



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:44 PM UTC

PDB ID : 1M6V / pdb_00001m6v
Title : Crystal Structure of the G359F (small subunit) Point Mutant of Carbamoyl Phosphate Synthetase
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 2002-07-17
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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

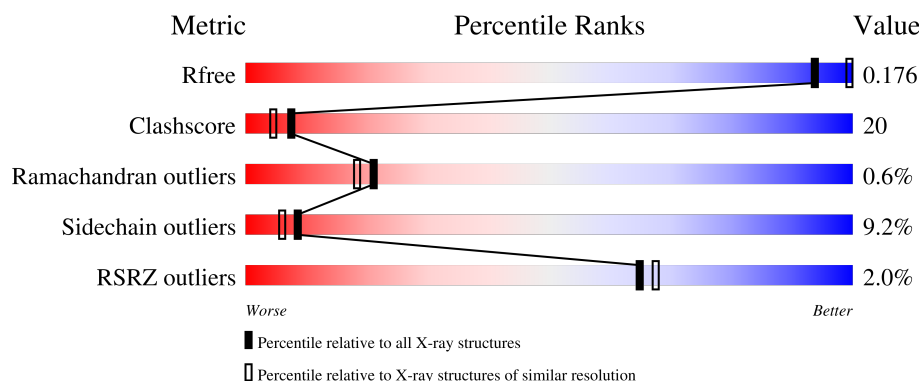
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1073	2% 64% 29% 5% .
1	C	1073	2% 64% 28% 7% .
1	E	1073	% 62% 31% 5% ..
1	G	1073	2% 56% 37% 6% .
2	B	382	4% 36% 49% 12% ...

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Mol	Chain	Length	Quality of chain
2	D	382	% 58% 35% 5% ••
2	F	382	% 47% 45% 5% ••
2	H	382	4% 40% 48% 9% ••

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48206 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1059	Total	C	N	O	S	0	6	0
			8190	5140	1425	1579	46			
1	C	1059	Total	C	N	O	S	0	5	0
			8196	5144	1431	1576	45			
1	E	1059	Total	C	N	O	S	0	6	0
			8189	5141	1426	1576	46			
1	G	1059	Total	C	N	O	S	0	6	0
			8197	5144	1428	1580	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	SEE REMARK 999	UNP P00968
C	46	ASN	LEU	SEE REMARK 999	UNP P00968
E	46	ASN	LEU	SEE REMARK 999	UNP P00968
G	46	ASN	LEU	SEE REMARK 999	UNP P00968

- Molecule 2 is a protein called carbamoyl-phosphate synthetase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	0	1	0
			2871	1812	504	545	10			
2	D	375	Total	C	N	O	S	0	2	0
			2877	1814	507	546	10			
2	F	375	Total	C	N	O	S	0	3	0
			2880	1818	505	546	11			
2	H	375	Total	C	N	O	S	0	1	0
			2871	1812	504	545	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	SEE REMARK 999	UNP P00907
B	359	PHE	GLY	engineered mutation	UNP P00907
D	183	GLN	GLU	SEE REMARK 999	UNP P00907
D	359	PHE	GLY	engineered mutation	UNP P00907
F	183	GLN	GLU	SEE REMARK 999	UNP P00907
F	359	PHE	GLY	engineered mutation	UNP P00907
H	183	GLN	GLU	SEE REMARK 999	UNP P00907
H	359	PHE	GLY	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

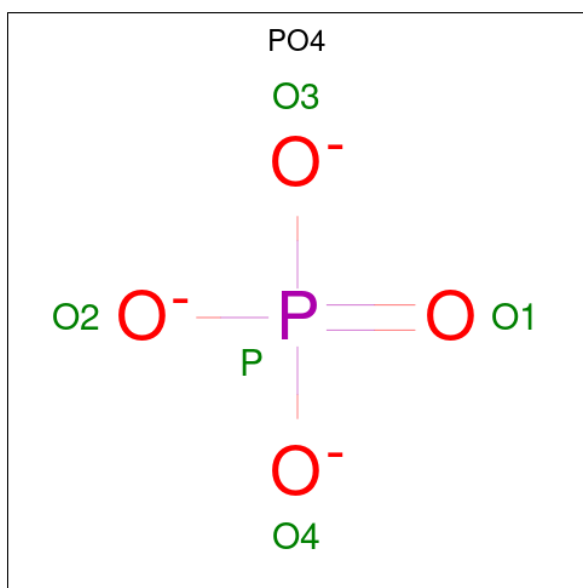
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total K 5 5	0	0
4	B	1	Total K 1 1	0	0
4	C	6	Total K 6 6	0	0
4	D	1	Total K 1 1	0	0
4	E	6	Total K 6 6	0	0
4	F	1	Total K 1 1	0	0
4	G	6	Total K 6 6	0	0

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

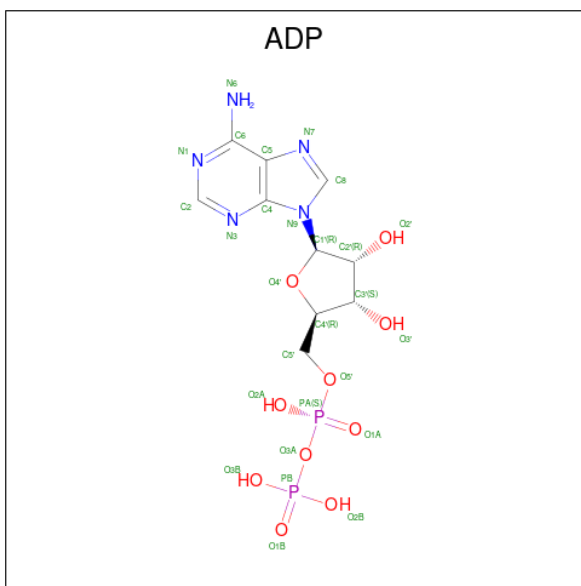
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Cl	0	0
			5	5		
5	B	1	Total	Cl	0	0
			1	1		
5	C	7	Total	Cl	0	0
			7	7		
5	D	1	Total	Cl	0	0
			1	1		
5	E	6	Total	Cl	0	0
			6	6		
5	F	1	Total	Cl	0	0
			1	1		
5	G	6	Total	Cl	0	0
			6	6		
5	H	1	Total	Cl	0	0
			1	1		

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



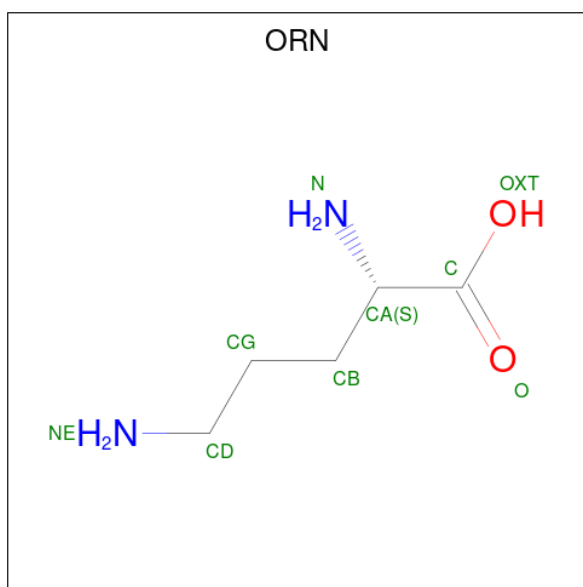
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

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



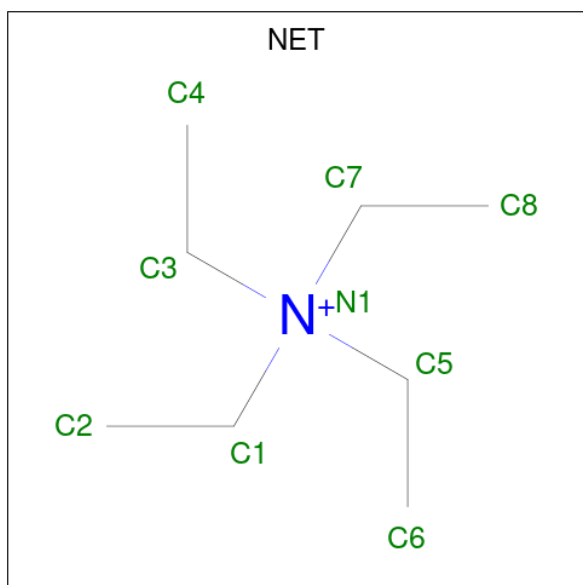
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	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 TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: C₈H₂₀N⁺).



