:A:556:SER:HB2	1:A:558:ASP:HB2	1.92	0.52
1:A:986:ILE:O	1:A:988:PRO:HD3	2.10	0.52
2:D:272:HIS:HA	2:D:349:SER:HB2	1.90	0.52
2:H:168:TYR:CE2	2:H:218:ILE:HG12	2.44	0.52
2:H:264:PRO:HB3	2:H:373:LEU:HB3	1.91	0.52
1:A:998:ARG:HA	1:A:999:PRO:C	2.32	0.52
1:C:734:LEU:HD12	1:C:734:LEU:C	2.35	0.52
2:D:246:ALA:HB3	2:D:247:PRO:CD	2.39	0.52
1:E:784:GLN:HE21	1:E:784:GLN:N	2.00	0.52
1:E:956[A]:ARG:HB3	1:E:1044:LEU:HD21	1.91	0.52
1:A:975:HIS:HE2	1:G:992:ASN:ND2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:HIS:HE2	1:G:992:ASN:HD21	1.58	0.52
2:D:272:HIS:HA	2:D:349:SER:CB	2.40	0.52
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.45	0.52
1:G:79:GLU:HG2	1:G:111:PHE:CZ	2.45	0.52
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.25	0.52
1:A:349:GLU:O	2:B:294:ASN:HB2	2.10	0.51
1:C:695:VAL:CG2	1:C:752:LEU:HD22	2.40	0.51
1:G:1:MET:HB2	1:G:224:LYS:HZ2	1.74	0.51
1:A:1023:ILE:HG22	1:A:1024:GLU:N	2.23	0.51
2:B:27:VAL:O	2:B:78:GLN:HG2	2.10	0.51
2:D:118:LEU:HD12	2:D:118:LEU:C	2.36	0.51
1:E:1061:LYS:HE2	11:E:4658:HOH:O	2.09	0.51
1:G:950:ARG:HD3	11:G:3654:HOH:O	2.10	0.51
1:A:101:GLU:OE2	1:A:101:GLU:HA	2.11	0.51
1:C:997:GLY:O	1:C:998:ARG:HG3	2.10	0.51
1:G:1030:ARG:HH11	1:G:1030:ARG:CG	2.23	0.51
2:D:279:SER:O	2:D:322:PRO:HG3	2.09	0.51
2:F:279:SER:O	2:F:322:PRO:HG3	2.10	0.51
1:G:1:MET:N	1:G:224:LYS:HE3	2.25	0.51
1:G:18:ILE:HG23	1:G:23:ALA:HA	1.91	0.51
1:G:47:VAL:HG13	1:G:47:VAL:O	2.10	0.51
2:H:174:SER:HB2	2:H:211:ASP:OD2	2.10	0.51
1:C:673:GLU:O	1:C:675:ARG:NH1	2.43	0.51
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.75	0.51
1:E:966:LYS:O	1:E:966:LYS:HG3	2.10	0.51
2:B:249:ASP:HB3	11:B:4178:HOH:O	2.10	0.51
2:B:364:ALA:N	2:B:365:PRO:CD	2.73	0.51
1:E:258:ASP:O	1:E:262:GLN:HG2	2.10	0.51
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.45	0.51
1:G:292:ASN:OD1	1:G:294:ARG:HB2	2.10	0.51
1:A:222:ARG:CZ	1:A:273:ARG:HG2	2.41	0.51
1:C:740:THR:O	1:C:741:ALA:O	2.29	0.51
1:E:3:LYS:HB2	1:E:42:TYR:OH	2.10	0.51
1:E:1001:ILE:O	1:E:1005:ILE:HG13	2.11	0.51
2:F:228:VAL:HA	2:F:231:MET:HE3	1.89	0.51
2:F:257:LYS:O	2:F:260:GLU:HB2	2.11	0.51
1:C:166:CYS:C	1:C:167:ILE:HD12	2.35	0.51
1:C:539:ASP:HB2	11:C:4614:HOH:O	2.09	0.51
1:E:1048:PHE:O	1:E:1052:MET:HG3	2.11	0.51
1:G:339:ILE:HD12	1:G:530:ASP:HA	1.93	0.51
1:G:713:VAL:HG23	1:G:755:PHE:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:734:LEU:CD1	1:G:738:PHE:CE2	2.94	0.51
1:G:772:MET:HE1	1:G:880:THR:HA	1.93	0.51
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.46	0.51
1:C:127:GLU:HB2	1:C:172:PHE:CZ	2.45	0.51
1:C:344:THR:HB	1:C:345:PRO:HD2	1.93	0.51
1:E:998:ARG:CG	1:E:999:PRO:HA	2.40	0.51
1:E:817:ALA:HB2	1:E:826:MET:SD	2.50	0.51
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.45	0.51
1:G:692:ASN:HA	1:G:752:LEU:O	2.11	0.51
2:H:158:LEU:HB3	2:H:242:PRO:HB2	1.92	0.51
2:B:66:ASN:HB3	2:B:93:ARG:O	2.12	0.50
1:C:669:ILE:HA	1:C:844:PRO:HG2	1.92	0.50
2:D:353:HIS:CE1	11:D:1634:HOH:O	2.64	0.50
1:E:62:ASP:OD2	11:E:4634:HOH:O	2.18	0.50
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.29	0.50
1:G:150:HIS:CD2	1:G:203:GLU:HB2	2.46	0.50
1:G:730:ASP:H	1:G:733:ASP:HB2	1.76	0.50
2:H:158:LEU:HB2	2:H:242:PRO:HB2	1.92	0.50
2:D:218:ILE:HD13	2:D:218:ILE:N	2.27	0.50
2:D:327:VAL:HG13	2:D:337:LEU:CD1	2.41	0.50
1:G:1000:HIS:NE2	1:G:1002:GLN:HB3	2.27	0.50
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.75	0.50
2:H:81:VAL:CG1	2:H:113:ILE:HD11	2.42	0.50
1:A:333:ASP:OD1	1:A:333:ASP:N	2.44	0.50
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.46	0.50
1:C:655:GLU:CD	1:C:666:PRO:HG2	2.36	0.50
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.46	0.50
1:E:126:ALA:CB	1:E:302:PRO:HG3	2.39	0.50
1:G:361:ARG:NH2	1:G:571:ARG:HG2	2.27	0.50
2:H:6:LEU:HD12	2:H:7:LEU:H	1.76	0.50
2:H:250:TYR:CD2	2:H:250:TYR:N	2.79	0.50
1:A:470:VAL:O	1:A:474:GLU:HG3	2.11	0.50
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.41	0.50
1:C:289:ASN:HB3	1:C:292:ASN:OD1	2.11	0.50
1:C:726:GLU:CG	1:C:727:ILE:N	2.74	0.50
2:H:153:LEU:HA	2:H:156:MET:HE3	1.94	0.50
1:A:728:VAL:HG12	1:A:733:ASP:HB3	1.92	0.50
1:G:698:ILE:O	1:G:701:ALA:HB3	2.12	0.50
1:G:729:TYR:HE1	1:G:1019:GLY:HA2	1.76	0.50
1:A:11:LEU:HA	1:A:45:ILE:O	2.11	0.50
1:A:950:ARG:HD3	11:A:4711:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LEU:HA	1:C:45:ILE:O	2.12	0.50
2:D:354:PRO:HB2	2:D:367:PHE:CE2	2.46	0.50
1:E:234:ILE:HG23	1:E:250:VAL:O	2.11	0.50
1:E:693:ALA:CB	1:E:708:ILE:HD11	2.42	0.50
1:G:550:GLU:CD	2:H:120:ARG:HH21	2.19	0.50
1:C:562:ILE:HG21	1:C:589:LEU:CD1	2.42	0.50
1:E:393:GLU:HA	1:E:496:GLY:HA3	1.94	0.50
1:G:947:LEU:HG	1:G:1014:ILE:CG2	2.41	0.50
2:D:232:ASN:N	2:D:233:PRO:HD3	2.27	0.50
2:F:202:LYS:NZ	2:F:355:GLU:OE1	2.43	0.50
1:A:710:TYR:HB3	1:A:729:TYR:O	2.11	0.50
2:B:290:HIS:HB2	2:B:312:HIS:NE2	2.27	0.50
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.47	0.50
2:D:174:SER:HB2	2:D:211:ASP:OD2	2.12	0.50
2:D:237:PHE:CZ	2:D:268:ILE:HD12	2.47	0.50
1:E:808:VAL:O	1:E:811[B]:GLN:HG3	2.11	0.50
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.93	0.50
1:G:294:ARG:HD2	5:G:4083:CL:CL	2.49	0.50
1:A:417:ASP:OD1	1:A:423:LYS:NZ	2.35	0.49
1:A:704:LYS:O	1:A:707:GLU:HB2	2.11	0.49
1:A:1001:ILE:O	1:A:1005:ILE:HG13	2.12	0.49
2:D:195:VAL:HG11	2:D:231:MET:HE1	1.94	0.49
2:D:370:PHE:O	2:D:374:ILE:HG13	2.12	0.49
1:E:358:LYS:HG2	1:E:359:ILE:N	2.26	0.49
2:F:32:PHE:O	2:F:291:HIS:HB2	2.11	0.49
2:H:16:HIS:O	2:H:113:ILE:HG22	2.12	0.49
2:B:290:HIS:HB2	2:B:312:HIS:CD2	2.47	0.49
1:C:288:VAL:O	1:C:290:PRO:HD3	2.12	0.49
1:C:713:VAL:O	1:C:713:VAL:HG12	2.12	0.49
2:D:324:ASN:ND2	2:D:324:ASN:H	2.06	0.49
1:E:67:GLU:HB3	1:E:68:PRO:HD2	1.94	0.49
1:G:636:LYS:HD3	11:G:3354:HOH:O	2.11	0.49
1:A:947:LEU:N	1:A:947:LEU:CD1	2.76	0.49
2:F:174:SER:HB2	2:F:211:ASP:OD2	2.12	0.49
2:F:322:PRO:HD2	2:F:325:LEU:HD12	1.93	0.49
1:G:103:GLU:HG3	1:G:104:ARG:N	2.19	0.49
1:G:167:ILE:N	1:G:167:ILE:CD1	2.75	0.49
2:F:376:GLN:O	2:F:376:GLN:HG2	2.08	0.49
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.47	0.49
1:C:321:LYS:NZ	1:C:611:ASP:OD1	2.39	0.49
1:C:972:ASP:OD2	1:C:991[B]:VAL:HG21	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:LEU:HA	2:B:273:GLN:OE1	2.13	0.49
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.47	0.49
2:F:249:ASP:OD2	2:F:250:TYR:N	2.45	0.49
1:G:434:ASP:HB2	11:G:3231:HOH:O	2.12	0.49
1:G:1005:ILE:HG21	1:G:1032:SER:HB3	1.93	0.49
1:G:1021:ARG:HG2	1:G:1021:ARG:NH1	2.16	0.49
2:H:71:GLU:C	2:H:203:ARG:HG3	2.37	0.49
1:A:278:GLU:HG2	11:A:4597:HOH:O	2.13	0.49
2:B:245:PRO:HG3	2:B:273:GLN:OE1	2.13	0.49
1:C:802:SER:OG	1:C:805:ILE:HB	2.13	0.49
1:E:738:PHE:O	1:E:741:ALA:HB3	2.12	0.49
2:F:269:SER:O	2:F:272:HIS:HB3	2.13	0.49
1:C:130:ARG:HG3	1:C:148:ILE:HG13	1.95	0.49
1:E:1020:ARG:HA	1:E:1020:ARG:HD3	1.46	0.49
1:G:441:ASP:OD2	1:G:444:ARG:NH1	2.44	0.49
1:G:641:GLN:CD	1:G:869:MET:HE1	2.38	0.49
1:A:106:GLY:HA2	11:A:4176:HOH:O	2.13	0.49
1:A:981:LEU:CD1	1:A:988:PRO:HG3	2.43	0.49
1:C:110:GLU:HG2	1:C:111:PHE:CD1	2.48	0.49
1:C:534:ALA:HB2	2:D:116:ARG:NH1	2.27	0.49
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.47	0.49
1:C:805:ILE:CD1	1:C:837:VAL:HG23	2.43	0.49
1:E:760:VAL:HG11	1:E:801:LEU:HD11	1.94	0.49
1:G:298:ILE:HG13	11:G:3128:HOH:O	2.11	0.49
1:G:738:PHE:O	1:G:741:ALA:HB3	2.13	0.49
1:G:951:GLU:HA	1:G:954:LYS:HD2	1.94	0.49
1:G:967:GLN:HG3	1:G:1054:LEU:HD13	1.95	0.49
1:G:1017:THR:HG22	1:G:1018:SER:N	2.28	0.49
2:D:212:ARG:HH11	2:D:212:ARG:CG	2.25	0.48
1:E:515:LYS:HD3	1:E:515:LYS:C	2.38	0.48
2:H:48:TYR:O	2:H:51:GLN:HB2	2.12	0.48
1:A:665:SER:O	1:A:669:ILE:HG13	2.12	0.48
2:B:334:ASP:CG	2:B:336:THR:HG23	2.38	0.48
1:G:710:TYR:HB3	1:G:729:TYR:O	2.12	0.48
1:A:602:ASN:CG	1:A:605:THR:HG23	2.38	0.48
1:E:493:LYS:HE2	1:E:517:ARG:HD3	1.95	0.48
1:E:686:LYS:C	1:E:687:LEU:HD23	2.38	0.48
1:A:562:ILE:HG21	1:A:589:LEU:HD12	1.94	0.48
1:A:726:GLU:CG	1:A:727:ILE:N	2.77	0.48
2:B:196:ALA:HB3	2:B:218:ILE:HD12	1.94	0.48
1:C:18:ILE:HG23	1:C:23:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:GLU:O	2:F:294:ASN:HB2	2.13	0.48
2:F:275:LEU:HD23	2:F:349:SER:OG	2.13	0.48
1:G:481:ILE:HD13	1:G:508:VAL:HG11	1.94	0.48
2:H:176:THR:O	2:H:180:GLY:N	2.40	0.48
1:A:558:ASP:HB3	1:A:559:ARG:H	1.38	0.48
2:F:48:TYR:HA	2:F:51:GLN:NE2	2.28	0.48
1:G:56:THR:OG1	1:G:855:LYS:NZ	2.34	0.48
1:G:67:GLU:HB3	1:G:68:PRO:HD2	1.94	0.48
1:G:830:PHE:CE1	1:G:839:LEU:HD13	2.48	0.48
1:C:209:SER:OG	1:C:211:ILE:HG13	2.14	0.48
2:D:306:MET:HE1	2:D:366:LEU:CD1	2.44	0.48
1:E:240:MET:HE3	7:E:4045:ADP:C4	2.48	0.48
1:E:347:SER:O	2:F:296:PRO:HB3	2.14	0.48
2:F:125:LYS:NZ	11:F:2862:HOH:O	2.46	0.48
2:F:201:ALA:CB	2:F:239:SER:HB2	2.38	0.48
1:A:954:LYS:O	1:A:980:VAL:HG11	2.14	0.48
1:A:972:ASP:OD1	1:A:989:ARG:HB3	2.14	0.48
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.48	0.48
1:E:671:ARG:NH2	1:E:819:GLU:O	2.47	0.48
2:F:34:THR:HA	2:F:56:THR:OG1	2.13	0.48
1:G:726:GLU:CG	1:G:727:ILE:N	2.77	0.48
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.49	0.48
1:A:167:ILE:N	1:A:167:ILE:CD1	2.77	0.48
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.29	0.48
1:C:993:LYS:O	1:C:1000:HIS:HB3	2.14	0.48
1:G:579:ASP:OD1	1:G:605:THR:HB	2.14	0.48
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.43	0.48
1:A:891:LYS:NZ	11:A:4492:HOH:O	2.47	0.48
1:C:698:ILE:O	1:C:702:VAL:HG23	2.14	0.48
2:D:269:SER:O	2:D:272:HIS:HB3	2.14	0.48
1:E:170:PRO:HA	1:E:204:LEU:HD23	1.95	0.48
1:E:448:SER:O	1:E:452:VAL:HG23	2.14	0.48
1:G:679:GLN:HG2	1:G:689:GLN:NE2	2.28	0.48
2:H:218:ILE:N	2:H:218:ILE:CD1	2.75	0.48
1:A:467:GLU:O	1:A:471:ARG:HG2	2.14	0.48
1:A:525:VAL:HG22	1:A:548:GLU:H	1.79	0.48
2:B:70:GLU:OE1	2:B:101:TYR:OH	2.27	0.48
1:C:4:ARG:CD	1:C:7:ILE:HD12	2.37	0.48
2:D:7:LEU:HD23	2:D:15:PHE:CD2	2.49	0.48
2:D:85:LEU:HD12	2:D:86:PRO:HD2	1.95	0.48
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:804:GLU:O	1:E:808:VAL:HG23	2.14	0.48
1:G:956:ARG:HB3	1:G:1044:LEU:HD21	1.96	0.48
1:A:89:THR:O	1:A:304:VAL:HG22	2.14	0.47
1:A:772:MET:CE	1:A:880:THR:HA	2.44	0.47
2:B:173:GLY:O	2:B:207:ARG:HG2	2.14	0.47
2:B:232:ASN:N	2:B:233:PRO:HD3	2.30	0.47
1:E:726:GLU:CG	1:E:727:ILE:N	2.77	0.47
2:F:322:PRO:HB2	2:F:324:ASN:HD22	1.77	0.47
1:G:805:ILE:HD12	1:G:832:VAL:CG1	2.43	0.47
2:H:322:PRO:CB	2:H:324:ASN:HD21	2.24	0.47
1:A:17:PRO:HG3	1:A:917:VAL:HG13	1.95	0.47
1:C:668:ALA:O	1:C:671:ARG:HB2	2.15	0.47
1:C:703:GLU:HA	1:C:703:GLU:OE2	2.14	0.47
1:G:246:ASP:C	1:G:360:PRO:HG3	2.40	0.47
1:G:738:PHE:HA	1:G:741:ALA:HB3	1.96	0.47
1:A:1:MET:HB2	1:A:224:LYS:NZ	2.29	0.47
1:A:730:ASP:H	1:A:733:ASP:HB2	1.77	0.47
1:E:278:GLU:HG2	11:E:4235:HOH:O	2.14	0.47
1:E:525:VAL:HG22	1:E:548:GLU:H	1.78	0.47
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.50	0.47
1:A:82:ARG:NH1	1:A:82:ARG:HG3	2.30	0.47
1:A:224:LYS:HE2	1:A:329:GLY:O	2.14	0.47
1:A:426:ARG:HD3	1:A:426:ARG:C	2.40	0.47
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.32	0.47
2:F:106:ASN:ND2	11:F:2545:HOH:O	2.47	0.47
2:F:164:THR:O	2:F:220:PRO:HB3	2.15	0.47
1:G:423:LYS:HB3	11:G:3274:HOH:O	2.14	0.47
1:A:951:GLU:HA	1:A:954:LYS:HD2	1.96	0.47
2:B:205:ILE:O	2:B:209:LEU:HG	2.15	0.47
2:B:222:GLN:HA	2:B:250:TYR:CD1	2.50	0.47
1:C:865:ALA:O	1:C:869:MET:HG3	2.13	0.47
1:C:992:ASN:O	1:C:1000:HIS:HA	2.14	0.47
1:G:906:LEU:O	1:G:912:ARG:NH2	2.31	0.47
1:A:728:VAL:HG11	1:A:734:LEU:HA	1.97	0.47
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.50	0.47
1:C:704:LYS:HD2	1:C:707:GLU:OE1	2.14	0.47
1:C:737:TYR:O	1:C:741:ALA:HB2	2.15	0.47
1:C:1000:HIS:CD2	1:C:1000:HIS:H	2.33	0.47
2:D:186:LYS:H	2:D:189:GLU:CD	2.22	0.47
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.50	0.47
2:H:8:VAL:HG12	2:H:9:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PHE:HA	1:A:165:PRO:C	2.40	0.47
1:A:693:ALA:HB2	1:A:708:ILE:HD11	1.96	0.47
1:A:734:LEU:CD1	1:A:738:PHE:CE2	2.98	0.47
1:C:167:ILE:HG13	1:C:181:ILE:HG12	1.96	0.47
1:E:698:ILE:CD1	1:E:698:ILE:N	2.77	0.47
1:E:841:GLU:HB2	11:E:4625:HOH:O	2.15	0.47
1:E:1017:THR:CG2	1:E:1023:ILE:HG13	2.43	0.47
2:F:236:ILE:O	2:F:265:VAL:HA	2.15	0.47
2:F:259:LEU:O	2:F:345:LYS:HE2	2.15	0.47
1:G:224:LYS:HE2	1:G:329:GLY:O	2.14	0.47
1:G:339:ILE:CD1	1:G:530:ASP:HA	2.45	0.47
1:G:863:LYS:O	1:G:867:ARG:HG3	2.14	0.47
1:G:946:LEU:C	1:G:947:LEU:HD12	2.39	0.47
1:G:1017:THR:CG2	1:G:1018:SER:N	2.77	0.47
1:G:1026:SER:CB	1:G:1030:ARG:HH12	2.22	0.47
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.95	0.47
2:H:322:PRO:HD2	2:H:325:LEU:HD12	1.97	0.47
1:A:184:ASN:O	1:A:188:PHE:HB2	2.15	0.47
1:C:64:THR:O	1:C:1065:VAL:HG23	2.14	0.47
1:C:240:MET:HE2	1:C:287:ALA:HB2	1.97	0.47
1:C:294:ARG:HD2	5:C:4038:CL:CL	2.51	0.47