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

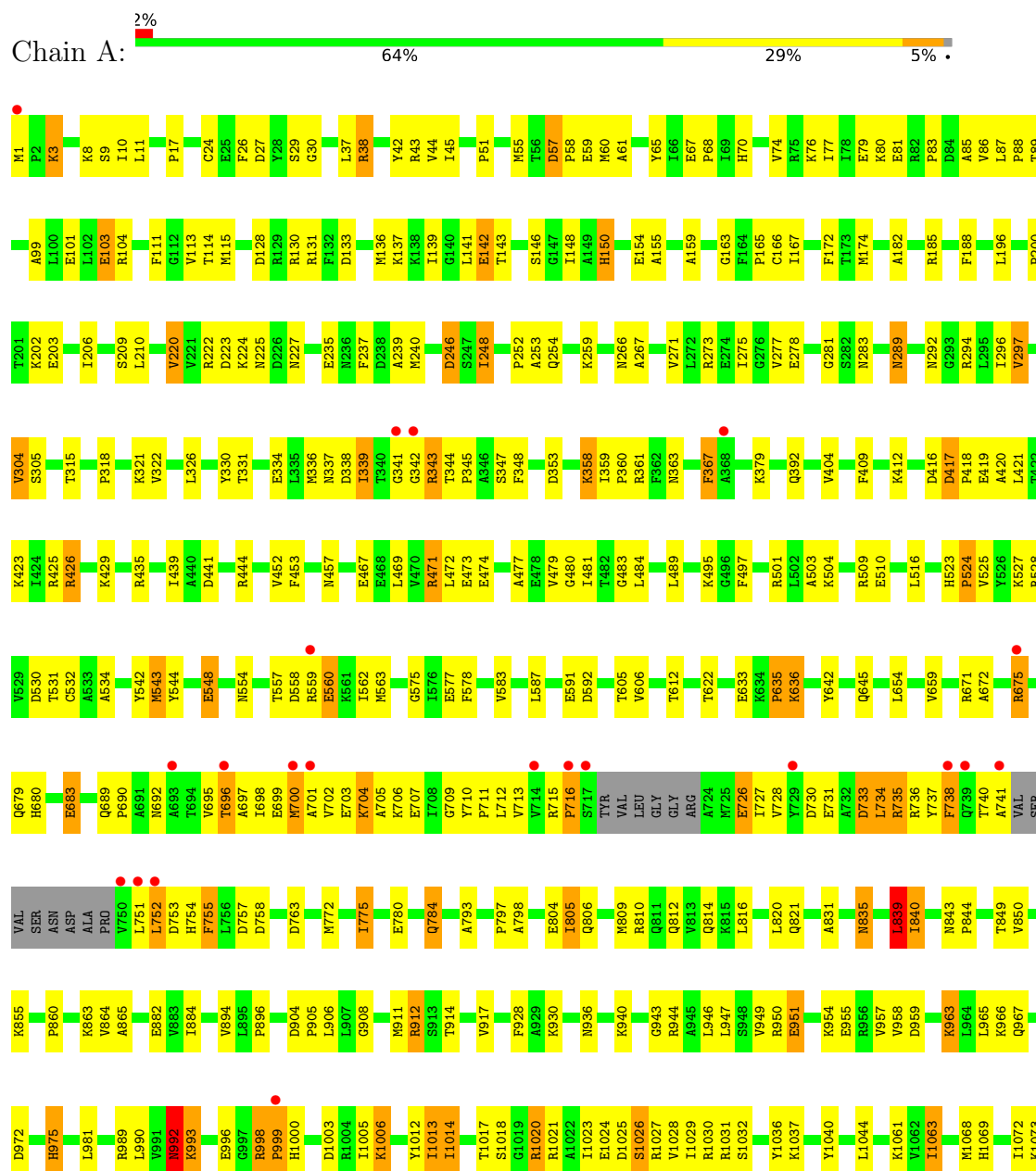
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	793	Total O 793 793	0	0
10	B	130	Total O 130 130	0	0
10	C	681	Total O 681 681	0	0
10	D	177	Total O 177 177	0	0
10	E	813	Total O 813 813	0	0
10	F	205	Total O 205 205	0	0
10	G	645	Total O 645 645	0	0
10	H	117	Total O 117 117	0	0

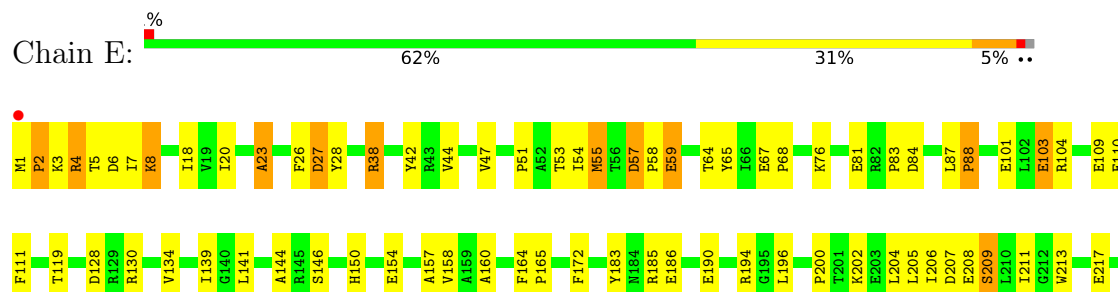
3 Residue-property plots

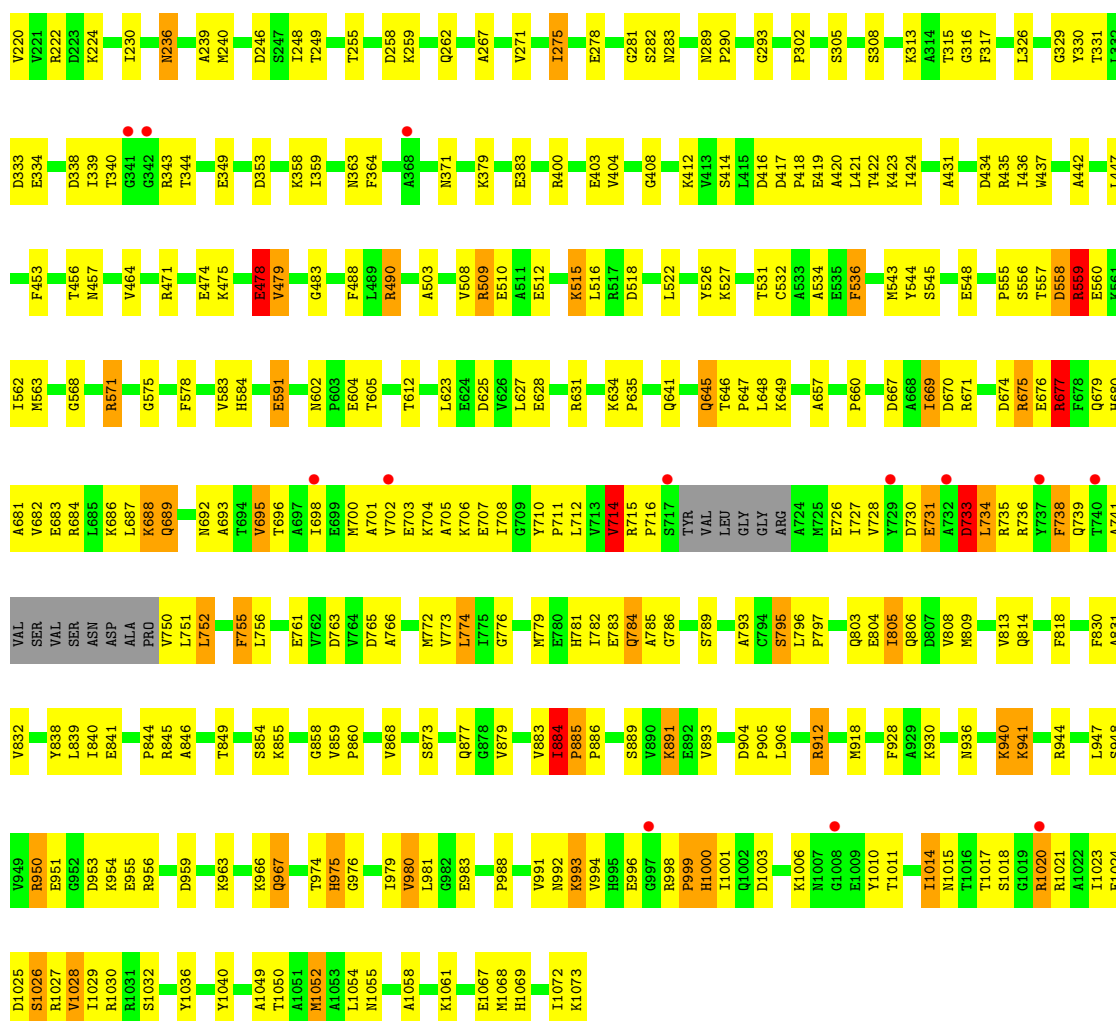
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: carbamoyl phosphate synthetase large chain

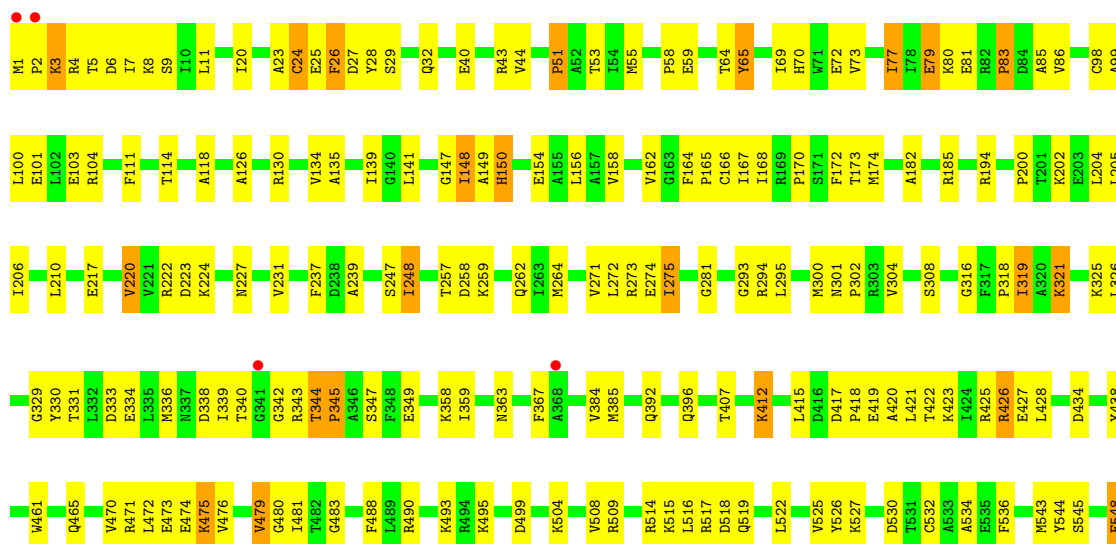


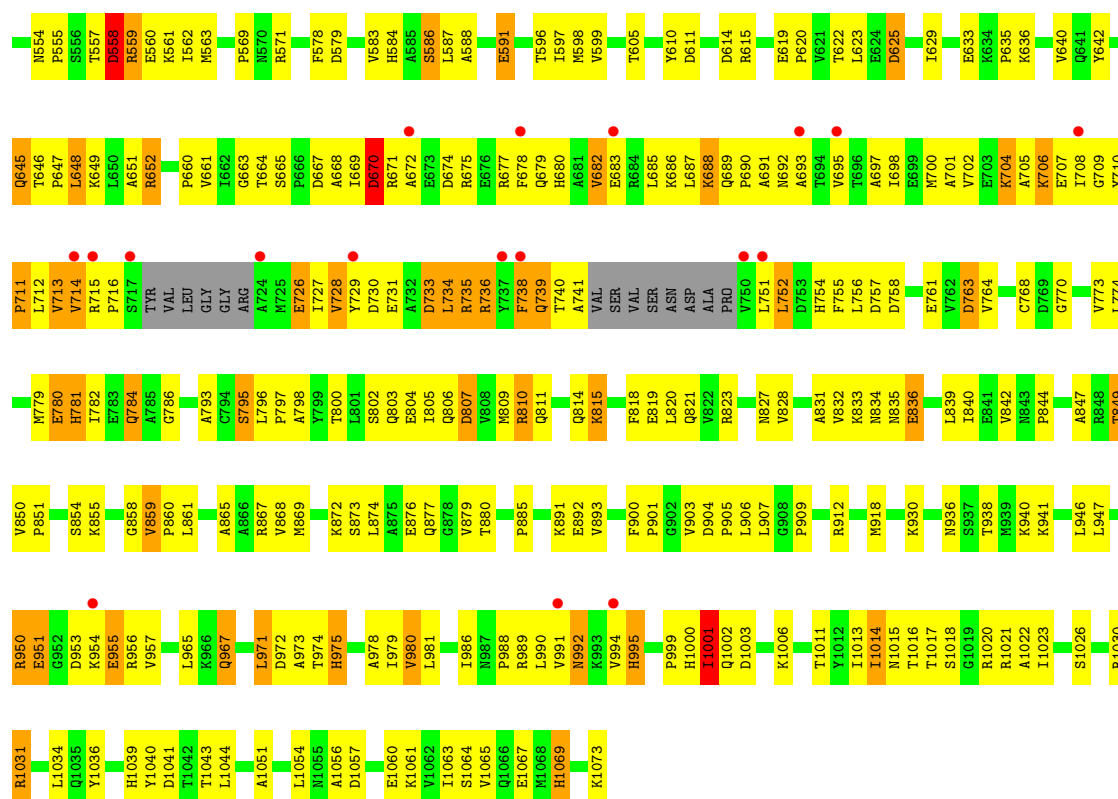
- Molecule 1: carbamoyl phosphate synthetase large chain