1:C:986:ILE:O	1:C:988:PRO:HD3	2.14	0.47
2:F:244:ASP:OD2	2:F:245:PRO:HD2	2.14	0.47
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.45	0.47
1:A:698:ILE:O	1:A:702:VAL:HG23	2.15	0.47
1:C:130:ARG:HB2	1:C:148:ILE:HD12	1.95	0.47
1:E:500:ALA:O	1:E:504:LYS:HG3	2.15	0.47
2:F:26:ALA:O	2:F:131:CYS:HA	2.15	0.47
1:A:1021:ARG:HH11	1:A:1021:ARG:HG2	1.80	0.47
1:C:74:VAL:CG1	1:C:102:LEU:HD11	2.42	0.47
1:C:808:VAL:HA	1:C:811[B]:GLN:OE1	2.14	0.47
1:E:904:ASP:O	1:E:906:LEU:N	2.45	0.47
2:F:83:ARG:O	2:F:112:ASP:HA	2.15	0.47
1:G:11:LEU:HA	1:G:45:ILE:O	2.14	0.47
1:G:939:MET:HE2	1:G:1050:THR:HG22	1.93	0.47
1:A:24:CYS:SG	1:A:576:ILE:HB	2.55	0.46
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.39	0.46
1:E:458:ILE:O	1:E:463:LEU:HD11	2.15	0.46
1:E:1017:THR:HG21	1:E:1023:ILE:HA	1.97	0.46
1:G:145:ARG:HB2	1:G:208:GLU:CD	2.40	0.46
1:G:453:PHE:CD1	1:G:453:PHE:C	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.28	0.46
2:H:40:GLN:HE21	2:H:70:GLU:HG2	1.80	0.46
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.53	0.46
1:A:313:LYS:HE2	1:A:608:THR:C	2.39	0.46
1:A:383:GLU:OE2	1:A:604:GLU:OE1	2.34	0.46
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.51	0.46
1:C:318:PRO:HB2	1:C:321:LYS:HB2	1.97	0.46
1:E:1017:THR:HG22	1:E:1018:SER:N	2.30	0.46
2:F:55:LEU:HD13	2:F:60:ILE:HD12	1.97	0.46
1:G:277:VAL:O	1:G:277:VAL:HG12	2.15	0.46
2:H:45:ASP:HB3	2:H:48:TYR:HD2	1.80	0.46
1:A:9:SER:OG	1:A:83:PRO:HA	2.16	0.46
1:A:469:LEU:O	1:A:473:GLU:HG3	2.15	0.46
2:D:173:GLY:O	2:D:207:ARG:HG2	2.15	0.46
1:E:678:PHE:O	1:E:681:ALA:N	2.48	0.46
1:G:148:ILE:CG2	1:G:149:ALA:N	2.78	0.46
2:H:325:LEU:HD23	2:H:325:LEU:HA	1.68	0.46
1:C:4:ARG:HD3	1:C:7:ILE:CD1	2.40	0.46
1:C:733:ASP:OD1	1:C:736:ARG:NH1	2.48	0.46
2:D:274:LEU:HD23	2:D:274:LEU:HA	1.69	0.46
1:E:734:LEU:O	1:E:737:TYR:HB3	2.14	0.46
2:H:144:LEU:HD12	2:H:144:LEU:O	2.16	0.46
1:A:40:GLU:HG2	1:A:325:LYS:HE2	1.97	0.46
1:A:772:MET:HE1	1:A:880:THR:CG2	2.44	0.46
2:B:121:LEU:O	2:B:121:LEU:HD12	2.15	0.46
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.16	0.46
1:C:51:PRO:HG3	1:C:918:MET:HB2	1.97	0.46
1:C:66:ILE:CG2	1:C:918:MET:HB3	2.45	0.46
2:F:152:GLY:O	2:F:156:MET:HE3	2.16	0.46
2:F:225:ALA:HA	2:F:258:PHE:CZ	2.49	0.46
1:G:702:VAL:O	1:G:706:LYS:HD3	2.15	0.46
1:A:796:LEU:HD23	1:A:796:LEU:C	2.40	0.46
1:C:885:PRO:HG2	11:C:4735:HOH:O	2.16	0.46
1:C:990:LEU:HD13	1:E:990:LEU:HD22	1.98	0.46
10:C:4036:NET:H71	10:C:4036:NET:H23	1.62	0.46
2:D:45:ASP:HB3	2:D:48:TYR:HD2	1.80	0.46
2:D:201:ALA:HB2	2:D:239:SER:CB	2.46	0.46
1:E:735:ARG:O	1:E:738:PHE:HB2	2.16	0.46
1:G:598:MET:HG3	1:G:599:VAL:N	2.31	0.46
1:G:874:LEU:HB3	1:G:879:VAL:O	2.16	0.46
1:C:77:ILE:O	1:C:81:GLU:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:GLU:H	1:C:365:GLU:HG3	1.04	0.46
1:E:412:LYS:HG2	1:E:438:TYR:CZ	2.51	0.46
1:E:1017:THR:CG2	1:E:1018:SER:N	2.78	0.46
2:F:46:PRO:HA	2:F:76:HIS:CG	2.50	0.46
2:H:249:ASP:HB3	11:H:3526:HOH:O	2.14	0.46
2:H:300:VAL:HG22	2:H:328:THR:O	2.16	0.46
2:F:332:LEU:HD12	2:F:332:LEU:HA	1.60	0.46
1:G:53:THR:OG1	1:G:56:THR:HG23	2.16	0.46
1:G:648:LEU:CD2	1:G:845:ARG:HD3	2.45	0.46
1:A:840:ILE:O	1:A:841:GLU:HB3	2.14	0.46
2:B:185:LYS:CD	2:B:190:LEU:HD21	2.46	0.46
1:C:130:ARG:HB2	1:C:148:ILE:CD1	2.45	0.46
1:G:315:THR:O	1:G:531:THR:HG22	2.15	0.46
1:G:1052:MET:O	1:G:1055:ASN:HB2	2.16	0.46
1:A:38[B]:ARG:HH11	1:A:38[B]:ARG:CG	2.20	0.46
1:A:764:VAL:HG11	1:A:813:VAL:HG21	1.97	0.46
1:A:814:GLN:NE2	11:A:4511:HOH:O	2.48	0.46
1:A:946:LEU:C	1:A:947:LEU:HD12	2.41	0.46
2:B:241:GLY:N	9:B:4012:GLN:OE1	2.39	0.46
1:C:710:TYR:HB3	1:C:729:TYR:O	2.15	0.46
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.45	0.46
2:H:222:GLN:HA	2:H:250:TYR:CD1	2.51	0.46
1:C:118:ALA:HA	11:C:4198:HOH:O	2.16	0.45
1:C:186:GLU:N	11:C:4608:HOH:O	2.43	0.45
1:C:1021:ARG:HH11	1:C:1021:ARG:CG	2.28	0.45
1:E:146:SER:HB3	1:E:207:ASP:OD1	2.15	0.45
1:G:763:ASP:HB3	1:G:779:MET:HE3	1.98	0.45
1:A:125:LYS:NZ	1:A:274:GLU:OE1	2.47	0.45
1:A:336[A]:MET:HB3	1:A:342:GLY:HA2	1.98	0.45
2:B:6:LEU:HD23	2:B:138:PRO:HB2	1.97	0.45
2:B:266:PHE:HB2	2:B:370:PHE:CD1	2.50	0.45
1:C:479:VAL:HG23	1:C:480:GLY:O	2.16	0.45
2:F:379:LYS:HB2	2:F:379:LYS:NZ	2.31	0.45
1:G:250:VAL:HA	1:G:356:VAL:O	2.16	0.45
1:G:475:LYS:CE	11:G:3293:HOH:O	2.64	0.45
1:G:726:GLU:HG3	1:G:727:ILE:N	2.30	0.45
2:H:208:MET:SD	2:H:355:GLU:HA	2.56	0.45
2:H:313:GLY:HA3	11:H:2933:HOH:O	2.15	0.45
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.45
1:A:32:GLN:OE1	1:A:320:ALA:HB3	2.16	0.45
1:E:400:ARG:HD3	11:E:4438:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:679:GLN:O	1:E:683:GLU:HB2	2.16	0.45
1:G:294:ARG:NH1	5:G:4083:CL:CL	2.86	0.45
1:C:220:VAL:C	1:C:221:VAL:HG23	2.42	0.45
1:C:715:ARG:HB2	1:C:751:LEU:HB2	1.98	0.45
1:C:805:ILE:CD1	1:C:837:VAL:CG2	2.94	0.45
1:C:975:HIS:HE2	1:E:992:ASN:HD21	1.63	0.45
2:D:298:LYS:O	2:D:329:HIS:HA	2.17	0.45
2:F:169:SER:HA	2:F:216:LEU:O	2.16	0.45
1:G:540:THR:CG2	1:G:541:ALA:N	2.78	0.45
1:G:559:ARG:HG3	1:G:559:ARG:HH11	1.81	0.45
1:G:833:LYS:O	1:G:836:GLU:HB2	2.15	0.45
1:A:1:MET:HB2	1:A:224:LYS:HZ2	1.81	0.45
1:A:384:VAL:HG22	1:A:385:MET:N	2.32	0.45
1:E:953:ASP:O	1:E:955:GLU:N	2.50	0.45
1:E:956[B]:ARG:HB3	1:E:1044:LEU:HD21	1.96	0.45
2:F:46:PRO:O	2:F:242:PRO:HG3	2.16	0.45
1:A:82:ARG:HG3	1:A:82:ARG:HH11	1.82	0.45
1:A:671:ARG:HG2	1:A:677:ARG:NH1	2.32	0.45
2:B:142:LEU:O	2:B:145:GLU:HB3	2.17	0.45
1:C:86:VAL:HG13	1:C:86:VAL:O	2.15	0.45
1:C:186:GLU:HB2	11:C:4608:HOH:O	2.16	0.45
1:C:698:ILE:N	1:C:698:ILE:CD1	2.79	0.45
2:D:39:TYR:CZ	2:D:61:GLY:HA2	2.51	0.45
2:D:298:LYS:HE2	2:D:303:ASN:OD1	2.16	0.45
1:E:669:ILE:HA	1:E:844:PRO:HG2	1.98	0.45
2:H:350:PHE:HD2	2:H:354:PRO:HD3	1.81	0.45
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.69	0.45
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.82	0.45
1:A:633:GLU:O	1:A:634:LYS:HB2	2.17	0.45
2:F:23:THR:HG23	2:F:134:ALA:O	2.16	0.45
1:G:40:GLU:HG2	1:G:325:LYS:HE2	1.98	0.45
1:G:475:LYS:HE3	11:G:3293:HOH:O	2.15	0.45
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.52	0.45
2:B:324:ASN:N	2:B:324:ASN:ND2	2.39	0.45
1:E:157:ALA:HA	11:E:4288:HOH:O	2.16	0.45
2:F:53:VAL:O	2:F:80:LEU:HD12	2.16	0.45
2:F:270:LEU:HB2	9:F:4056:GLN:HG2	1.98	0.45
1:A:250:VAL:HA	1:A:356:VAL:O	2.17	0.45
1:A:901:PRO:C	1:A:903:VAL:H	2.25	0.45
2:B:57:TYR:CE1	2:B:58:PRO:HD2	2.52	0.45
2:B:232:ASN:N	2:B:233:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:ALA:HB3	11:D:1800:HOH:O	2.17	0.45
1:E:167:ILE:N	1:E:167:ILE:CD1	2.80	0.45
1:G:128:ASP:CG	1:G:131:ARG:HG3	2.42	0.45
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.98	0.45
1:A:38[A]:ARG:HH11	1:A:38[A]:ARG:CG	2.17	0.45
1:A:998:ARG:CG	1:A:999:PRO:HA	2.46	0.45
2:B:321:LEU:HD21	2:B:337:LEU:HD21	1.99	0.45
2:B:367:PHE:O	2:B:370:PHE:HB3	2.17	0.45
1:C:456:THR:O	1:C:457:ASN:HB2	2.16	0.45
1:C:901:PRO:C	1:C:903:VAL:H	2.25	0.45
2:D:2:ILE:HD12	2:D:3:LYS:N	2.32	0.45
2:D:2:ILE:HD12	2:D:3:LYS:H	1.81	0.45
1:E:704:LYS:O	1:E:707:GLU:HB2	2.17	0.45
1:E:995:HIS:CD2	1:E:995:HIS:H	2.33	0.45
1:G:301:ASN:HA	1:G:302:PRO:HD3	1.87	0.45
1:G:820:LEU:O	1:G:821:GLN:HB2	2.17	0.45
2:H:275:LEU:HD12	2:H:275:LEU:O	2.17	0.45
1:A:509:ARG:O	1:A:512:GLU:HB2	2.16	0.44
1:C:99:ALA:HB1	1:C:115:MET:HE2	1.99	0.44
1:C:213:TRP:HH2	1:C:294:ARG:HD3	1.82	0.44
1:C:325:LYS:O	1:C:330:TYR:HB2	2.16	0.44
1:E:1:MET:HB2	1:E:224:LYS:HZ1	1.81	0.44
1:E:215:GLU:OE1	7:E:4045:ADP:O3'	2.31	0.44
2:F:185:LYS:HD2	2:F:190:LEU:HD21	1.99	0.44
1:G:473[B]:GLU:OE1	1:G:501:ARG:NH2	2.43	0.44
1:G:698:ILE:H	1:G:698:ILE:CD1	2.29	0.44
2:H:240:ASN:HB2	9:H:4079:GLN:OE1	2.16	0.44
1:E:176:GLY:N	7:E:4045:ADP:O2B	2.43	0.44
1:E:503:ALA:HB1	1:E:508:VAL:O	2.18	0.44
2:F:5:ALA:HB2	2:F:19:ALA:HB2	2.00	0.44
2:F:218:ILE:N	2:F:218:ILE:CD1	2.79	0.44
2:H:253:THR:O	2:H:256:GLN:HB2	2.17	0.44
2:B:344:ASP:OD2	2:B:344:ASP:N	2.39	0.44
7:C:4029:ADP:H5'2	11:C:4571:HOH:O	2.17	0.44
2:D:327:VAL:HG23	11:D:1624:HOH:O	2.16	0.44
1:E:805:ILE:CD1	1:E:837:VAL:CG2	2.95	0.44
1:G:79:GLU:CG	1:G:111:PHE:CZ	3.00	0.44
1:G:87:LEU:HD12	1:G:87:LEU:HA	1.66	0.44
1:G:254:GLN:NE2	2:H:57:TYR:OH	2.50	0.44
1:G:632:ILE:HG13	1:G:633:GLU:N	2.32	0.44
1:G:693:ALA:HB3	1:G:708:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:882:GLU:HB3	11:G:3372:HOH:O	2.16	0.44
2:H:196:ALA:HA	2:H:237:PHE:O	2.17	0.44
1:A:730:ASP:O	1:A:733:ASP:HB2	2.18	0.44
1:A:1021:ARG:HH11	1:A:1021:ARG:HG3	1.82	0.44
2:B:363:ALA:C	2:B:365:PRO:HD2	2.43	0.44
1:C:948:SER:O	1:C:1015:ASN:HA	2.17	0.44
1:C:994:VAL:HG23	11:C:4748:HOH:O	2.17	0.44
1:E:157:ALA:O	1:E:160:ALA:HB3	2.18	0.44
1:E:384:VAL:HG22	1:E:385:MET:N	2.32	0.44
1:E:417:ASP:OD2	1:E:418:PRO:HD2	2.16	0.44
1:E:750:VAL:O	1:E:750:VAL:HG12	2.17	0.44
1:G:76:LYS:HD2	1:G:76:LYS:HA	1.71	0.44
1:G:150:HIS:HD2	1:G:203:GLU:HB2	1.82	0.44
1:G:683:GLU:OE2	1:G:683:GLU:HA	2.15	0.44
1:C:559:ARG:HG3	1:C:559:ARG:NH1	2.31	0.44
1:C:772:MET:HE1	1:C:880:THR:O	2.18	0.44
1:C:998:ARG:CB	1:C:999:PRO:HA	2.46	0.44
2:D:150:PHE:CD2	2:D:151:PRO:HD2	2.53	0.44
2:D:226:GLU:O	2:D:230:LYS:HG3	2.17	0.44
2:D:286:MET:HE2	2:D:315:ALA:CB	2.37	0.44
1:G:675:ARG:CD	1:G:675:ARG:H	2.28	0.44
1:A:220:VAL:O	1:A:281:GLY:HA2	2.17	0.44
1:E:283:ASN:HB2	11:E:4666:HOH:O	2.17	0.44
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.43	0.44
1:G:784:GLN:NE2	1:G:784:GLN:N	2.40	0.44
1:A:129:ARG:HB3	1:A:205:LEU:HD22	1.99	0.44
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.98	0.44
2:B:102:LEU:HA	2:B:102:LEU:HD23	1.74	0.44
1:C:675:ARG:H	1:C:675:ARG:HD3	1.83	0.44
1:C:831:ALA:HB2	1:C:840:ILE:HD11	1.99	0.44
2:F:286:MET:HE1	2:F:312:HIS:CE1	2.53	0.44
1:G:654:LEU:HD22	1:G:659:VAL:HG21	1.98	0.44
1:G:726:GLU:HG3	1:G:727:ILE:H	1.83	0.44
2:H:374:ILE:O	2:H:377:TYR:HB3	2.18	0.44
1:A:675:ARG:HG3	1:A:751:LEU:HD21	1.98	0.44
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.82	0.44
1:C:998:ARG:HA	1:C:999:PRO:C	2.41	0.44
2:F:199:PHE:O	2:F:241:GLY:HA3	2.18	0.44
2:B:13:THR:HG22	2:B:15:PHE:CE2	2.52	0.44
2:B:218:ILE:N	2:B:218:ILE:CD1	2.80	0.44
1:C:158:VAL:HG11	1:C:206:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:666:PRO:O	1:C:669:ILE:HB	2.18	0.44
1:C:671:ARG:NH2	1:C:819:GLU:O	2.51	0.44
1:C:686:LYS:O	1:C:687:LEU:HD23	2.18	0.44
1:E:612:THR:O	1:E:612:THR:HG22	2.16	0.44
1:E:903:VAL:O	1:E:905:PRO:HD3	2.18	0.44
1:G:563:MET:HB3	1:G:638:VAL:HG22	1.99	0.44
1:G:946:LEU:HB3	1:G:1013:ILE:HG12	1.99	0.44
1:G:994:VAL:HG13	1:G:1000:HIS:CE1	2.53	0.44
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.48	0.43
2:B:199:PHE:O	2:B:241:GLY:HA3	2.18	0.43
2:B:265:VAL:O	2:B:347:ALA:HA	2.18	0.43
1:C:772:MET:SD	1:C:880:THR:HG22	2.57	0.43
1:C:775:ILE:HG13	1:C:810:ARG:HG2	2.00	0.43
1:E:57:ASP:HA	1:E:58:PRO:HD3	1.79	0.43
1:E:148:ILE:CG2	1:E:149:ALA:N	2.81	0.43
1:E:885:PRO:HA	1:E:886:PRO:HD3	1.81	0.43
2:F:373:LEU:HA	2:F:373:LEU:HD23	1.78	0.43
1:G:947:LEU:HD12	1:G:947:LEU:N	2.33	0.43
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.45	0.43
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.99	0.43
1:A:612:THR:O	1:A:612:THR:HG22	2.18	0.43
1:C:384:VAL:HB	1:C:569:PRO:HG3	1.99	0.43
1:E:713:VAL:O	1:E:713:VAL:HG12	2.17	0.43
1:E:761:GLU:C	1:E:762:VAL:HG23	2.43	0.43
1:E:808:VAL:HG13	1:E:811[B]:GLN:NE2	2.32	0.43
10:E:4058:NET:H31	10:E:4058:NET:H63	1.53	0.43
1:G:104:ARG:HB2	11:G:2906:HOH:O	2.18	0.43
1:G:308:SER:HB3	11:G:3571:HOH:O	2.17	0.43
1:G:1021:ARG:CG	1:G:1021:ARG:NH1	2.78	0.43
2:H:279:SER:O	2:H:322:PRO:HG3	2.18	0.43
2:H:321:LEU:HA	2:H:321:LEU:HD12	1.78	0.43
1:A:598:MET:HE2	1:A:598:MET:HB2	1.90	0.43
1:C:426:ARG:HD3	1:C:426:ARG:C	2.43	0.43
1:C:920:VAL:O	1:C:930:LYS:HD3	2.18	0.43
1:E:335:LEU:C	1:E:336:MET:HE2	2.43	0.43
1:E:385:MET:HG2	1:E:386:ALA:N	2.32	0.43
1:G:710:TYR:HA	1:G:711:PRO:C	2.42	0.43
1:G:734:LEU:CD1	1:G:738:PHE:CD2	3.02	0.43
1:G:1001:ILE:HD13	1:G:1002:GLN:N	2.32	0.43
2:H:5:ALA:HB2	2:H:19:ALA:HB2	1.99	0.43
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:ASP:OD2	1:C:827:ASN:HB2	2.18	0.43
1:C:1013:ILE:O	1:C:1040:TYR:HA	2.19	0.43
1:E:659:VAL:HG13	1:E:660:PRO:HD2	2.00	0.43
1:A:479:VAL:CG2	1:A:483:GLY:HA3	2.49	0.43
1:A:828:VAL:CG1	1:A:839:LEU:HD11	2.49	0.43
1:E:1:MET:CB	1:E:224:LYS:NZ	2.76	0.43
2:F:205:ILE:HG12	2:F:355:GLU:HG3	2.00	0.43
1:G:358:LYS:HG2	1:G:359:ILE:N	2.31	0.43
1:G:456:THR:O	1:G:457:ASN:HB2	2.18	0.43
1:G:965:LEU:HD23	1:G:965:LEU:HA	1.87	0.43
2:B:255:ILE:HA	2:B:258:PHE:HD2	1.84	0.43
1:C:895:LEU:HA	1:C:896:PRO:HD3	1.83	0.43
1:C:956:ARG:HB3	1:C:1044:LEU:HD21	1.99	0.43
1:C:1063:ILE:CD1	1:C:1068:MET:CG	2.93	0.43
1:E:472:LEU:O	1:E:476:VAL:HG23	2.19	0.43
2:F:163:THR:OG1	2:F:164:THR:N	2.50	0.43
1:G:24:CYS:HB2	1:G:604:GLU:HB3	2.00	0.43
1:G:385:MET:HG3	1:G:386:ALA:N	2.34	0.43
2:H:17:GLY:HA3	2:H:110:ILE:HD11	2.01	0.43
1:A:671:ARG:CG	1:A:677:ARG:NH1	2.81	0.43
1:A:793:ALA:HA	1:A:891:LYS:O	2.19	0.43
2:B:324:ASN:HA	2:B:343:THR:OG1	2.18	0.43
2:B:350:PHE:CB	2:B:366:LEU:HD22	2.47	0.43
1:C:1061:LYS:HD3	11:C:4585:HOH:O	2.18	0.43
2:D:376:GLN:HA	2:D:379:LYS:NZ	2.33	0.43
1:E:735:ARG:O	1:E:738:PHE:N	2.51	0.43
1:G:509:ARG:HB2	1:G:509:ARG:NH1	2.32	0.43
1:A:38[B]:ARG:NH1	1:A:38[B]:ARG:CG	2.80	0.43
1:A:682:VAL:HG11	1:A:689:GLN:NE2	2.32	0.43
1:A:954:LYS:HB3	1:A:980:VAL:HG11	2.01	0.43
2:B:249:ASP:HA	2:B:252:ILE:HD12	2.00	0.43
2:B:269:SER:OG	9:B:4012:GLN:HG2	2.18	0.43
1:E:579:ASP:OD1	1:E:605:THR:HB	2.19	0.43
2:F:272:HIS:HB2	2:F:349:SER:HB2	2.01	0.43
2:F:313:GLY:H	9:F:4056:GLN:C	2.27	0.43
1:G:339:ILE:HD11	1:G:531:THR:HG23	2.00	0.43
1:G:588:ALA:O	1:G:591:GLU:HB3	2.19	0.43
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.48	0.43
1:G:1017:THR:HG22	1:G:1023:ILE:HG13	1.99	0.43
1:G:1021:ARG:O	1:G:1025:ASP:OD2	2.36	0.43
1:A:951:GLU:C	1:A:953:ASP:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ILE:HD12	1:C:167:ILE:N	2.33	0.43
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	1.99	0.43
1:E:765:ASP:O	1:E:776:GLY:N	2.51	0.43
7:E:4051:ADP:H5'2	11:E:4614:HOH:O	2.18	0.43
1:G:339:ILE:HD12	1:G:529:VAL:O	2.19	0.43
1:G:905:PRO:HG2	1:G:1030:ARG:HB3	2.00	0.43
1:G:944:ARG:NH1	1:G:972:ASP:OD1	2.52	0.43
2:H:28:GLY:HA2	2:H:150:PHE:CE2	2.54	0.43
2:H:299:ASP:CG	2:H:302:LYS:HD3	2.43	0.43
2:D:259:LEU:HD13	2:D:342:ARG:HH12	1.82	0.43
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.54	0.43
2:F:102:LEU:HD23	2:F:102:LEU:HA	1.84	0.43
1:G:370:ALA:HB2	1:G:900:PHE:HB3	2.00	0.43
1:G:695:VAL:HG11	1:G:701:ALA:N	2.34	0.43
1:G:733:ASP:HA	1:G:736:ARG:HH11	1.83	0.43
2:H:66:ASN:HB3	2:H:93:ARG:O	2.18	0.43
2:H:334:ASP:OD2	2:H:336:THR:HG23	2.19	0.43
1:A:267:ALA:O	1:A:271:VAL:HG23	2.19	0.42
1:A:738:PHE:O	1:A:741:ALA:HB3	2.19	0.42
2:D:33:ASN:HA	2:D:291:HIS:O	2.18	0.42
2:D:178:THR:HG22	2:D:179:GLY:N	2.32	0.42
1:E:456:THR:O	1:E:457:ASN:HB2	2.19	0.42
2:H:209:LEU:HA	2:H:209:LEU:HD23	1.79	0.42
1:C:550:GLU:CD	2:D:120:ARG:HH21	2.26	0.42
1:E:569:PRO:O	1:E:571:ARG:HD2	2.19	0.42
1:E:854:SER:HA	1:E:859:VAL:O	2.19	0.42
2:F:86:PRO:HA	11:F:2685:HOH:O	2.19	0.42
2:B:208:MET:O	2:B:211:ASP:HB2	2.19	0.42
1:C:677:ARG:O	1:C:680:HIS:HB2	2.19	0.42
1:C:778:ILE:HD11	1:C:810:ARG:HG3	2.02	0.42
1:E:548:GLU:HG2	2:F:114:ASP:HB2	2.01	0.42
1:E:1070:ALA:HB3	11:E:4646:HOH:O	2.19	0.42
2:H:190:LEU:HA	2:H:191:PRO:HD3	1.93	0.42
2:H:373:LEU:HD23	2:H:373:LEU:HA	1.74	0.42
1:A:259:LYS:HD3	2:B:175:TRP:CZ3	2.55	0.42
1:C:1:MET:N	1:C:224:LYS:HE3	2.34	0.42
1:C:221:VAL:O	1:C:228:CYS:HA	2.19	0.42
1:C:493:LYS:HD2	1:C:493:LYS:HA	1.86	0.42
2:D:333:PHE:HD1	2:D:333:PHE:HA	1.77	0.42
1:E:534:ALA:HB1	2:F:120:ARG:HG2	2.01	0.42
1:E:808:VAL:CA	1:E:811[B]:GLN:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:196:ALA:HB3	2:F:218:ILE:HD12	2.01	0.42
1:G:267:ALA:O	1:G:271:VAL:HG23	2.19	0.42
1:G:915:GLY:HA2	11:G:2979:HOH:O	2.18	0.42
2:H:367:PHE:O	2:H:370:PHE:HB3	2.19	0.42
1:A:35:LYS:HD2	11:A:4141:HOH:O	2.19	0.42
1:A:868:VAL:HA	1:A:872:LYS:O	2.19	0.42
2:B:87:LEU:HD12	2:B:87:LEU:HA	1.72	0.42
2:D:208:MET:O	2:D:211:ASP:HB2	2.20	0.42
1:E:714:VAL:HG13	1:E:752:LEU:HD12	2.00	0.42
1:E:891:LYS:HG2	1:E:892:GLU:N	2.33	0.42
1:E:940:LYS:HG3	1:E:1011:THR:HB	2.01	0.42
2:F:342:ARG:HD2	2:F:342:ARG:HA	1.92	0.42
1:G:361:ARG:O	1:G:380:SER:HB2	2.19	0.42
1:G:402:LEU:O	1:G:403:GLU:HB2	2.19	0.42
1:G:482:THR:HG22	1:G:483:GLY:N	2.34	0.42
1:G:735:ARG:O	1:G:738:PHE:HB2	2.19	0.42
1:G:1032:SER:O	1:G:1036:TYR:HD1	2.02	0.42
1:A:775:ILE:HD13	1:A:775:ILE:HA	1.86	0.42
1:C:730:ASP:H	1:C:733:ASP:HB2	1.84	0.42
2:D:325:LEU:HD23	2:D:325:LEU:HA	1.82	0.42
1:E:493:LYS:HD2	1:E:493:LYS:HA	1.78	0.42
1:E:755:PHE:CE1	7:E:4051:ADP:C2	3.08	0.42
2:F:66:ASN:OD1	2:F:68:ALA:HB3	2.19	0.42
1:G:170:PRO:HA	1:G:204:LEU:HD23	2.01	0.42
1:G:185:ARG:O	1:G:188:PHE:HB3	2.19	0.42
1:G:329:GLY:CA	11:G:2959:HOH:O	2.68	0.42
1:G:828:VAL:CG1	1:G:839:LEU:HD11	2.50	0.42
1:G:905:PRO:HB2	1:G:1040:TYR:HH	1.82	0.42
1:G:965:LEU:HG	1:G:971:LEU:HD11	2.02	0.42
1:A:548:GLU:OE1	2:B:83:ARG:HD3	2.19	0.42
1:A:981:LEU:HD12	1:A:988:PRO:HG3	2.02	0.42
1:E:217:GLU:HG2	1:E:285:GLN:HG2	2.01	0.42
1:E:403:GLU:CD	1:E:646:THR:HG23	2.44	0.42
1:E:426:ARG:C	1:E:426:ARG:HD3	2.44	0.42
2:F:91:ASN:OD1	2:F:93:ARG:HB2	2.19	0.42
1:G:975:HIS:CD2	1:G:975:HIS:C	2.96	0.42
1:A:336[B]:MET:HB3	1:A:342:GLY:HA2	2.02	0.42
1:C:257:THR:HG23	1:C:260:GLU:OE2	2.19	0.42
1:C:840:ILE:O	1:C:841:GLU:HB3	2.20	0.42
1:C:892:GLU:OE1	8:C:4033:ORN:NE	2.52	0.42
2:D:212:ARG:CG	2:D:212:ARG:NH1	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:ALA:HA	1:E:114:THR:O	2.20	0.42
2:F:46:PRO:HA	2:F:76:HIS:CB	2.50	0.42
1:G:987:ASN:HA	1:G:988:PRO:HD2	1.91	0.42
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.68	0.42
2:H:376:GLN:O	2:H:376:GLN:HG3	2.20	0.42
1:A:1021:ARG:CG	1:A:1021:ARG:NH1	2.80	0.42
1:C:563:MET:HE3	1:C:563:MET:HB2	1.75	0.42
1:E:10:ILE:HD13	1:E:37:LEU:HD13	2.02	0.42
1:E:248:ILE:HA	1:E:358:LYS:O	2.20	0.42
1:E:528:ARG:HG2	1:E:543:MET:HG2	2.01	0.42
1:A:528:ARG:HG2	1:A:543:MET:HG2	2.02	0.42
1:C:40:GLU:CG	1:C:325:LYS:HE2	2.49	0.42
1:C:358:LYS:HG2	1:C:359:ILE:N	2.32	0.42
1:C:1064:SER:OG	1:C:1067:GLU:HG3	2.20	0.42
1:E:514:ARG:HD3	11:E:4483:HOH:O	2.20	0.42
1:E:1001:ILE:CD1	1:E:1002:GLN:N	2.79	0.42
1:G:48:ASN:O	1:G:66:ILE:HA	2.20	0.42
2:H:7:LEU:HD23	2:H:15:PHE:CD2	2.54	0.42
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.20	0.41
1:A:191:ILE:HD13	1:A:191:ILE:HG21	1.91	0.41
1:A:702:VAL:O	1:A:706:LYS:HD3	2.20	0.41
1:C:24:CYS:HB2	1:C:604:GLU:HB3	2.02	0.41
1:C:1064:SER:O	1:C:1068:MET:HG3	2.20	0.41
1:E:882:GLU:HB3	11:E:4757:HOH:O	2.19	0.41
2:F:228:VAL:HG11	2:F:258:PHE:CE1	2.55	0.41
1:G:240:MET:HE3	7:G:4068:ADP:C4	2.54	0.41
1:G:752:LEU:HD12	1:G:752:LEU:HA	1.72	0.41
2:H:150:PHE:CE1	2:H:152:GLY:HA2	2.55	0.41
1:A:659:VAL:HG12	1:A:660:PRO:N	2.34	0.41
1:A:954:LYS:C	1:A:957:VAL:HG12	2.45	0.41
2:D:364:ALA:N	2:D:365:PRO:CD	2.83	0.41
1:E:765:ASP:OD2	1:E:827:ASN:HB2	2.20	0.41
2:F:325:LEU:HD23	2:F:325:LEU:HA	1.83	0.41
1:G:755:PHE:CD1	7:G:4074:ADP:C2	3.08	0.41
1:A:734:LEU:CD1	1:A:738:PHE:CD2	3.03	0.41
1:A:905:PRO:HB2	1:A:1040:TYR:HH	1.83	0.41
2:B:75:VAL:HG11	2:B:107:ILE:HG13	2.02	0.41
1:C:662:ILE:HD13	1:C:662:ILE:HG21	1.84	0.41
1:C:967:GLN:HG3	1:C:1054:LEU:CD1	2.45	0.41
2:D:163:THR:OG1	2:D:164:THR:N	2.54	0.41
1:E:489:LEU:HD12	1:E:489:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:734:LEU:O	1:G:737:TYR:HB3	2.20	0.41
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.36	0.41
1:G:981:LEU:HD23	1:G:981:LEU:HA	1.87	0.41
2:H:197:TYR:HB3	2:H:199:PHE:CZ	2.55	0.41
1:A:225:ASN:ND2	1:A:331:THR:HG21	2.36	0.41
1:A:654:LEU:HD22	1:A:659:VAL:HG21	2.02	0.41
2:B:64:GLY:C	2:B:65:THR:HG23	2.45	0.41
2:B:240:ASN:HB2	9:B:4012:GLN:OE1	2.21	0.41
1:C:453:PHE:CD1	1:C:453:PHE:C	2.97	0.41
1:C:994:VAL:HG23	1:C:1001:ILE:HD11	2.01	0.41
2:D:172:GLN:O	2:D:207:ARG:HA	2.21	0.41
2:D:190:LEU:HB2	2:D:215:ARG:HB3	2.02	0.41
2:D:229:LEU:HD23	2:D:229:LEU:HA	1.82	0.41
1:E:726:GLU:HG3	1:E:727:ILE:H	1.84	0.41
1:G:726:GLU:OE1	1:G:1020:ARG:HD3	2.20	0.41
2:H:201:ALA:HB2	2:H:239:SER:CB	2.51	0.41
1:A:654:LEU:O	1:A:659:VAL:HG23	2.20	0.41
1:A:698:ILE:HG22	1:A:699:GLU:N	2.36	0.41
1:C:4:ARG:NH1	11:C:4132:HOH:O	2.54	0.41
1:C:34:CYS:SG	1:C:46:LEU:HD22	2.60	0.41
1:C:278:GLU:C	1:C:279:THR:HG23	2.45	0.41
1:C:525:VAL:HG12	1:C:551:CYS:HB2	2.03	0.41
1:C:571:ARG:HD3	1:C:571:ARG:N	2.35	0.41
1:C:682:VAL:HG13	1:C:687:LEU:HB2	2.02	0.41
2:D:171:THR:O	2:D:185:LYS:N	2.47	0.41
1:E:942:HIS:CD2	1:E:942:HIS:C	2.96	0.41
1:G:516:LEU:HA	1:G:516:LEU:HD12	1.77	0.41
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.35	0.41
2:H:181:LEU:HA	2:H:182:PRO:HD3	1.91	0.41
1:A:353:ASP:N	1:A:353:ASP:OD2	2.51	0.41
1:C:964:LEU:O	1:C:969:PHE:HB2	2.20	0.41
2:D:369:HIS:O	2:D:372:GLU:HB2	2.20	0.41
1:E:58:PRO:HD2	1:E:59:GLU:OE2	2.20	0.41
1:E:78:ILE:HG23	1:E:83:PRO:HD2	2.02	0.41
1:E:532:CYS:O	1:E:533:ALA:HB3	2.21	0.41
1:E:1021:ARG:CG	1:E:1021:ARG:NH1	2.80	0.41
2:F:286:MET:CE	2:F:312:HIS:ND1	2.83	0.41
2:F:374:ILE:O	2:F:374:ILE:HG22	2.19	0.41
1:G:479:VAL:HG23	1:G:480:GLY:O	2.20	0.41
1:G:622:THR:OG1	1:G:625:ASP:OD1	2.27	0.41
2:H:95:THR:HG21	11:H:3459:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:376:GLN:HG2	2:H:377:TYR:N	2.35	0.41
1:C:85:ALA:HA	1:C:114:THR:O	2.20	0.41
2:D:188:ASP:OD2	2:D:188:ASP:N	2.51	0.41
1:E:615:ARG:NE	1:E:633:GLU:OE1	2.44	0.41
1:E:670:ASP:CB	1:E:677:ARG:HH21	2.24	0.41
10:E:4058:NET:H42	10:E:4058:NET:H22	2.03	0.41
2:F:212:ARG:HG3	2:F:212:ARG:HH11	1.86	0.41
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.20	0.41
1:G:469:LEU:O	1:G:473[B]:GLU:HB2	2.20	0.41
2:H:354:PRO:HB2	2:H:367:PHE:CE2	2.56	0.41
1:C:57:ASP:HB2	1:C:60:MET:HG2	2.03	0.41
1:C:886:PRO:HD2	1:C:887:TYR:CD1	2.56	0.41
1:C:932:GLN:HG2	1:C:937:SER:HB3	2.02	0.41
2:D:43:LEU:HB3	2:D:75:VAL:HG13	2.03	0.41
2:D:259:LEU:HD23	2:D:259:LEU:HA	1.87	0.41
2:F:228:VAL:HG11	2:F:258:PHE:CZ	2.55	0.41
1:G:895:LEU:HA	1:G:896:PRO:HD3	1.98	0.41
2:H:350:PHE:HB2	2:H:366:LEU:HD22	2.03	0.41
1:A:4:ARG:NE	1:A:7:ILE:HD12	2.36	0.41
1:A:947:LEU:HA	1:A:1014:ILE:HG23	2.03	0.41
1:A:1048:PHE:O	1:A:1051:ALA:HB3	2.21	0.41
2:B:285:LYS:HG3	2:B:314:PHE:CZ	2.54	0.41
1:C:43:ARG:NH2	1:C:81:GLU:OE2	2.50	0.41
2:D:371:ILE:O	2:D:374:ILE:HB	2.20	0.41
1:E:411:PRO:HD2	11:E:4697:HOH:O	2.20	0.41
1:E:832:VAL:HA	1:E:836:GLU:O	2.21	0.41
2:F:29:GLU:HB2	2:F:153:LEU:HD22	2.01	0.41
2:F:142:LEU:HA	2:F:142:LEU:HD12	1.78	0.41
2:F:205:ILE:HD13	2:F:268:ILE:HD12	2.03	0.41
2:F:354:PRO:HB2	2:F:367:PHE:CE2	2.55	0.41
1:G:861:LEU:HA	1:G:861:LEU:HD23	1.75	0.41
1:A:294:ARG:HD2	5:A:4016:CL:CL	2.58	0.41
1:A:930:LYS:HG3	1:A:1058:ALA:CB	2.51	0.41
1:A:930:LYS:HG3	1:A:1058:ALA:HB1	2.03	0.41
1:A:1012:TYR:C	1:A:1013:ILE:HG13	2.45	0.41
2:D:364:ALA:C	2:D:366:LEU:N	2.78	0.41
2:F:306:MET:HE1	2:F:366:LEU:HD11	2.03	0.41
2:F:322:PRO:CB	2:F:324:ASN:HD21	2.31	0.41
2:F:327:VAL:HG13	2:F:337:LEU:CD1	2.51	0.41
1:G:734:LEU:HD12	1:G:738:PHE:CD2	2.55	0.41
1:G:780:GLU:OE2	1:G:798:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:GLY:HA3	2:H:358:PRO:CB	2.51	0.41
2:H:323:ALA:C	2:H:325:LEU:H	2.28	0.41
1:A:713:VAL:HG23	1:A:755:PHE:HB2	2.03	0.40
1:A:957:VAL:HG13	1:A:958:VAL:N	2.36	0.40
1:C:78:ILE:O	1:C:82:ARG:N	2.34	0.40
1:C:516:LEU:HD12	1:C:516:LEU:HA	1.59	0.40
1:E:1:MET:CB	1:E:224:LYS:HZ1	2.32	0.40
1:E:148:ILE:HG22	1:E:149:ALA:N	2.36	0.40
1:E:1001:ILE:HD13	1:E:1029:ILE:HG13	2.03	0.40
2:F:62:ASN:OD1	2:F:86:PRO:HG3	2.22	0.40
1:G:250:VAL:HG12	1:G:357:THR:HG23	2.03	0.40
1:G:620:PRO:HB2	1:G:622:THR:HG23	2.02	0.40
1:G:656:ALA:C	1:G:658:GLY:H	2.29	0.40
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.37	0.40
1:G:982:GLY:C	1:G:984:ALA:N	2.79	0.40
1:A:126:ALA:HB3	1:A:302:PRO:HG3	2.02	0.40
1:C:475:LYS:O	1:C:479:VAL:HG13	2.20	0.40
1:C:805:ILE:HD11	1:C:837:VAL:HG23	2.03	0.40
2:F:286:MET:CE	2:F:312:HIS:O	2.69	0.40
1:G:362:PHE:CD2	1:G:433:ALA:HB1	2.56	0.40
1:G:472:LEU:O	1:G:476:VAL:HG23	2.21	0.40
1:G:788:HIS:ND1	1:G:790:GLY:N	2.60	0.40
2:H:156:MET:HE2	2:H:156:MET:HB2	1.51	0.40
2:H:250:TYR:H	2:H:250:TYR:HD2	1.63	0.40
1:A:1006:LYS:HB3	1:A:1006:LYS:HE3	2.00	0.40
2:B:34:THR:HA	2:B:56:THR:OG1	2.22	0.40
1:C:6:ASP:N	1:C:6:ASP:OD2	2.49	0.40
1:C:873:SER:O	1:C:877:GLN:HG3	2.21	0.40
2:D:294:ASN:OD1	2:D:294:ASN:N	2.54	0.40
1:G:1031:ARG:HE	1:G:1031:ARG:HB3	1.56	0.40
2:H:236:ILE:HD12	2:H:263:ILE:CG2	2.51	0.40
2:H:296:PRO:HB2	2:H:332:LEU:HB2	2.02	0.40
1:A:732:ALA:O	1:A:736:ARG:HB2	2.21	0.40
1:C:561:LYS:HE2	11:C:4472:HOH:O	2.21	0.40
1:C:678:PHE:C	1:C:680:HIS:N	2.79	0.40
1:C:701:ALA:O	1:C:705:ALA:N	2.49	0.40
1:E:484:LEU:HD23	1:E:484:LEU:HA	1.96	0.40
1:E:713:VAL:HG23	1:E:755:PHE:HB2	2.04	0.40
1:E:950:ARG:HH11	1:E:950:ARG:HD2	1.68	0.40
2:F:246:ALA:N	2:F:247:PRO:HD2	2.36	0.40
2:F:274:LEU:HD23	2:F:274:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:PHE:O	2:H:291:HIS:HB2	2.20	0.40
1:A:165:PRO:HA	1:A:182:ALA:O	2.21	0.40
1:A:345:PRO:HG3	2:B:332:LEU:HB3	2.03	0.40
1:A:1004:ARG:HD2	1:A:1010:TYR:OH	2.20	0.40
1:C:630:VAL:HG11	1:C:659:VAL:HG22	2.04	0.40
1:C:809:MET:O	1:C:813:VAL:HG23	2.21	0.40
2:D:139:ASP:OD2	2:D:142:LEU:HB2	2.21	0.40
2:D:345:LYS:HB3	2:D:346:PRO:HD2	2.04	0.40
1:E:761:GLU:HB3	1:E:781:HIS:ND1	2.36	0.40
2:F:181:LEU:HA	2:F:182:PRO:HD3	1.98	0.40
2:F:299:ASP:OD1	2:F:302:LYS:HD2	2.22	0.40
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.56	0.40
1:G:712:LEU:O	1:G:727:ILE:HA	2.20	0.40
1:G:839:LEU:HD12	1:G:839:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