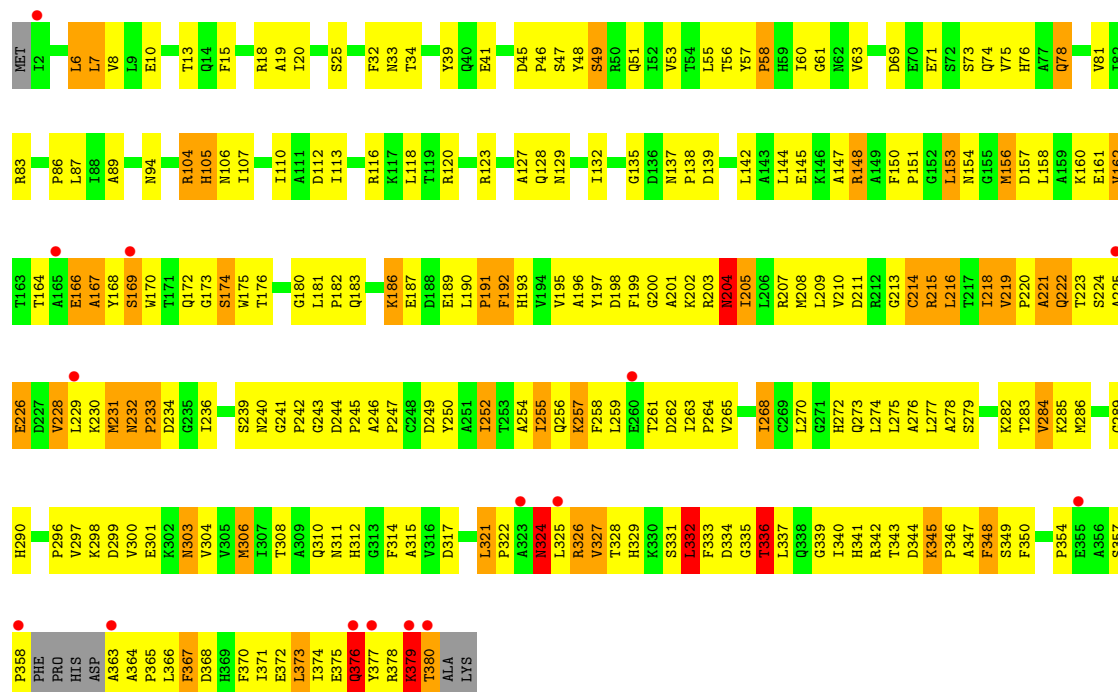


• Molecule 1: carbamoyl phosphate synthetase large chain

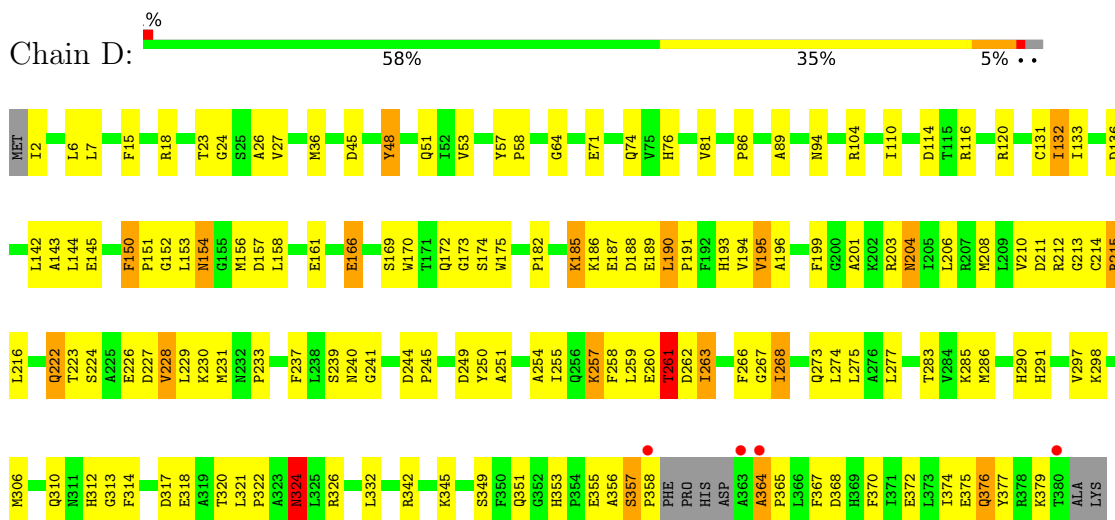




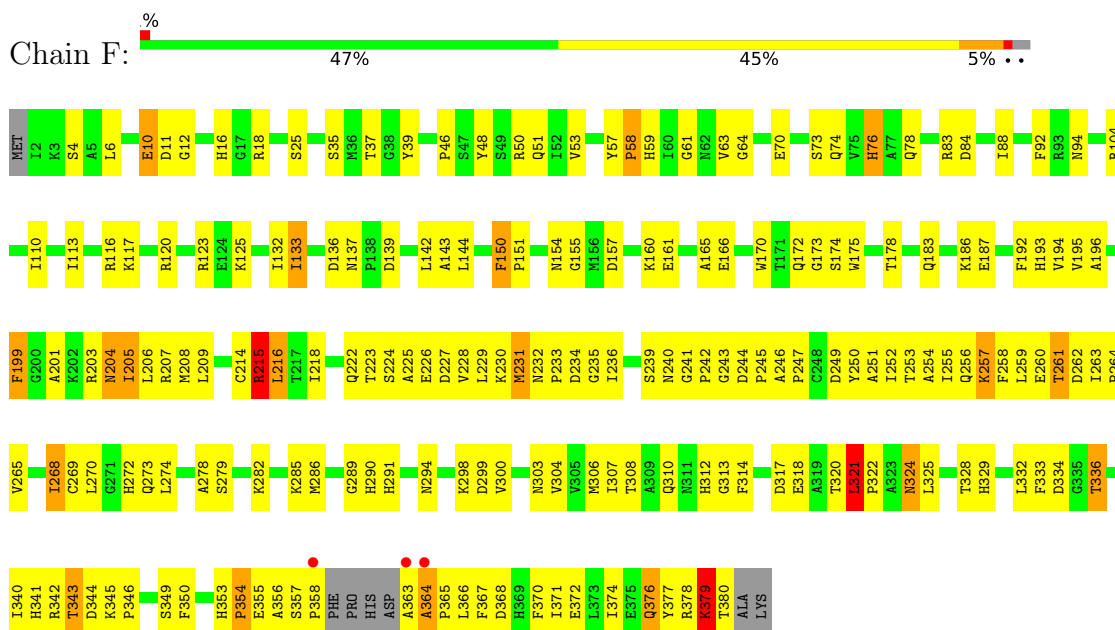
• Molecule 2: carbamoyl-phosphate synthetase small chain



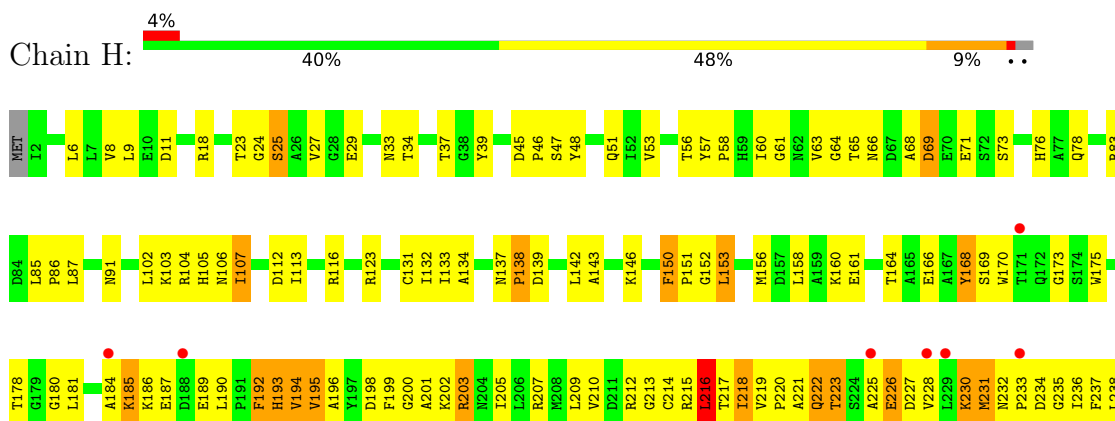
• Molecule 2: carbamoyl-phosphate synthetase small chain

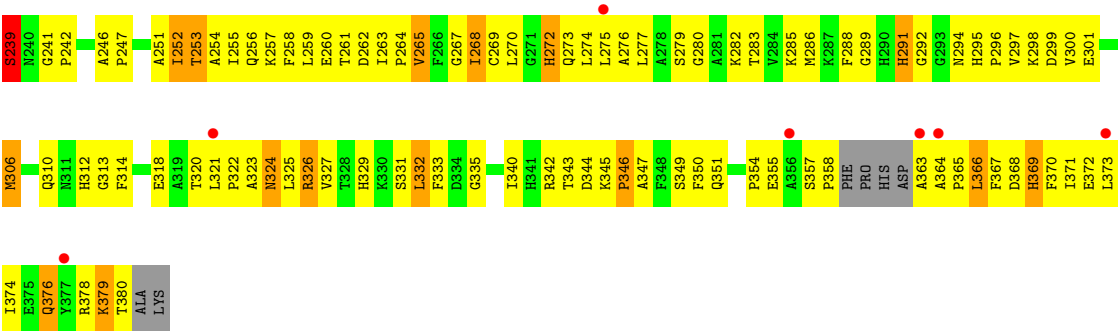


• Molecule 2: carbamoyl-phosphate synthetase small chain



• Molecule 2: carbamoyl-phosphate synthetase small chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.50Å 164.20Å 331.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-2.10) 92.3 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.09Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.174 , 0.245 0.176 , 0.176	Depositor DCC
R_{free} test set	44498 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 122.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48206	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.20	2/8340 (0.0%)	1.64	90/11273 (0.8%)
1	C	1.19	4/8350 (0.0%)	1.65	94/11288 (0.8%)
1	E	1.19	2/8339 (0.0%)	1.63	91/11272 (0.8%)
1	G	1.16	2/8351 (0.0%)	1.65	79/11291 (0.7%)
2	B	1.12	0/2934	1.67	37/3981 (0.9%)
2	D	1.16	1/2944 (0.0%)	1.69	34/3996 (0.9%)
2	F	1.13	1/2951 (0.0%)	1.67	34/4003 (0.8%)
2	H	1.09	1/2934 (0.0%)	1.64	26/3981 (0.7%)
All	All	1.17	13/45143 (0.0%)	1.65	485/61085 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	1	0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	634	LYS	CA-C	-6.44	1.49	1.53
1	E	879	VAL	CA-C	-6.13	1.45	1.52
1	C	1069	HIS	ND1-CE1	-5.88	1.26	1.32
1	C	179	GLY	N-CA	5.73	1.49	1.44
1	A	683	GLU	CD-OE2	5.54	1.35	1.25
1	E	478	GLU	CA-C	-5.45	1.45	1.52
2	F	137	ASN	CA-C	-5.37	1.47	1.52
1	C	1009	GLU	CD-OE2	5.36	1.35	1.25
1	A	850	VAL	CA-CB	-5.31	1.51	1.54
1	G	554[A]	ASN	N-CA	5.04	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	554[B]	ASN	N-CA	5.04	1.50	1.46
2	H	210	VAL	CA-CB	-5.03	1.48	1.54
2	D	132	ILE	CA-C	-5.01	1.46	1.52