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	1058/1073 (99%)	1004 (95%)	51 (5%)	3 (0%)	36	36
1	C	1059/1073 (99%)	1005 (95%)	50 (5%)	4 (0%)	30	28
1	E	1062/1073 (99%)	1004 (94%)	56 (5%)	2 (0%)	43	44
1	G	1056/1073 (98%)	991 (94%)	59 (6%)	6 (1%)	21	18
2	B	377/382 (99%)	362 (96%)	15 (4%)	0	100	100
2	D	377/382 (99%)	357 (95%)	18 (5%)	2 (0%)	24	22
2	F	377/382 (99%)	358 (95%)	19 (5%)	0	100	100
2	H	377/382 (99%)	353 (94%)	22 (6%)	2 (0%)	24	22
All	All	5743/5820 (99%)	5434 (95%)	290 (5%)	19 (0%)	36	36

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	ASP
1	E	954	LYS
1	G	558	ASP
1	G	873	SER
1	A	975	HIS
1	C	739	GLN
1	E	975	HIS
1	G	739	GLN
1	G	975	HIS
2	D	229	LEU
2	H	269	SER
2	D	127	ALA
1	C	951	GLU
1	G	2	PRO
1	G	788	HIS
1	A	698	ILE
1	C	2	PRO
2	H	243	GLY
1	C	698	ILE

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	871/878 (99%)	809 (93%)	62 (7%)	13	11
1	C	872/878 (99%)	802 (92%)	70 (8%)	11	8
1	E	875/878 (100%)	810 (93%)	65 (7%)	13	10
1	G	869/878 (99%)	780 (90%)	89 (10%)	7	4
2	B	308/310 (99%)	272 (88%)	36 (12%)	5	3
2	D	308/310 (99%)	281 (91%)	27 (9%)	9	7
2	F	308/310 (99%)	274 (89%)	34 (11%)	6	3
2	H	308/310 (99%)	280 (91%)	28 (9%)	9	6
All	All	4719/4752 (99%)	4308 (91%)	411 (9%)	9	7

All (411) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	8	LYS
1	A	38[A]	ARG
1	A	38[B]	ARG
1	A	46	LEU
1	A	49	SER
1	A	103	GLU
1	A	138	LYS
1	A	202	LYS
1	A	220	VAL
1	A	275	ILE
1	A	300	MET
1	A	312	SER
1	A	313	LYS
1	A	326	LEU
1	A	343	ARG
1	A	358	LYS
1	A	416	ASP
1	A	548	GLU
1	A	559	ARG
1	A	576	ILE
1	A	591	GLU
1	A	652[A]	ARG
1	A	652[B]	ARG
1	A	671	ARG
1	A	675	ARG
1	A	677	ARG
1	A	688	LYS
1	A	696	THR
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS
1	A	708	ILE
1	A	712	LEU
1	A	714	VAL
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	757	ASP
1	A	763	ASP
1	A	784	GLN
1	A	805	ILE

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Mol	Chain	Res	Type
1	A	815	LYS
1	A	835	ASN
1	A	855	LYS
1	A	880	THR
1	A	891	LYS
1	A	895	LEU
1	A	906	LEU
1	A	912	ARG
1	A	930	LYS
1	A	940	LYS
1	A	947	LEU
1	A	950	ARG
1	A	951	GLU
1	A	967	GLN
1	A	992	ASN
1	A	1006	LYS
1	A	1018	SER
1	A	1021	ARG
1	A	1072	ILE
1	A	1073	LYS
2	B	2	ILE
2	B	6	LEU
2	B	18	ARG
2	B	25	SER
2	B	35	SER
2	B	50	ARG
2	B	87	LEU
2	B	113	ILE
2	B	154	ASN
2	B	157	ASP
2	B	166	GLU
2	B	174	SER
2	B	183	GLU
2	B	186	LYS
2	B	215	ARG
2	B	218	ILE
2	B	219	VAL
2	B	222	GLN
2	B	238	LEU
2	B	239	SER
2	B	257	LYS
2	B	269	SER

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Mol	Chain	Res	Type
2	B	282	LYS
2	B	301	GLU
2	B	302	LYS
2	B	304	VAL
2	B	306	MET
2	B	321	LEU
2	B	324	ASN
2	B	326	ARG
2	B	332	LEU
2	B	333	PHE
2	B	357	SER
2	B	366	LEU
2	B	372	GLU
2	B	379	LYS
1	C	1	MET
1	C	5	THR
1	C	38	ARG
1	C	43	ARG
1	C	46	LEU
1	C	55	MET
1	C	82	ARG
1	C	103	GLU
1	C	174	MET
1	C	202	LYS
1	C	299	GLU
1	C	313	LYS
1	C	321	LYS
1	C	343	ARG
1	C	358	LYS
1	C	363	ASN
1	C	365	GLU
1	C	412	LYS
1	C	414	SER
1	C	422	THR
1	C	423	LYS
1	C	479	VAL
1	C	482	THR
1	C	509	ARG
1	C	515	LYS
1	C	559	ARG
1	C	571	ARG
1	C	591	GLU

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Mol	Chain	Res	Type
1	C	652	ARG
1	C	665	SER
1	C	671	ARG
1	C	675	ARG
1	C	683	GLU
1	C	696	THR
1	C	698	ILE
1	C	704	LYS
1	C	706	LYS
1	C	728	VAL
1	C	733	ASP
1	C	734	LEU
1	C	735	ARG
1	C	751	LEU
1	C	763	ASP
1	C	772	MET
1	C	784	GLN
1	C	792	SER
1	C	800	THR
1	C	805	ILE
1	C	812	GLN
1	C	849	THR
1	C	855	LYS
1	C	906	LEU
1	C	912	ARG
1	C	940	LYS
1	C	950	ARG
1	C	951	GLU
1	C	956	ARG
1	C	963	LYS
1	C	967	GLN
1	C	992	ASN
1	C	1000	HIS
1	C	1014	ILE
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1032	SER
1	C	1061	LYS
1	C	1063	ILE
1	C	1072	ILE
1	C	1073	LYS