All (485) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	THR	CA-C-N	10.99	135.16	120.65
1	A	557	THR	C-N-CA	10.99	135.16	120.65
1	G	885	PRO	O-C-N	10.42	126.11	121.31
1	C	885	PRO	N-CA-CB	10.42	108.64	103.22
2	B	105	HIS	CA-CB-CG	-9.84	103.96	113.80
1	A	839	LEU	CA-C-N	-9.68	113.27	122.66
1	A	839	LEU	C-N-CA	-9.68	113.27	122.66
2	B	367	PHE	CA-CB-CG	-9.49	104.31	113.80
1	E	884	ILE	CA-C-N	9.44	126.55	119.66
1	E	884	ILE	C-N-CA	9.44	126.55	119.66
2	H	53	VAL	N-CA-C	9.20	121.42	107.99
1	C	885	PRO	O-C-N	9.18	125.47	121.15
1	C	207	ASP	CA-CB-CG	9.18	121.78	112.60
2	B	174	SER	N-CA-C	8.90	122.28	110.53
1	C	738	PHE	CA-CB-CG	-8.89	104.91	113.80
1	A	738	PHE	CA-CB-CG	-8.86	104.94	113.80
1	E	793	ALA	N-CA-C	-8.73	97.60	110.52
2	F	76	HIS	CA-CB-CG	-8.63	105.17	113.80
2	B	106	ASN	CA-CB-CG	-8.56	104.04	112.60
1	A	367	PHE	CA-CB-CG	-8.48	105.32	113.80
1	A	457	ASN	CA-CB-CG	-8.34	104.26	112.60
1	G	885	PRO	N-CA-CB	8.33	107.85	103.19
1	C	680	HIS	CA-CB-CG	-8.06	105.73	113.80
1	A	908	GLY	CA-C-N	8.04	127.70	119.82
1	A	908	GLY	C-N-CA	8.04	127.70	119.82
1	E	885	PRO	O-C-N	8.02	125.00	121.31
2	D	353	HIS	CB-CA-C	-7.97	102.36	110.65
1	G	150	HIS	CA-CB-CG	-7.94	105.86	113.80
1	A	558	ASP	N-CA-C	7.92	119.61	110.97
2	B	311	ASN	CA-CB-CG	7.86	120.46	112.60
1	G	793	ALA	N-CA-C	-7.81	100.46	110.53
1	E	782	ILE	N-CA-C	-7.76	103.67	110.74
1	G	738	PHE	CA-CB-CG	-7.73	106.07	113.80
1	C	605	THR	N-CA-C	7.72	122.38	110.42
2	B	348	PHE	CA-CB-CG	-7.60	106.20	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	660	PRO	N-CA-CB	7.60	107.75	102.35
1	E	88	PRO	CB-CA-C	-7.57	101.60	109.92
1	E	338	ASP	N-CA-C	7.56	120.18	111.11
1	A	992	ASN	CA-CB-CG	-7.52	105.08	112.60
1	G	557	THR	N-CA-C	-7.50	103.97	113.72
1	E	738	PHE	CA-CB-CG	-7.49	106.31	113.80
1	G	1039	HIS	CA-CB-CG	-7.44	106.36	113.80
1	C	793	ALA	N-CA-C	-7.43	100.52	110.55
1	G	559	ARG	N-CA-C	7.33	120.47	110.35
1	E	996	GLU	CA-C-N	-7.32	110.77	122.92
1	E	996	GLU	C-N-CA	-7.32	110.77	122.92
1	A	612	THR	N-CA-C	7.25	120.05	111.71
1	C	959	ASP	CA-CB-CG	-7.21	105.39	112.60
2	D	150	PHE	CA-C-O	7.21	125.76	119.71
1	E	283	ASN	CA-CB-CG	7.18	119.78	112.60
2	H	216	LEU	N-CA-C	7.17	121.22	109.24
1	G	26	PHE	CA-CB-CG	-7.13	106.67	113.80
2	F	353	HIS	CB-CA-C	-7.09	102.30	110.17
2	D	132	ILE	CB-CA-C	-7.07	100.29	110.83
1	A	246	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	699	GLU	CA-C-N	7.03	129.69	120.28
1	A	699	GLU	C-N-CA	7.03	129.69	120.28
2	B	216	LEU	CB-CA-C	-7.01	96.55	109.37
1	E	44	VAL	N-CA-C	7.00	118.22	107.99
1	A	26	PHE	CA-CB-CG	-6.99	106.81	113.80
1	C	771	GLU	N-CA-C	-6.98	104.64	113.43
1	A	210	LEU	N-CA-C	-6.97	102.81	112.30
2	F	199	PHE	CA-CB-CG	-6.97	106.83	113.80
1	C	26	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	906	LEU	N-CA-CB	-6.92	98.80	110.83
2	D	368	ASP	CB-CA-C	6.91	123.41	110.63
2	F	370	PHE	N-CA-C	-6.90	103.45	110.97
2	F	16	HIS	CA-CB-CG	-6.90	106.90	113.80
1	G	569	PRO	CB-CA-C	-6.88	102.42	111.23
1	A	248	ILE	N-CA-C	-6.88	98.42	108.87
1	G	716	PRO	N-CA-CB	6.87	109.85	103.39
1	E	239	ALA	N-CA-C	6.86	118.69	110.19
2	F	174	SER	N-CA-C	6.84	119.66	110.35
1	C	858	GLY	CA-C-N	-6.83	116.76	123.04
1	C	858	GLY	C-N-CA	-6.83	116.76	123.04
1	G	880	THR	N-CA-CB	-6.81	101.20	111.15
1	E	23	ALA	N-CA-C	6.81	118.89	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	221	ALA	N-CA-C	6.79	119.25	111.11
1	G	23	ALA	N-CA-C	6.79	118.86	109.29
1	A	44	VAL	N-CA-C	6.70	117.95	108.36
1	C	44	VAL	N-CA-C	6.70	117.78	107.99
2	H	239	SER	N-CA-C	6.70	118.65	110.41
1	A	592	ASP	CA-CB-CG	6.70	119.30	112.60
1	E	27	ASP	N-CA-C	-6.70	103.91	111.14
2	F	4	SER	N-CA-C	6.69	119.94	110.50
2	H	112	ASP	N-CA-C	6.68	120.76	111.74
2	D	204	ASN	N-CA-C	6.68	119.57	111.82
1	C	338	ASP	CA-CB-CG	6.68	119.28	112.60
2	B	232	ASN	CA-CB-CG	-6.67	105.92	112.60
2	B	58	PRO	CA-C-N	-6.66	113.31	122.30
2	B	58	PRO	C-N-CA	-6.66	113.31	122.30
1	E	557	THR	CA-C-N	6.64	134.23	121.54
1	E	557	THR	C-N-CA	6.64	134.23	121.54
1	A	543	MET	N-CA-C	6.64	120.34	109.85
2	F	150	PHE	CA-C-O	6.63	126.00	119.51
1	C	1057	ASP	N-CA-CB	6.62	120.91	110.84
1	A	999	PRO	N-CA-CB	6.62	109.88	102.60
1	C	536	PHE	CA-CB-CG	-6.62	107.18	113.80
2	D	249	ASP	CA-CB-CG	6.60	119.20	112.60
1	G	953	ASP	CA-CB-CG	6.58	119.18	112.60
2	H	216	LEU	N-CA-CB	6.57	122.90	111.00
1	A	417	ASP	CA-CB-CG	6.56	119.16	112.60
2	B	74	GLN	N-CA-C	6.56	117.24	108.38
1	C	1039	HIS	CA-CB-CG	-6.56	107.24	113.80
1	G	319	ILE	N-CA-C	6.55	117.05	110.23
2	F	136	ASP	CA-C-N	-6.55	113.87	123.30
2	F	136	ASP	C-N-CA	-6.55	113.87	123.30
1	E	605	THR	N-CA-C	6.54	120.14	110.46
1	A	305	SER	N-CA-CB	-6.51	100.95	111.24
1	C	557	THR	N-CA-C	-6.50	105.65	113.97
1	A	605	THR	N-CA-C	6.50	120.13	110.52
1	E	431	ALA	N-CA-C	6.49	119.64	110.23
2	D	89	ALA	N-CA-C	-6.47	99.09	109.96
1	A	840	ILE	N-CA-C	-6.46	106.67	111.90
1	C	938	THR	CB-CA-C	-6.46	100.62	111.02
1	E	536	PHE	CA-CB-CG	-6.45	107.35	113.80
1	G	248	ILE	N-CA-C	-6.45	100.44	109.21
1	C	367	PHE	CA-CB-CG	-6.45	107.35	113.80
1	C	857	THR	CA-C-N	-6.44	113.45	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	857	THR	C-N-CA	-6.44	113.45	122.86
1	A	716	PRO	N-CA-CB	6.43	110.01	103.25
1	E	26	PHE	CA-CB-CG	-6.42	107.38	113.80
1	E	207	ASP	CA-CB-CG	6.41	119.01	112.60
1	G	995	HIS	CA-CB-CG	-6.40	107.40	113.80
1	C	67	GLU	O-C-N	6.37	125.79	121.71
1	C	659	VAL	N-CA-C	6.37	115.19	108.95
1	G	786	GLY	N-CA-C	-6.37	106.91	114.48
1	E	860	PRO	N-CA-CB	6.36	106.97	102.65
1	A	554	ASN	N-CA-CB	6.35	118.70	111.66
1	C	476	VAL	O-C-N	6.34	128.28	121.94
1	E	1000	HIS	CA-CB-CG	-6.32	107.48	113.80
1	C	516	LEU	N-CA-CB	-6.32	100.83	110.12
1	G	682	VAL	N-CA-C	-6.30	104.19	110.62
1	G	83	PRO	CB-CA-C	-6.30	103.16	111.23
2	B	370	PHE	CA-CB-CG	-6.29	107.51	113.80
2	D	215	ARG	CA-C-N	-6.29	113.50	122.94
2	D	215	ARG	C-N-CA	-6.29	113.50	122.94
1	C	988	PRO	CB-CA-C	-6.28	101.74	111.22
1	A	928	PHE	CA-CB-CG	-6.27	107.53	113.80
1	C	782	ILE	N-CA-C	-6.27	104.74	110.82
1	G	239	ALA	N-CA-C	6.26	117.96	110.19
1	E	733	ASP	CA-CB-CG	6.26	118.86	112.60
1	G	605	THR	N-CA-C	6.26	120.12	110.42
1	E	364	PHE	N-CA-C	6.26	118.90	111.33
1	A	532	CYS	N-CA-C	6.25	120.18	111.56
1	C	688	LYS	N-CA-C	6.24	118.46	108.41
1	G	536	PHE	CA-CB-CG	-6.24	107.56	113.80
2	B	214	CYS	N-CA-C	6.24	118.34	108.67
2	F	92	PHE	CA-CB-CG	-6.24	107.56	113.80
1	A	88	PRO	CB-CA-C	-6.21	101.31	111.56
1	A	304	VAL	N-CA-C	-6.21	103.28	110.05
1	C	961	ALA	CA-C-O	6.21	127.14	120.55
2	F	11	ASP	CA-CB-CG	6.21	118.81	112.60
1	E	716	PRO	N-CA-CB	6.21	109.11	103.34
1	G	210	LEU	N-CA-C	-6.21	103.86	112.30
1	A	992	ASN	N-CA-C	6.20	119.62	109.76
1	A	882	GLU	CA-C-N	-6.18	115.08	123.12
1	A	882	GLU	C-N-CA	-6.18	115.08	123.12
1	C	532	CYS	N-CA-C	6.17	120.07	111.56
1	G	518	ASP	O-C-N	6.15	128.41	122.07
2	B	53	VAL	N-CA-C	6.15	117.64	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	557	THR	CA-C-O	6.14	125.54	118.97
1	E	1028	VAL	CA-C-N	-6.12	112.72	120.56
1	E	1028	VAL	C-N-CA	-6.12	112.72	120.56
2	D	356	ALA	N-CA-C	6.10	120.21	109.96
1	E	209	SER	N-CA-C	6.10	119.19	110.10
1	C	57	ASP	CA-C-N	6.08	125.97	119.28
1	C	57	ASP	C-N-CA	6.08	125.97	119.28
1	C	209	SER	N-CA-C	6.07	119.26	110.28
1	C	172	PHE	CA-CB-CG	-6.05	107.75	113.80
1	E	559	ARG	CD-NE-CZ	6.05	132.87	124.40
2	B	204	ASN	N-CA-CB	6.04	119.00	109.82
1	G	1069	HIS	CA-CB-CG	-6.04	107.77	113.80
1	E	583	VAL	CA-C-N	6.03	128.64	120.38
1	E	583	VAL	C-N-CA	6.03	128.64	120.38
1	C	51	PRO	CB-CA-C	-6.03	103.31	112.11
1	G	584	HIS	CA-CB-CG	-6.03	107.78	113.80
1	C	88	PRO	CB-CA-C	-6.02	103.29	109.92
1	C	417	ASP	CB-CA-C	6.01	119.53	109.85
1	E	657	ALA	CA-C-N	-5.99	112.43	122.25
1	E	657	ALA	C-N-CA	-5.99	112.43	122.25
2	B	216	LEU	N-CA-C	5.97	119.45	109.95
1	E	625	ASP	CA-CB-CG	-5.96	106.64	112.60
1	E	255	THR	N-CA-C	5.96	119.86	112.59
2	H	215	ARG	N-CA-C	-5.95	101.67	110.48
1	G	543	MET	N-CA-C	5.94	119.24	109.85
2	B	162	VAL	CB-CA-C	-5.94	104.41	110.88
1	C	620	PRO	N-CA-CB	5.94	108.59	103.31
1	C	993	LYS	N-CA-C	-5.94	102.65	110.43
2	F	379[A]	LYS	N-CA-C	-5.93	105.14	112.38
2	F	379[B]	LYS	N-CA-C	-5.93	105.14	112.38
2	F	308	THR	N-CA-C	5.93	118.89	109.81
1	A	209	SER	N-CA-C	5.92	119.04	110.28
1	A	266	ASN	CA-C-N	5.91	128.12	120.44
1	A	266	ASN	C-N-CA	5.91	128.12	120.44
1	E	928	PHE	CA-CB-CG	-5.91	107.89	113.80
1	C	786	GLY	N-CA-C	-5.90	107.45	114.48
1	G	625	ASP	CA-CB-CG	-5.90	106.70	112.60
2	H	260	GLU	N-CA-C	-5.90	106.42	113.97
1	C	971	LEU	N-CA-C	5.90	119.33	109.95
1	A	558	ASP	N-CA-CB	-5.89	101.31	109.91
1	E	194	ARG	CA-C-N	5.87	126.46	119.94
1	E	194	ARG	C-N-CA	5.87	126.46	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	635	PRO	CB-CA-C	-5.87	102.36	111.40
1	C	482	THR	N-CA-CB	-5.87	101.48	110.16
2	F	58	PRO	N-CA-C	5.87	121.68	113.53
2	H	150	PHE	CA-C-O	5.87	124.64	119.71
1	A	57	ASP	CA-C-O	5.86	125.29	119.49
2	F	83	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	G	1036	TYR	CA-CB-CG	-5.85	103.38	113.90
1	C	210	LEU	N-CA-C	-5.84	104.36	112.30
1	E	571	ARG	CB-CA-C	-5.83	97.85	111.09
1	E	993	LYS	N-CA-C	-5.82	102.85	110.53
1	C	949	VAL	N-CA-C	5.82	117.55	109.29
1	G	367	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	993	LYS	N-CA-C	-5.80	101.70	110.28
2	H	346	PRO	N-CA-CB	5.80	106.31	102.25
1	G	344	THR	CB-CA-C	5.79	117.59	108.84
1	A	24	CYS	N-CA-C	5.79	119.16	111.75
1	C	517	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	A	417	ASP	CA-C-N	5.78	125.40	119.56
1	A	417	ASP	C-N-CA	5.78	125.40	119.56
1	A	575	GLY	N-CA-C	5.78	120.88	112.55
1	C	319	ILE	N-CA-C	5.78	116.24	110.23
1	G	554[A]	ASN	CA-CB-CG	5.78	118.38	112.60
1	G	554[B]	ASN	CA-CB-CG	5.78	118.38	112.60
1	G	918	MET	CA-C-N	-5.78	118.11	122.33
1	G	918	MET	C-N-CA	-5.78	118.11	122.33
1	A	348	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	949	VAL	N-CA-C	5.77	117.73	108.85
1	C	557	THR	CA-C-N	5.76	128.32	120.54
1	C	557	THR	C-N-CA	5.76	128.32	120.54
1	E	578	PHE	CA-CB-CG	-5.74	108.06	113.80
1	C	1069	HIS	CB-CA-C	5.73	121.24	110.63
2	D	215	ARG	O-C-N	-5.73	116.34	123.04
1	A	622	THR	CA-CB-OG1	-5.73	101.01	109.60
2	H	192	PHE	N-CA-C	5.72	118.99	110.52
2	F	53	VAL	N-CA-C	5.72	116.34	107.99
2	B	89	ALA	N-CA-C	-5.72	100.39	109.59
1	A	283	ASN	CA-CB-CG	5.71	118.31	112.60
2	F	321	LEU	N-CA-C	5.71	116.60	109.57
1	C	39	GLU	CB-CA-C	-5.71	101.32	110.79