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Mol	Chain	Res	Type
2	D	6	LEU
2	D	18	ARG
2	D	27	VAL
2	D	42	ILE
2	D	47	SER
2	D	50	ARG
2	D	87	LEU
2	D	125	LYS
2	D	166	GLU
2	D	174	SER
2	D	178	THR
2	D	183	GLU
2	D	186	LYS
2	D	218	ILE
2	D	222	GLN
2	D	257	LYS
2	D	261	THR
2	D	269	SER
2	D	282	LYS
2	D	301	GLU
2	D	324	ASN
2	D	326	ARG
2	D	332	LEU
2	D	333	PHE
2	D	366	LEU
2	D	372	GLU
2	D	379	LYS
1	E	4	ARG
1	E	5	THR
1	E	46	LEU
1	E	55	MET
1	E	103	GLU
1	E	153[A]	GLU
1	E	153[B]	GLU
1	E	174	MET
1	E	275	ILE
1	E	299	GLU
1	E	307	SER
1	E	321	LYS
1	E	343	ARG
1	E	358	LYS
1	E	363	ASN

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Mol	Chain	Res	Type
1	E	412	LYS
1	E	428	LEU
1	E	478[A]	GLU
1	E	478[B]	GLU
1	E	490	ARG
1	E	515	LYS
1	E	519	GLN
1	E	548	GLU
1	E	559	ARG
1	E	571	ARG
1	E	591	GLU
1	E	671	ARG
1	E	675	ARG
1	E	677	ARG
1	E	680	HIS
1	E	696	THR
1	E	698	ILE
1	E	700	MET
1	E	702	VAL
1	E	704	LYS
1	E	706	LYS
1	E	714	VAL
1	E	733	ASP
1	E	734	LEU
1	E	735	ARG
1	E	750	VAL
1	E	751	LEU
1	E	784	GLN
1	E	805	ILE
1	E	835	ASN
1	E	839	LEU
1	E	855	LYS
1	E	906	LEU
1	E	912[A]	ARG
1	E	912[B]	ARG
1	E	940	LYS
1	E	950	ARG
1	E	951	GLU
1	E	956[A]	ARG
1	E	956[B]	ARG
1	E	963	LYS
1	E	966	LYS

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Mol	Chain	Res	Type
1	E	993	LYS
1	E	998	ARG
1	E	1000	HIS
1	E	1020	ARG
1	E	1021	ARG
1	E	1061	LYS
1	E	1072	ILE
1	E	1073	LYS
2	F	6	LEU
2	F	18	ARG
2	F	25	SER
2	F	50	ARG
2	F	73	SER
2	F	87	LEU
2	F	106	ASN
2	F	153	LEU
2	F	166	GLU
2	F	169	SER
2	F	175	TRP
2	F	183	GLU
2	F	186	LYS
2	F	205	ILE
2	F	215	ARG
2	F	218	ILE
2	F	222	GLN
2	F	228	VAL
2	F	236	ILE
2	F	239	SER
2	F	255	ILE
2	F	257	LYS
2	F	261	THR
2	F	263	ILE
2	F	282	LYS
2	F	301	GLU
2	F	306	MET
2	F	321	LEU
2	F	324	ASN
2	F	332	LEU
2	F	366	LEU
2	F	372	GLU
2	F	376	GLN
2	F	379	LYS

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Mol	Chain	Res	Type
1	G	4	ARG
1	G	8	LYS
1	G	20	ILE
1	G	43	ARG
1	G	46	LEU
1	G	49	SER
1	G	55	MET
1	G	59	GLU
1	G	76	LYS
1	G	114	THR
1	G	145	ARG
1	G	174	MET
1	G	207	ASP
1	G	236	ASN
1	G	275	ILE
1	G	297	VAL
1	G	307	SER
1	G	313	LYS
1	G	321	LYS
1	G	326	LEU
1	G	343	ARG
1	G	363	ASN
1	G	385	MET
1	G	387	ILE
1	G	412	LYS
1	G	416	ASP
1	G	422	THR
1	G	428	LEU
1	G	479	VAL
1	G	482	THR
1	G	489	LEU
1	G	509	ARG
1	G	519	GLN
1	G	543	MET
1	G	548	GLU
1	G	558	ASP
1	G	559	ARG
1	G	571	ARG
1	G	591	GLU
1	G	652	ARG
1	G	665	SER
1	G	671	ARG

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Mol	Chain	Res	Type
1	G	675	ARG
1	G	682	VAL
1	G	683	GLU
1	G	688	LYS
1	G	704	LYS
1	G	706	LYS
1	G	712	LEU
1	G	714	VAL
1	G	733	ASP
1	G	734	LEU
1	G	735	ARG
1	G	751	LEU
1	G	752	LEU
1	G	763	ASP
1	G	772	MET
1	G	784	GLN
1	G	800	THR
1	G	805	ILE
1	G	815	LYS
1	G	845	ARG
1	G	849	THR
1	G	855	LYS
1	G	880	THR
1	G	881	LYS
1	G	884	ILE
1	G	906	LEU
1	G	912	ARG
1	G	940	LYS
1	G	949	VAL
1	G	950	ARG
1	G	956	ARG
1	G	963	LYS
1	G	966	LYS
1	G	967	GLN
1	G	983	GLU
1	G	1001	ILE
1	G	1006	LYS
1	G	1014	ILE
1	G	1020	ARG
1	G	1021	ARG
1	G	1026	SER
1	G	1030	ARG

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Mol	Chain	Res	Type
1	G	1031	ARG
1	G	1059	THR
1	G	1061	LYS
1	G	1063	ILE
1	G	1073	LYS
2	H	2	ILE
2	H	6	LEU
2	H	7	LEU
2	H	25	SER
2	H	47	SER
2	H	78	GLN
2	H	87	LEU
2	H	104	ARG
2	H	110	ILE
2	H	125	LYS
2	H	153	LEU
2	H	166	GLU
2	H	192	PHE
2	H	216	LEU
2	H	218	ILE
2	H	222	GLN
2	H	223	THR
2	H	257	LYS
2	H	263	ILE
2	H	306	MET
2	H	321	LEU
2	H	324	ASN
2	H	332	LEU
2	H	340	ILE
2	H	357	SER
2	H	366	LEU
2	H	376	GLN
2	H	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	689	GLN
1	A	784	GLN
1	A	803	GLN
1	A	814	GLN

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Mol	Chain	Res	Type
1	A	834	ASN
1	A	835	ASN
1	A	932	GLN
1	A	936	ASN
1	A	967	GLN
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1007	ASN
1	A	1015	ASN
1	A	1035	GLN
1	A	1055	ASN
1	A	1071	GLN
2	B	51	GLN
2	B	78	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	105	GLN
1	C	266	ASN
1	C	457	ASN
1	C	645	GLN
1	C	689	GLN
1	C	784	GLN
1	C	803	GLN
1	C	812	GLN
1	C	843	ASN
1	C	898	ASN
1	C	942	HIS
1	C	987	ASN
1	C	992	ASN
1	C	1000	HIS
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	74	GLN
2	D	222	GLN
2	D	324	ASN
2	D	351	GLN
1	E	105	GLN

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Mol	Chain	Res	Type
1	E	266	ASN
1	E	457	ASN
1	E	679	GLN
1	E	784	GLN
1	E	803	GLN
1	E	827	ASN
1	E	843	ASN
1	E	936	ASN
1	E	942	HIS
1	E	967	GLN
1	E	992	ASN
1	E	1000	HIS
1	E	1002	GLN
1	E	1007	ASN
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	51	GLN
2	F	78	GLN
2	F	106	ASN
2	F	204	ASN
2	F	222	GLN
2	F	324	ASN
2	F	351	GLN
1	G	105	GLN
1	G	266	ASN
1	G	457	ASN
1	G	523	HIS
1	G	784	GLN
1	G	803	GLN
1	G	834	ASN
1	G	932	GLN
1	G	936	ASN
1	G	942	HIS
1	G	992	ASN
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN
1	G	1071	GLN
2	H	51	GLN
2	H	78	GLN
2	H	324	ASN

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Mol	Chain	Res	Type
2	H	351	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 89 ligands modelled in this entry, 60 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	GLN	F	4056	-	8,9,9	1.49	2 (25%)	8,11,11	1.53	1 (12%)
9	GLN	H	4079	-	8,9,9	1.27	1 (12%)	8,11,11	1.26	0
9	GLN	A	4013	-	8,9,9	1.41	1 (12%)	8,11,11	1.08	0
7	ADP	C	4029	3,4	28,29,29	1.19	3 (10%)	43,45,45	1.02	3 (6%)
9	GLN	C	4035	-	8,9,9	1.27	1 (12%)	8,11,11	1.05	1 (12%)
8	ORN	G	4078	-	7,8,8	0.75	0	6,9,9	0.57	0
6	PO4	E	4050	3,4	4,4,4	2.47	3 (75%)	6,6,6	1.19	1 (16%)
7	ADP	G	4068	3	28,29,29	1.16	3 (10%)	43,45,45	1.21	5 (11%)
8	ORN	C	4033	-	7,8,8	1.17	1 (14%)	6,9,9	0.91	0
7	ADP	A	4007	3,4	28,29,29	1.36	2 (7%)	43,45,45	0.92	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	A	4000	3	28,29,29	1.46	4 (14%)	43,45,45	0.88	1 (2%)
9	GLN	E	4057	-	8,9,9	1.41	2 (25%)	8,11,11	1.34	1 (12%)
6	PO4	A	4006	3,4	4,4,4	2.45	2 (50%)	6,6,6	1.03	0
10	NET	E	4058	-	8,8,8	0.58	0	10,10,10	0.77	0
8	ORN	A	4011	-	7,8,8	1.11	0	6,9,9	1.39	0
7	ADP	E	4045	3	28,29,29	1.17	2 (7%)	43,45,45	0.94	3 (6%)
9	GLN	G	4080	-	8,9,9	1.35	1 (12%)	8,11,11	0.64	0
10	NET	A	4014	-	8,8,8	0.73	0	10,10,10	0.59	0
8	ORN	E	4055	-	7,8,8	1.03	0	6,9,9	0.65	0
7	ADP	E	4051	3,4	28,29,29	1.06	2 (7%)	43,45,45	0.89	1 (2%)
9	GLN	B	4012	-	8,9,9	1.16	1 (12%)	8,11,11	1.50	2 (25%)
9	GLN	D	4034	-	8,9,9	1.25	1 (12%)	8,11,11	2.18	3 (37%)
7	ADP	G	4074	3,4	28,29,29	1.33	4 (14%)	43,45,45	1.00	2 (4%)
6	PO4	G	4073	3,4	4,4,4	2.03	2 (50%)	6,6,6	1.06	0
10	NET	C	4036	-	8,8,8	0.57	0	10,10,10	0.49	0
6	PO4	E	4067	-	4,4,4	1.45	0	6,6,6	0.71	0
10	NET	G	4081	-	8,8,8	0.70	0	10,10,10	0.48	0
6	PO4	C	4028	3,4	4,4,4	2.98	3 (75%)	6,6,6	1.18	0
7	ADP	C	4023	3	28,29,29	1.36	3 (10%)	43,45,45	0.83	0

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
9	GLN	F	4056	-	-	2/9/9/9	-
9	GLN	H	4079	-	-	5/9/9/9	-
9	GLN	A	4013	-	-	4/9/9/9	-
7	ADP	C	4029	3,4	-	3/16/32/32	0/3/3/3
9	GLN	C	4035	-	-	2/9/9/9	-
8	ORN	G	4078	-	-	6/8/8/8	-
7	ADP	G	4068	3	-	1/16/32/32	0/3/3/3
8	ORN	C	4033	-	-	6/8/8/8	-
7	ADP	A	4007	3,4	-	4/16/32/32	0/3/3/3
9	GLN	E	4057	-	-	1/9/9/9	-
7	ADP	A	4000	3	-	2/16/32/32	0/3/3/3
10	NET	E	4058	-	-	3/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ORN	A	4011	-	-	5/8/8/8	-
7	ADP	E	4045	3	-	2/16/32/32	0/3/3/3
9	GLN	G	4080	-	-	0/9/9/9	-
10	NET	A	4014	-	-	0/12/12/12	-
8	ORN	E	4055	-	-	5/8/8/8	-
7	ADP	E	4051	3,4	-	4/16/32/32	0/3/3/3
9	GLN	B	4012	-	-	6/9/9/9	-
9	GLN	D	4034	-	-	2/9/9/9	-
7	ADP	G	4074	3,4	-	1/16/32/32	0/3/3/3
10	NET	C	4036	-	-	3/12/12/12	-
10	NET	G	4081	-	-	0/12/12/12	-
7	ADP	C	4023	3	-	3/16/32/32	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4000	ADP	PA-O3A	-5.20	1.53	1.59
7	C	4023	ADP	PA-O3A	-4.85	1.54	1.59
7	A	4007	ADP	PA-O3A	-4.62	1.54	1.59
6	C	4028	PO4	P-O4	-3.90	1.43	1.54
6	C	4028	PO4	P-O2	-3.56	1.44	1.54
7	G	4074	ADP	O3'-C3'	3.55	1.51	1.43
7	C	4029	ADP	O3'-C3'	3.44	1.51	1.43
7	G	4074	ADP	PA-O3A	-3.39	1.55	1.59
6	A	4006	PO4	P-O2	-3.23	1.45	1.54
6	G	4073	PO4	P-O2	-3.12	1.45	1.54
9	C	4035	GLN	CA-N	-3.01	1.33	1.48
9	E	4057	GLN	CA-N	-2.92	1.33	1.48
9	H	4079	GLN	CA-N	-2.92	1.33	1.48
6	E	4050	PO4	P-O3	-2.90	1.46	1.54
6	A	4006	PO4	P-O4	-2.88	1.46	1.54
9	G	4080	GLN	CA-N	-2.88	1.34	1.48
7	E	4045	ADP	PA-O3A	-2.85	1.56	1.59
9	F	4056	GLN	CA-N	-2.82	1.34	1.48
6	E	4050	PO4	P-O2	-2.82	1.46	1.54
7	G	4068	ADP	O3'-C3'	2.78	1.49	1.43
9	A	4013	GLN	CA-N	-2.74	1.34	1.48
7	E	4045	ADP	O3'-C3'	2.73	1.49	1.43
7	C	4023	ADP	O2'-C2'	2.67	1.49	1.43
6	E	4050	PO4	P-O4	-2.65	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	4033	ORN	O-C	2.63	1.29	1.22
9	B	4012	GLN	CA-N	-2.59	1.35	1.48
9	F	4056	GLN	O-C	2.51	1.29	1.22
7	C	4029	ADP	O2'-C2'	2.48	1.49	1.43
7	G	4074	ADP	O2'-C2'	2.48	1.49	1.43
9	D	4034	GLN	CA-N	-2.45	1.36	1.48
7	G	4068	ADP	PA-O3A	-2.45	1.56	1.59
7	E	4051	ADP	C2-N1	2.36	1.38	1.33
7	C	4029	ADP	C2-N1	2.36	1.38	1.33
9	E	4057	GLN	O-C	2.35	1.29	1.22
7	A	4000	ADP	O3'-C3'	2.34	1.48	1.43
6	C	4028	PO4	P-O3	-2.28	1.48	1.54
7	A	4007	ADP	C2-N3	-2.27	1.29	1.33
6	G	4073	PO4	P-O4	-2.20	1.48	1.54
7	G	4068	ADP	O2'-C2'	2.20	1.48	1.43
7	A	4000	ADP	C2-N1	2.18	1.37	1.33
7	G	4074	ADP	C2-N3	-2.14	1.30	1.33
7	A	4000	ADP	C2-N3	-2.14	1.30	1.33
7	E	4051	ADP	O2'-C2'	2.12	1.48	1.43
7	C	4023	ADP	PA-O2A	-2.01	1.46	1.55