1	A	61	ALA	N-CA-C	5.70	117.45	108.96
1	A	998	ARG	C-N-CD	-5.68	108.09	120.60
2	D	53	VAL	N-CA-C	5.68	116.92	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	240	MET	CA-C-N	-5.68	116.72	123.08
1	E	240	MET	C-N-CA	-5.68	116.72	123.08
1	E	408	GLY	N-CA-C	-5.67	102.72	110.20
1	A	225	ASN	CA-CB-CG	-5.67	106.93	112.60
2	H	195	VAL	N-CA-CB	5.67	117.79	110.99
1	G	980	VAL	N-CA-C	5.66	116.39	110.62
1	E	532	CYS	N-CA-C	5.66	119.29	111.71
1	C	248	ILE	N-CA-C	-5.65	101.44	108.89
2	D	261	THR	N-CA-CB	-5.65	102.59	110.38
1	G	900	PHE	CA-C-N	5.65	125.49	119.28
1	G	900	PHE	C-N-CA	5.65	125.49	119.28
1	A	635	PRO	CB-CA-C	-5.64	104.00	111.23
2	D	166	GLU	N-CA-CB	5.64	120.34	111.20
1	E	584	HIS	CA-CB-CG	-5.64	108.16	113.80
1	G	867	ARG	CA-CB-CG	-5.64	102.81	114.10
2	F	368	ASP	CB-CA-C	5.64	121.06	110.63
1	C	559	ARG	N-CA-C	5.63	118.44	109.65
1	E	999	PRO	N-CA-CB	5.62	108.78	102.60
2	H	11	ASP	CA-CB-CG	5.61	118.21	112.60
1	E	786	GLY	N-CA-C	-5.60	107.23	113.79
1	C	625	ASP	CA-CB-CG	-5.60	107.00	112.60
1	G	670	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	1012	TYR	CA-C-N	-5.60	114.64	122.75
1	A	1012	TYR	C-N-CA	-5.60	114.64	122.75
1	C	27	ASP	N-CA-C	-5.58	104.83	111.69
1	A	27	ASP	N-CA-C	-5.58	105.20	112.23
1	A	417	ASP	CA-C-O	5.57	123.44	119.32
1	C	204	LEU	CB-CA-C	-5.56	98.34	109.35
2	H	105	HIS	CA-CB-CG	-5.56	108.24	113.80
2	H	210	VAL	CB-CA-C	-5.56	104.76	112.04
1	G	859	VAL	CA-C-N	5.55	126.78	119.84
1	G	859	VAL	C-N-CA	5.55	126.78	119.84
1	A	560	GLU	N-CA-CB	5.55	119.52	110.37
2	D	186	LYS	CB-CA-C	5.55	119.54	109.83
1	E	1072	ILE	N-CA-C	5.54	116.75	108.54
1	A	793	ALA	N-CA-C	-5.54	102.33	110.52
2	D	136	ASP	CA-C-N	-5.54	116.69	122.89
2	D	136	ASP	C-N-CA	-5.54	116.69	122.89
2	F	183	GLN	N-CA-C	-5.54	102.69	110.50
1	E	575	GLY	O-C-N	5.53	128.68	122.82
2	F	356	ALA	N-CA-C	5.52	118.63	109.46
2	D	157	ASP	CA-CB-CG	5.52	118.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	660	PRO	N-CA-CB	5.52	106.41	102.65
1	E	992	ASN	CB-CA-C	-5.52	100.43	109.53
1	E	57	ASP	CA-C-N	5.51	125.86	119.47
1	E	57	ASP	C-N-CA	5.51	125.86	119.47
2	F	240	ASN	N-CA-C	-5.51	102.60	110.59
1	C	558	ASP	N-CA-C	5.50	117.71	111.11
1	E	424	ILE	CB-CA-C	-5.50	104.84	111.88
1	C	435	ARG	N-CA-C	5.50	120.44	111.37
2	B	303	ASN	CA-CB-CG	-5.49	107.11	112.60
2	D	324	ASN	N-CA-C	-5.49	106.43	113.02
1	G	640	VAL	CB-CA-C	-5.47	104.41	111.20
1	E	57	ASP	N-CA-CB	-5.47	101.09	110.01
2	D	367	PHE	CA-CB-CG	-5.47	108.33	113.80
1	C	678	PHE	CA-CB-CG	-5.47	108.33	113.80
1	C	554	ASN	CA-C-O	5.46	124.63	120.26
1	G	810	ARG	N-CA-CB	5.46	118.63	110.22
1	E	83	PRO	CB-CA-C	-5.46	103.95	111.21
1	G	715	ARG	CB-CA-C	-5.46	104.11	110.17
2	H	327	VAL	CB-CA-C	-5.45	105.34	111.23
1	C	996	GLU	CA-C-N	-5.45	110.74	121.41
1	C	996	GLU	C-N-CA	-5.45	110.74	121.41
1	A	51	PRO	CB-CA-C	-5.44	104.16	112.11
1	C	1060	GLU	N-CA-C	5.44	117.02	111.14
2	F	137	ASN	O-C-N	5.43	126.37	121.04
2	B	299	ASP	CA-CB-CG	5.43	118.03	112.60
1	E	885	PRO	CA-C-N	5.42	125.89	120.04
1	E	885	PRO	C-N-CA	5.42	125.89	120.04
1	G	807	ASP	CA-C-N	-5.42	113.73	120.56
1	G	807	ASP	C-N-CA	-5.42	113.73	120.56
1	C	23	ALA	N-CA-C	5.42	116.93	109.29
1	A	150	HIS	CA-CB-CG	-5.42	108.39	113.80
1	E	560	GLU	N-CA-C	-5.41	100.35	108.96
1	G	65	TYR	N-CA-C	5.41	117.81	107.75
2	F	10	GLU	CB-CG-CD	-5.40	103.42	112.60
1	C	908	GLY	CA-C-N	5.40	125.11	119.82
1	C	908	GLY	C-N-CA	5.40	125.11	119.82
1	C	821	GLN	CA-C-N	-5.39	113.62	121.71
1	C	821	GLN	C-N-CA	-5.39	113.62	121.71
1	E	4	ARG	CA-C-N	-5.39	113.26	122.11
1	E	4	ARG	C-N-CA	-5.39	113.26	122.11
1	G	20	ILE	CA-C-N	-5.39	114.98	122.86
1	G	20	ILE	C-N-CA	-5.39	114.98	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	VAL	CB-CA-C	-5.39	103.59	110.98
2	B	193	HIS	CA-CB-CG	-5.39	108.41	113.80
1	G	661	VAL	N-CA-C	5.38	115.33	108.12
1	E	557	THR	N-CA-C	-5.38	107.37	114.31
1	A	633	GLU	CA-C-N	-5.38	117.94	123.10
1	A	633	GLU	C-N-CA	-5.38	117.94	123.10
1	C	301	ASN	CA-C-N	5.38	126.56	119.84
1	C	301	ASN	C-N-CA	5.38	126.56	119.84
1	E	714	VAL	N-CA-C	5.38	115.05	106.88
2	B	32	PHE	CA-CB-CG	5.38	119.17	113.80
1	E	558	ASP	N-CA-CB	-5.37	101.42	110.49
1	A	1013	ILE	CA-C-N	-5.37	115.96	123.10
1	A	1013	ILE	C-N-CA	-5.37	115.96	123.10
1	G	682	VAL	O-C-N	5.37	127.08	121.87
1	G	711	PRO	N-CA-CB	5.37	108.51	102.60
1	G	518	ASP	CA-C-N	5.37	127.73	120.38
1	G	518	ASP	C-N-CA	5.37	127.73	120.38
1	E	316	GLY	N-CA-C	-5.37	107.86	115.43
1	E	868	VAL	CB-CA-C	-5.36	105.11	111.97
1	G	518	ASP	CA-CB-CG	-5.35	107.25	112.60
2	H	242	PRO	N-CA-C	5.34	119.00	110.40
1	E	755	PHE	CA-CB-CG	-5.34	108.46	113.80
1	E	248	ILE	N-CA-C	-5.34	101.84	108.89
1	A	1029	ILE	CB-CA-C	-5.34	105.03	112.02
1	E	404	VAL	N-CA-C	-5.34	107.10	112.17
2	F	133	ILE	N-CA-CB	5.32	118.56	111.64
1	A	911	MET	N-CA-C	5.32	118.22	109.76
1	C	339	ILE	N-CA-C	5.32	119.49	112.04
2	D	297	VAL	CA-C-N	-5.31	114.71	122.19
2	D	297	VAL	C-N-CA	-5.31	114.71	122.19
2	F	336	THR	N-CA-C	5.30	117.56	110.35
1	A	713	VAL	N-CA-CB	5.30	117.41	111.21
1	E	490	ARG	NE-CZ-NH1	5.29	126.79	121.50
2	B	332	LEU	CA-C-O	5.29	125.86	119.31
1	A	150	HIS	N-CA-C	-5.28	106.85	113.72
1	A	606	VAL	N-CA-C	-5.28	104.36	111.44
2	D	74	GLN	N-CA-C	5.28	116.17	108.14
2	B	19	ALA	CA-C-N	-5.28	116.24	122.36
2	B	19	ALA	C-N-CA	-5.28	116.24	122.36
1	A	700	MET	CA-C-N	5.28	127.81	120.63
1	A	700	MET	C-N-CA	5.28	127.81	120.63
1	C	169	ARG	CA-C-O	5.27	123.70	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	532	CYS	N-CA-C	5.26	118.82	111.56
1	G	558	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	726	GLU	N-CA-C	5.26	117.07	108.55
1	C	18	ILE	CB-CA-C	-5.26	104.32	111.15
1	G	1001	ILE	N-CA-CB	-5.25	102.56	111.23
1	C	902	GLY	CA-C-N	-5.25	114.89	122.45
1	C	902	GLY	C-N-CA	-5.25	114.89	122.45
2	D	214	CYS	N-CA-C	5.25	117.31	108.96
1	E	677	ARG	CA-C-O	5.25	126.52	120.90
1	E	555	PRO	N-CA-CB	5.25	107.92	103.35
1	C	445	ALA	CA-C-N	-5.24	114.35	122.69
1	C	445	ALA	C-N-CA	-5.24	114.35	122.69
2	H	203	ARG	N-CA-C	5.24	117.40	111.11
1	G	51	PRO	CB-CA-C	-5.24	104.03	112.21
1	A	142	GLU	CB-CA-C	5.24	118.47	109.51
2	B	327	VAL	CA-C-N	-5.24	113.52	122.11
2	B	327	VAL	C-N-CA	-5.24	113.52	122.11
1	G	781	HIS	CB-CA-C	-5.24	101.03	109.72
2	H	333	PHE	CA-CB-CG	-5.24	108.56	113.80
1	C	3	LYS	N-CA-C	5.23	117.81	109.96
1	A	339	ILE	N-CA-C	5.23	119.77	112.50
1	E	185	ARG	CD-NE-CZ	5.22	131.72	124.40
2	F	260	GLU	N-CA-C	-5.22	106.75	113.23
1	G	345	PRO	CB-CA-C	-5.22	103.33	111.22
1	G	578	PHE	CA-CB-CG	-5.22	108.58	113.80
1	C	906	LEU	N-CA-CB	-5.22	102.29	110.69
1	G	900	PHE	O-C-N	5.22	125.61	121.17
2	B	132	ILE	CB-CA-C	-5.22	102.88	110.81
1	C	407	THR	CA-C-O	5.22	124.93	119.03
1	C	65	TYR	N-CA-C	5.21	117.22	107.99
1	A	87	LEU	CA-C-O	5.20	123.92	119.71
1	C	431	ALA	N-CA-C	5.20	117.78	110.23
1	E	893	VAL	CB-CA-C	-5.20	104.62	111.70
2	D	76	HIS	CA-CB-CG	-5.19	108.61	113.80
1	C	417	ASP	CA-C-O	5.19	124.27	119.24
1	G	499	ASP	CB-CA-C	-5.19	101.86	110.68
2	H	369	HIS	CA-CB-CG	-5.19	108.61	113.80
2	F	10	GLU	N-CA-CB	5.18	118.33	110.14
1	E	230	ILE	CB-CA-C	-5.18	104.06	111.31
1	G	173	THR	N-CA-CB	5.18	120.70	111.69
1	A	975	HIS	N-CA-C	5.17	121.81	110.80
1	A	578	PHE	CA-CB-CG	-5.17	108.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	LEU	O-C-N	-5.16	117.33	123.22
1	E	562	ILE	N-CA-CB	5.16	118.84	111.82
2	B	112	ASP	N-CA-C	5.16	118.88	112.58
1	C	791	ASP	CA-CB-CG	-5.16	107.44	112.60
1	G	27	ASP	N-CA-C	-5.16	105.57	111.14
2	D	195	VAL	N-CA-CB	5.15	117.24	111.21
1	A	239	ALA	N-CA-C	5.15	116.58	110.19
2	B	308	THR	CB-CA-C	-5.15	100.56	110.24
1	C	835	ASN	CA-CB-CG	-5.15	107.45	112.60
1	E	64	THR	CA-C-N	-5.15	115.55	123.07
1	E	64	THR	C-N-CA	-5.15	115.55	123.07
1	E	317	PHE	CA-C-N	5.14	126.27	119.84
1	E	317	PHE	C-N-CA	5.14	126.27	119.84
2	D	86	PRO	CB-CA-C	-5.14	104.65	111.23
1	A	345	PRO	CB-CA-C	-5.14	103.15	110.75
1	A	755	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	1005	ILE	CA-C-N	-5.14	113.40	120.28
1	A	1005	ILE	C-N-CA	-5.14	113.40	120.28
1	E	612	THR	N-CA-C	5.14	117.78	111.82
1	C	665	SER	N-CA-C	5.13	116.98	109.84
2	F	70	GLU	CG-CD-OE2	-5.13	106.61	118.40
1	G	907	LEU	N-CA-C	5.13	118.07	110.48
1	G	425	ARG	N-CA-C	5.12	116.55	111.07
1	E	205	LEU	N-CA-CB	5.12	118.64	110.65
2	F	307	ILE	N-CA-C	-5.12	100.51	107.99
1	A	775	ILE	N-CA-CB	5.12	116.69	110.95
1	E	371	ASN	N-CA-C	-5.12	102.29	109.96
2	B	148	ARG	CA-C-N	5.11	127.13	120.28
2	B	148	ARG	C-N-CA	5.11	127.13	120.28
1	E	453	PHE	CA-CB-CG	-5.11	108.69	113.80
2	H	69	ASP	N-CA-C	5.11	119.15	113.02
2	D	48	TYR	CA-CB-CG	-5.10	104.72	113.90
1	C	457	ASN	CA-CB-CG	-5.10	107.50	112.60
2	F	215	ARG	N-CA-C	-5.10	101.40	109.76
1	G	44	VAL	N-CA-C	5.10	115.44	107.99
2	D	45	ASP	CA-CB-CG	5.10	117.70	112.60
1	E	543	MET	N-CA-C	5.09	117.90	109.85
2	B	379	LYS	CA-C-N	5.09	130.86	121.70
2	B	379	LYS	C-N-CA	5.09	130.86	121.70
2	H	369	HIS	CB-CA-C	-5.09	102.89	110.88
2	D	114	ASP	CA-CB-CG	5.09	117.69	112.60
1	G	210	LEU	N-CA-CB	5.08	119.93	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	271	VAL	N-CA-C	5.08	115.51	110.23
1	G	688	LYS	N-CA-C	5.07	116.96	107.99
2	D	260	GLU	N-CA-C	-5.07	107.23	113.41
2	D	132	ILE	CA-C-N	-5.06	115.95	122.99
2	D	132	ILE	C-N-CA	-5.06	115.95	122.99
1	C	233	SER	N-CA-C	-5.06	101.90	109.95
1	A	360	PRO	N-CA-CB	5.06	108.03	103.33
2	B	204	ASN	CA-CB-CG	5.06	117.66	112.60
1	G	1011	THR	N-CA-C	-5.06	107.15	113.72
1	E	305	SER	N-CA-C	5.05	114.81	108.45
2	B	324	ASN	CA-CB-CG	-5.04	107.56	112.60
1	E	785	ALA	CA-C-N	-5.04	117.44	123.44
1	E	785	ALA	C-N-CA	-5.04	117.44	123.44
1	G	316	GLY	N-CA-C	-5.04	108.33	115.43
1	A	289	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	343	ARG	N-CA-C	-5.03	105.26	111.40
2	H	193	HIS	CA-CB-CG	-5.03	108.77	113.80
2	D	240	ASN	N-CA-C	-5.03	103.30	110.59
1	C	154	GLU	CB-CG-CD	5.03	121.14	112.60
1	G	532	CYS	N-CA-CB	-5.03	104.25	111.54
1	A	524	PRO	CB-CA-C	-5.02	103.32	110.75
2	F	150	PHE	CA-C-N	5.02	124.80	119.28
2	F	150	PHE	C-N-CA	5.02	124.80	119.28
2	H	112	ASP	CA-C-N	-5.02	115.79	122.77
2	H	112	ASP	C-N-CA	-5.02	115.79	122.77
1	G	971	LEU	N-CA-C	5.02	117.67	109.59
2	H	168	TYR	N-CA-C	5.01	116.04	108.07
1	C	411	PRO	CB-CA-C	-5.01	105.00	111.46
2	H	288	PHE	CB-CA-C	5.00	117.48	109.27
1	C	329	GLY	N-CA-C	5.00	120.64	114.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	216	LEU	CA