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	4034	GLN	CG-CB-CA	-3.96	104.78	113.86
7	E	4051	ADP	O2A-PA-O3A	3.69	117.25	107.27
7	G	4068	ADP	O3B-PB-O3A	-3.66	92.38	104.64
7	C	4029	ADP	O2A-PA-O3A	3.01	115.40	107.27
9	D	4034	GLN	CB-CA-C	-2.99	102.53	110.45
7	G	4074	ADP	O3B-PB-O3A	2.88	114.30	104.64
9	F	4056	GLN	CG-CB-CA	-2.82	107.39	113.86
7	G	4068	ADP	O3'-C3'-C2'	2.73	120.57	111.82
7	G	4074	ADP	O3'-C3'-C2'	2.71	120.51	111.82
9	E	4057	GLN	OXT-C-O	-2.68	117.99	124.08
9	B	4012	GLN	CB-CA-C	-2.65	103.42	110.45
9	D	4034	GLN	OE1-CD-CG	-2.52	113.45	121.04
7	A	4007	ADP	C2'-C3'-C4'	-2.50	97.79	102.61
7	G	4068	ADP	O2'-C2'-C3'	2.49	119.78	111.82
7	G	4068	ADP	N6-C6-N1	2.47	123.88	118.38
7	E	4045	ADP	O4'-C1'-N9	2.30	112.50	108.09
9	B	4012	GLN	OXT-C-O	-2.21	119.07	124.08
7	E	4045	ADP	O2A-PA-O3A	2.20	113.22	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	4035	GLN	OXT-C-O	-2.20	119.09	124.08
7	C	4029	ADP	O3'-C3'-C2'	2.13	118.66	111.82
7	E	4045	ADP	C3'-C2'-C1'	2.13	105.49	101.46
7	A	4000	ADP	O3B-PB-O3A	-2.13	97.49	104.64
7	C	4029	ADP	O2'-C2'-C3'	2.11	118.59	111.82
6	E	4050	PO4	O3-P-O1	-2.07	103.61	110.95
7	G	4068	ADP	O3B-PB-O2B	2.04	115.45	107.80

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	4029	ADP	PA-O3A-PB-O3B
7	E	4051	ADP	PA-O3A-PB-O3B
8	A	4011	ORN	N-CA-CB-CG
8	A	4011	ORN	C-CA-CB-CG
8	C	4033	ORN	N-CA-CB-CG
8	C	4033	ORN	C-CA-CB-CG
8	E	4055	ORN	N-CA-CB-CG
8	E	4055	ORN	C-CA-CB-CG
8	G	4078	ORN	N-CA-CB-CG
9	A	4013	GLN	C-CA-CB-CG
9	B	4012	GLN	C-CA-CB-CG
9	C	4035	GLN	N-CA-CB-CG
9	C	4035	GLN	C-CA-CB-CG
9	E	4057	GLN	C-CA-CB-CG
9	H	4079	GLN	N-CA-CB-CG
9	H	4079	GLN	C-CA-CB-CG
9	B	4012	GLN	CA-CB-CG-CD
8	E	4055	ORN	OXT-C-CA-N
8	G	4078	ORN	OXT-C-CA-N
10	C	4036	NET	C8-C7-N1-C3
10	C	4036	NET	C8-C7-N1-C5
10	C	4036	NET	C8-C7-N1-C1
8	C	4033	ORN	OXT-C-CA-N
8	E	4055	ORN	CA-CB-CG-CD
7	A	4007	ADP	PA-O3A-PB-O1B
7	E	4051	ADP	PA-O3A-PB-O1B
9	H	4079	GLN	NE2-CD-CG-CB
8	C	4033	ORN	O-C-CA-N
8	E	4055	ORN	O-C-CA-N
8	G	4078	ORN	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
10	E	4058	NET	C4-C3-N1-C5
7	A	4007	ADP	PA-O3A-PB-O3B
9	H	4079	GLN	OE1-CD-CG-CB
8	G	4078	ORN	C-CA-CB-CG
10	E	4058	NET	C4-C3-N1-C1
7	A	4000	ADP	PB-O3A-PA-O1A
7	E	4045	ADP	PB-O3A-PA-O1A
9	B	4012	GLN	OE1-CD-CG-CB
8	C	4033	ORN	CA-CB-CG-CD
9	A	4013	GLN	N-CA-CB-CG
10	E	4058	NET	C4-C3-N1-C7
7	C	4023	ADP	C5'-O5'-PA-O1A
7	E	4045	ADP	C5'-O5'-PA-O1A
8	G	4078	ORN	CA-CB-CG-CD
8	A	4011	ORN	OXT-C-CA-N
7	G	4074	ADP	PA-O3A-PB-O1B
9	B	4012	GLN	NE2-CD-CG-CB
8	A	4011	ORN	CA-CB-CG-CD
9	F	4056	GLN	OE1-CD-CG-CB
9	F	4056	GLN	NE2-CD-CG-CB
7	A	4007	ADP	PB-O3A-PA-O2A
7	C	4029	ADP	PB-O3A-PA-O2A
7	E	4051	ADP	PB-O3A-PA-O2A
8	G	4078	ORN	NE-CD-CG-CB
8	A	4011	ORN	O-C-CA-N
9	H	4079	GLN	CA-CB-CG-CD
7	G	4068	ADP	PB-O3A-PA-O1A
7	C	4029	ADP	PA-O3A-PB-O1B
9	B	4012	GLN	OXT-C-CA-N
9	D	4034	GLN	OXT-C-CA-N
7	A	4007	ADP	PB-O3A-PA-O1A
7	C	4023	ADP	PB-O3A-PA-O1A
7	E	4051	ADP	PB-O3A-PA-O1A
9	A	4013	GLN	OXT-C-CA-N
9	D	4034	GLN	NE2-CD-CG-CB
8	C	4033	ORN	NE-CD-CG-CB
9	B	4012	GLN	N-CA-CB-CG
9	A	4013	GLN	O-C-CA-N
7	A	4000	ADP	PB-O3A-PA-O2A
7	C	4023	ADP	PB-O3A-PA-O2A

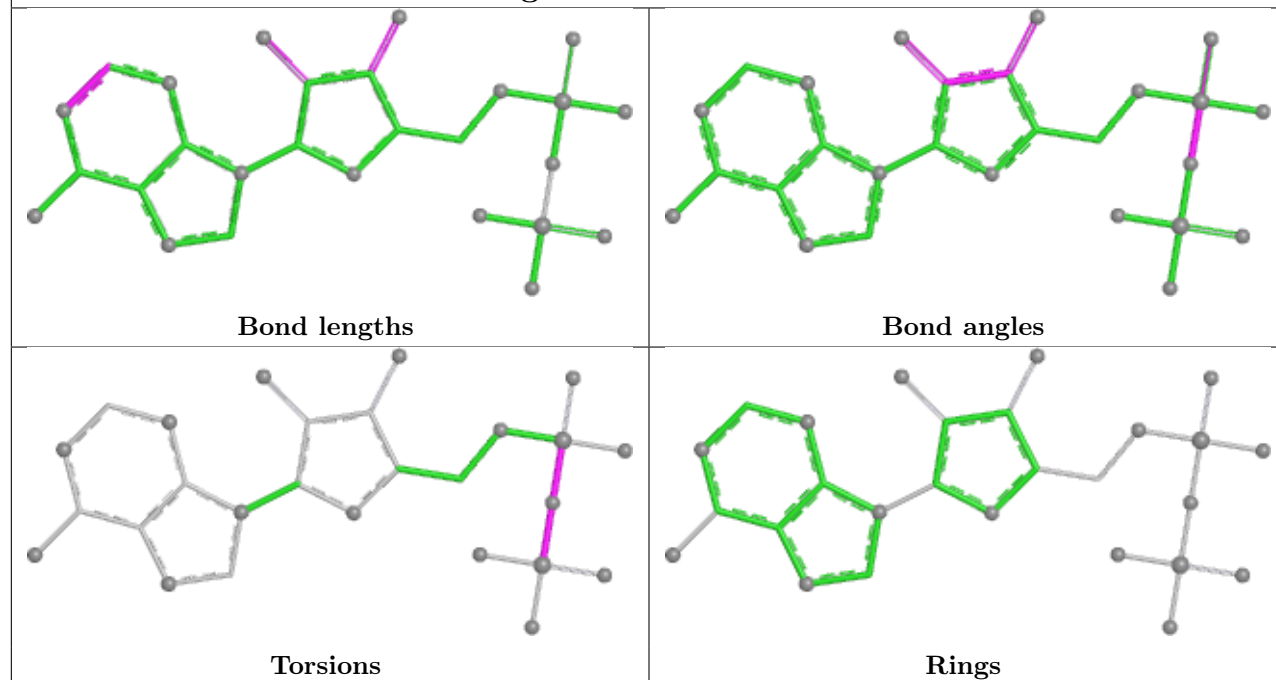
There are no ring outliers.

13 monomers are involved in 24 short contacts:

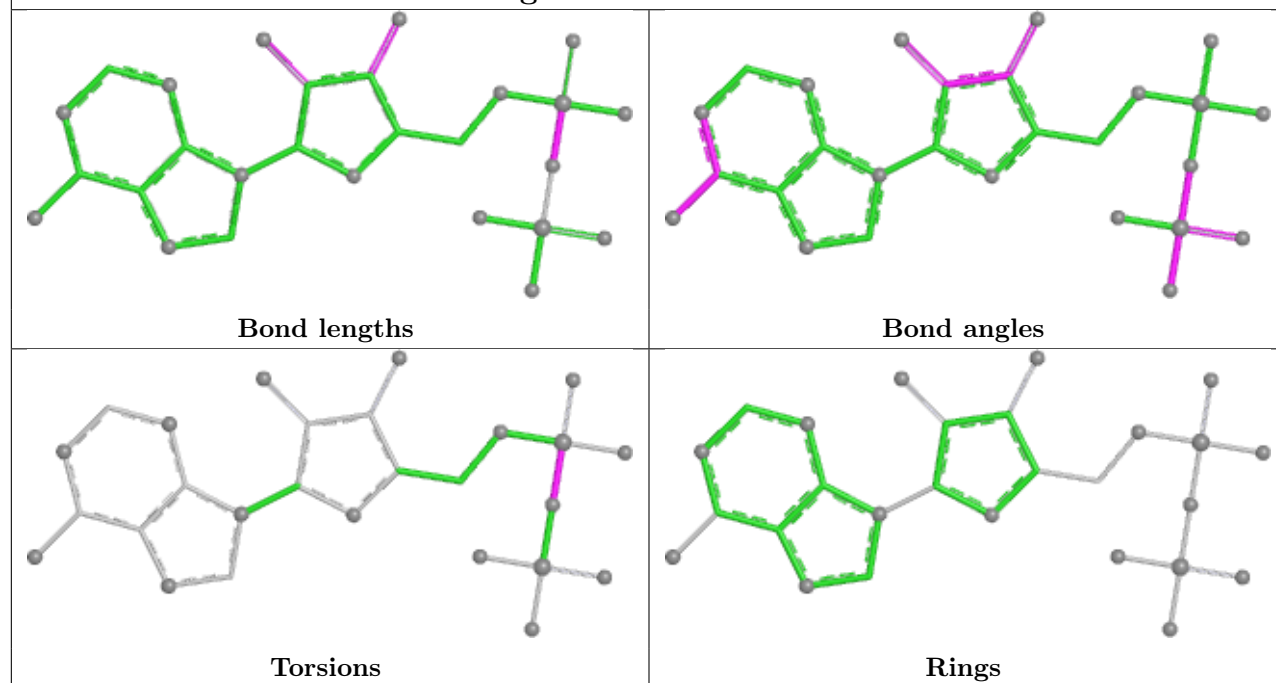
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	4056	GLN	4	0
9	H	4079	GLN	2	0
7	C	4029	ADP	1	0
7	G	4068	ADP	1	0
8	C	4033	ORN	1	0
10	E	4058	NET	2	0
8	A	4011	ORN	1	0
7	E	4045	ADP	3	0
7	E	4051	ADP	2	0
9	B	4012	GLN	3	0
9	D	4034	GLN	2	0
7	G	4074	ADP	1	0
10	C	4036	NET	1	0

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.