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	8190	0	8213	248	0
1	C	8196	0	8236	252	0
1	E	8189	0	8219	270	0
1	G	8197	0	8218	348	0
2	B	2871	0	2850	225	0
2	D	2877	0	2852	111	0
2	F	2880	0	2859	161	0
2	H	2871	0	2850	213	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	5	0	0	1	0
4	B	1	0	0	0	0
4	C	6	0	0	1	0
4	D	1	0	0	0	0
4	E	6	0	0	1	0
4	F	1	0	0	0	0
4	G	6	0	0	0	0
5	A	5	0	0	0	0
5	B	1	0	0	0	0
5	C	7	0	0	1	0
5	D	1	0	0	1	0
5	E	6	0	0	0	0
5	F	1	0	0	0	0
5	G	6	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	3	0
7	C	54	0	24	1	0
7	E	54	0	24	1	0
7	G	54	0	24	0	0
8	A	9	0	11	0	0
8	C	9	0	11	2	0
8	E	9	0	11	1	0
8	G	9	0	11	2	0
9	A	9	0	20	3	0
9	C	9	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	9	0	20	0	0
9	G	9	0	20	0	0
10	A	793	0	0	25	0
10	B	130	0	0	3	0
10	C	681	0	0	14	0
10	D	177	0	0	2	0
10	E	813	0	0	19	0
10	F	205	0	0	10	0
10	G	645	0	0	15	0
10	H	117	0	0	6	0
All	All	48206	0	44517	1809	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 20.