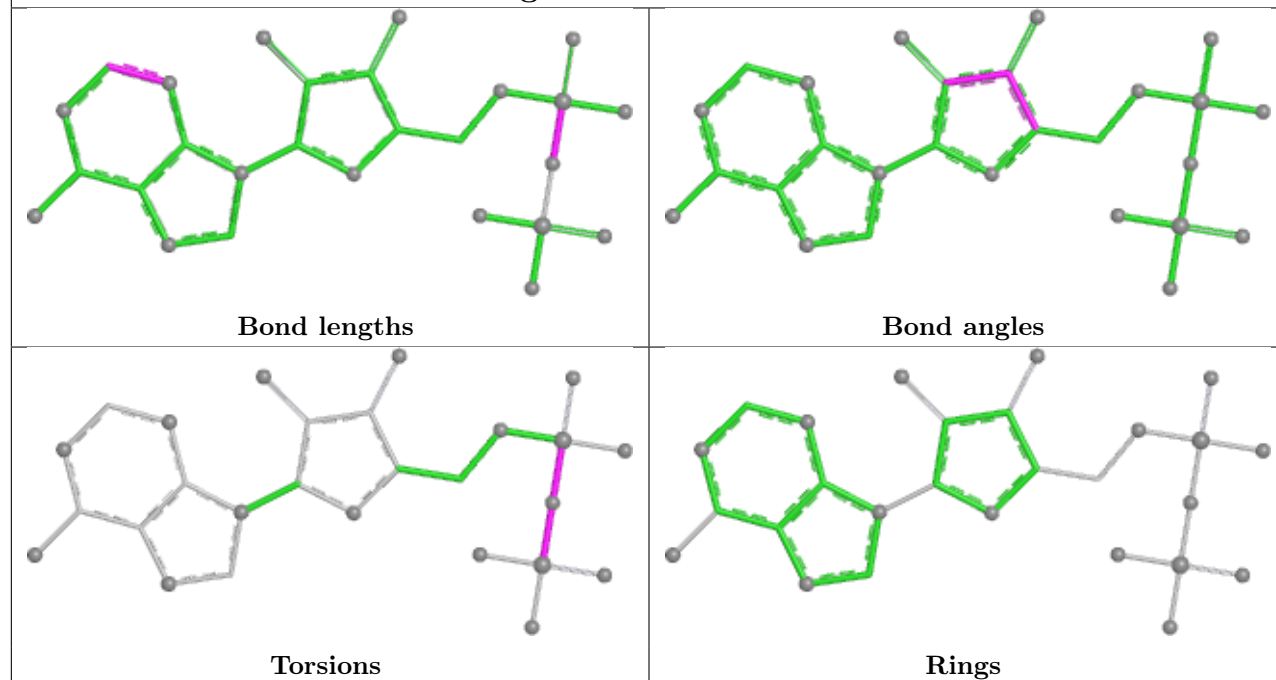
Ligand ADP C 4029



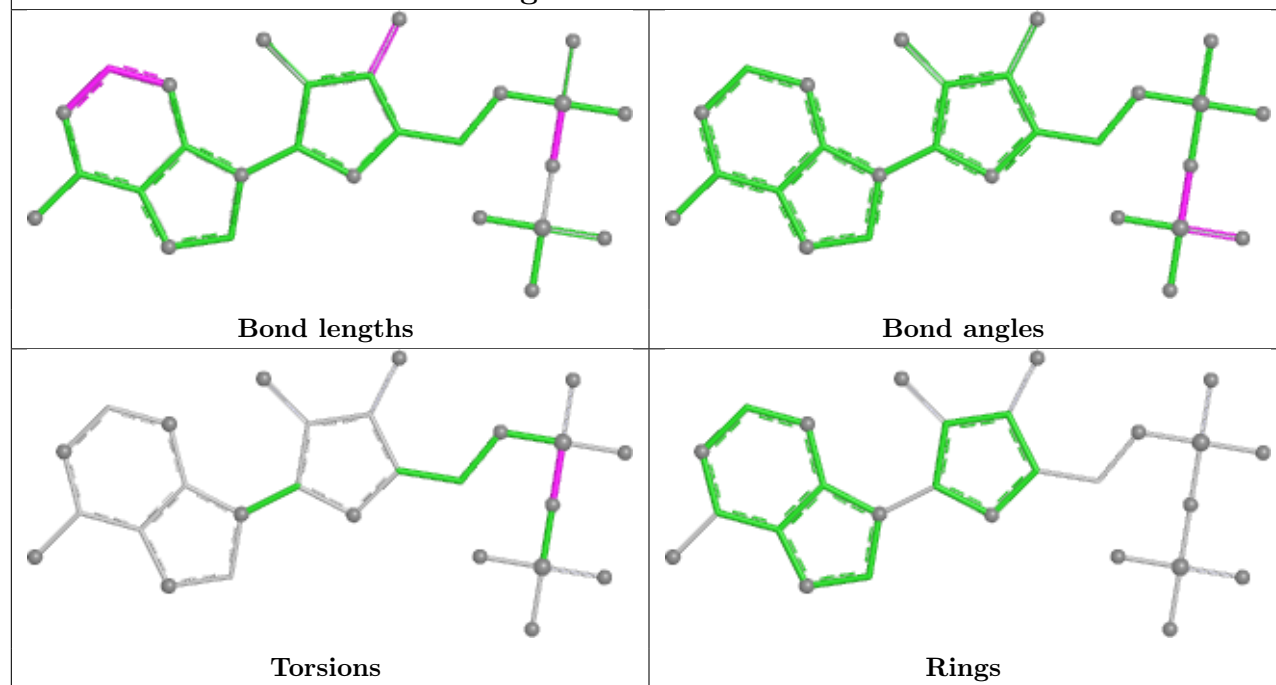
Ligand ADP G 4068



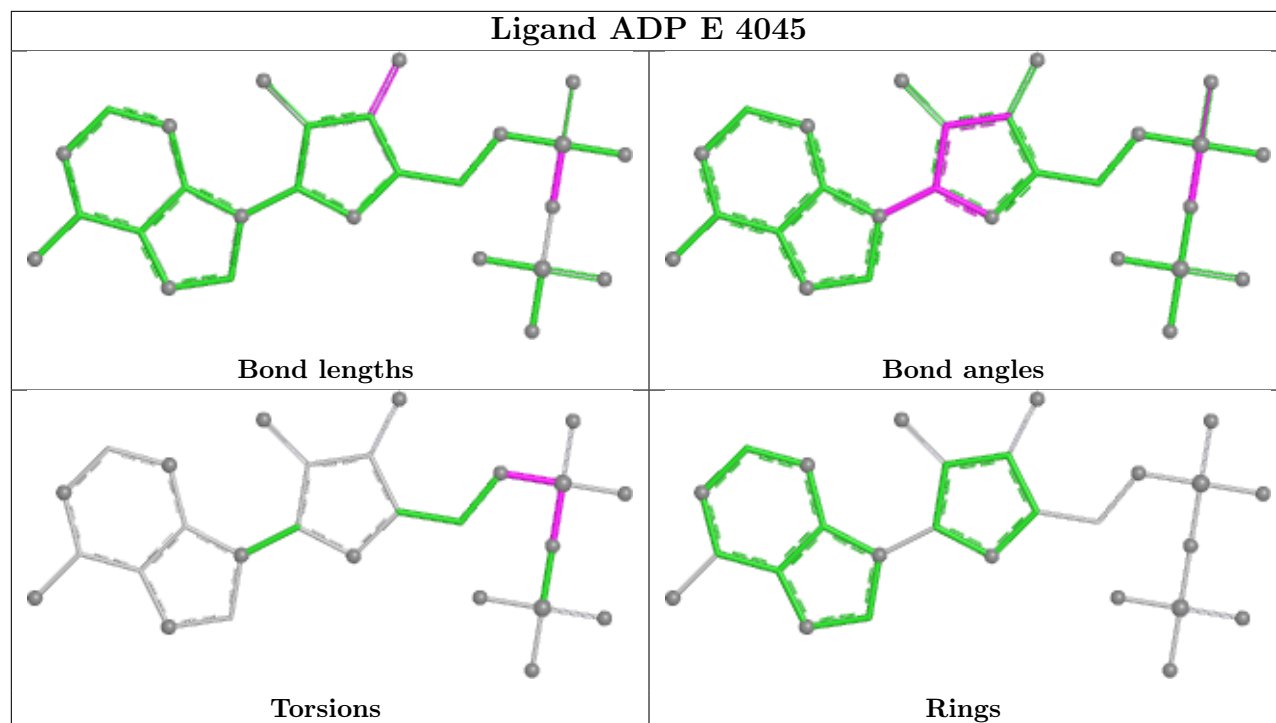
Ligand ADP A 4007



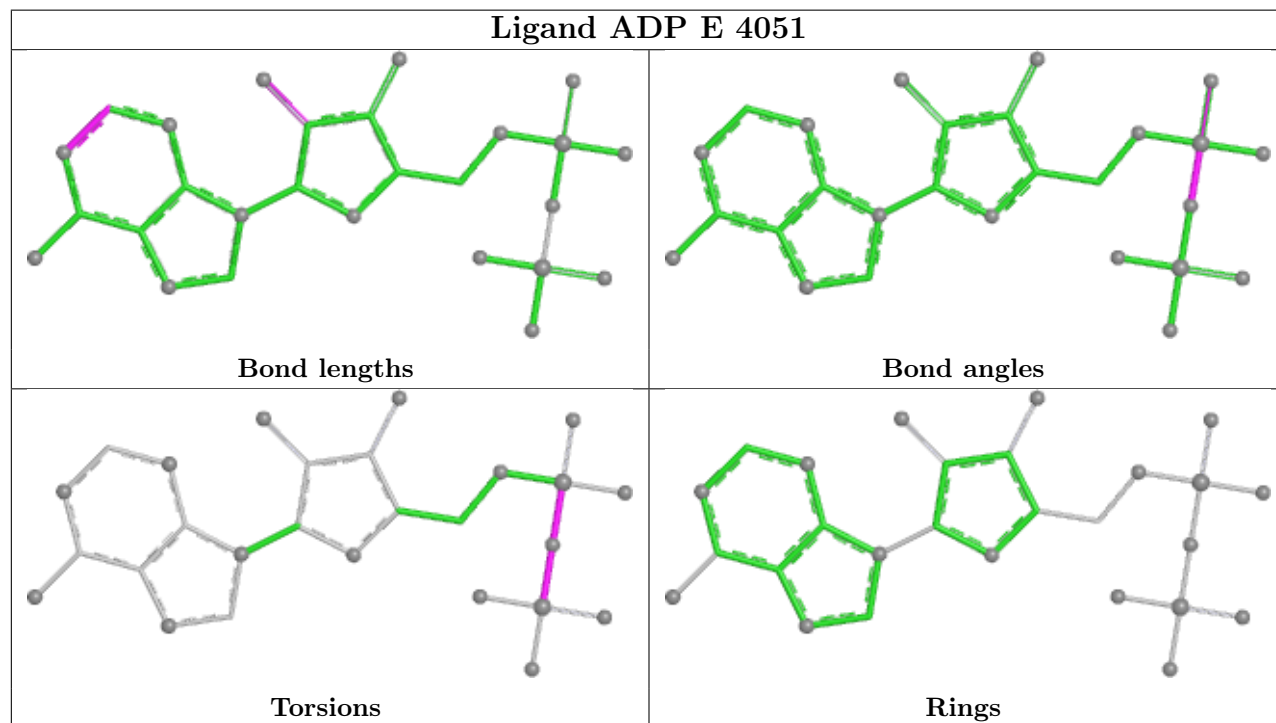
Ligand ADP A 4000

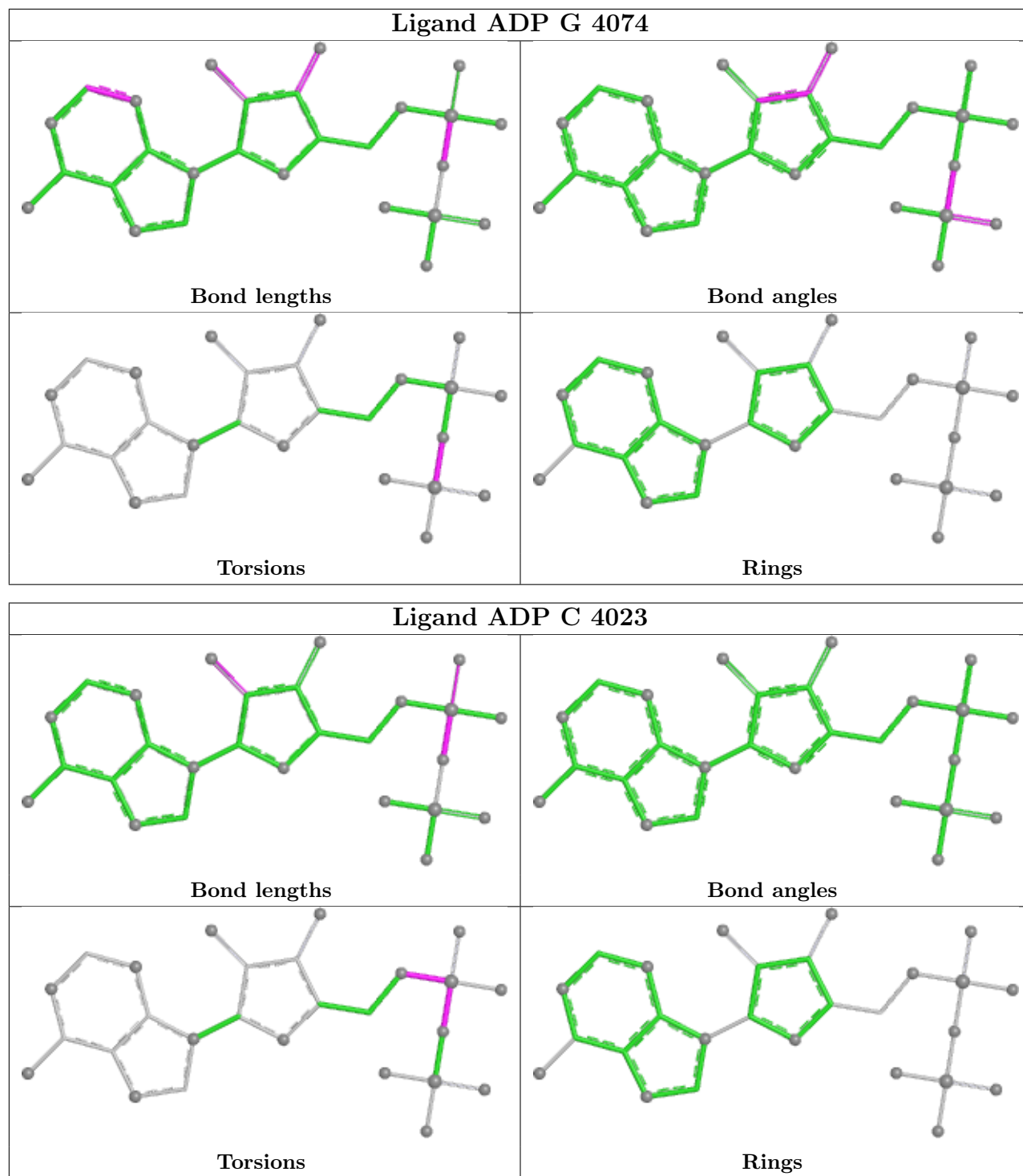


Ligand ADP E 4045



Ligand ADP E 4051





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.