All (1809) 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)
4:A:4009:K:K	10:A:4434:HOH:O	1.26	1.26
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.28	1.15
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.25	1.14
2:H:228:VAL:HA	2:H:231:MET:HE2	1.30	1.11
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.30	1.11
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.32	1.10
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.31	1.08
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.11	1.06
2:B:261:THR:HG22	2:B:263:ILE:H	1.12	1.06
1:C:1:MET:HB2	1:C:224:LYS:HE3	1.29	1.06
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.37	1.04
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.19	1.03
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.37	1.03
2:D:324:ASN:HD22	2:D:324:ASN:H	1.07	1.00
1:E:1:MET:HB2	1:E:224:LYS:HE3	1.43	1.00
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.45	0.98
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.27	0.98
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.29	0.96
4:E:4052:K:K	10:E:1604:HOH:O	1.76	0.96
2:B:324:ASN:HD22	2:B:324:ASN:H	1.14	0.96
2:B:324:ASN:HD22	2:B:324:ASN:N	1.58	0.96
1:E:784:GLN:HE21	1:E:784:GLN:H	0.96	0.95
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.49	0.94
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.49	0.94
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.31	0.94
2:H:354:PRO:HB3	2:H:363:ALA:HB1	1.49	0.94
1:G:698:ILE:HD12	1:G:698:ILE:H	1.31	0.93
1:A:784:GLN:HE21	1:A:784:GLN:H	0.93	0.93
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.48	0.92
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.85	0.92
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.84	0.92
2:F:196:ALA:HB3	2:F:218:ILE:HD12	1.50	0.92
2:H:261:THR:HG22	2:H:263:ILE:H	1.31	0.91
1:G:674:ASP:HB3	1:G:677:ARG:HB2	1.49	0.91
2:F:150:PHE:CD2	2:F:151:PRO:HD2	2.04	0.91
2:D:261:THR:HG23	2:D:263:ILE:H	1.35	0.90
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.54	0.90
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.02	0.89
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.53	0.89
2:B:376:GLN:HA	2:B:379:LYS:HZ3	1.34	0.89
2:F:286[A]:MET:HE3	2:F:289:GLY:HA2	1.53	0.89
2:D:187:GLU:HG2	2:D:215:ARG:CD	2.03	0.89
1:A:784:GLN:H	1:A:784:GLN:NE2	1.72	0.88
1:E:1:MET:HB2	1:E:224:LYS:CE	2.02	0.88
1:C:59:GLU:HG2	1:C:60:MET:HE2	1.55	0.88
1:E:57:ASP:HB3	1:E:59:GLU:OE1	1.74	0.88
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.03	0.88
2:D:286:MET:HE1	2:D:312:HIS:ND1	1.90	0.87
1:E:784:GLN:H	1:E:784:GLN:NE2	1.73	0.87
4:C:4029:K:K	10:C:4440:HOH:O	1.85	0.87
2:H:228:VAL:HA	2:H:231:MET:CE	2.04	0.87
2:B:324:ASN:H	2:B:324:ASN:ND2	1.72	0.86
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.57	0.86
1:G:784:GLN:NE2	1:G:784:GLN:H	1.73	0.86
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.91	0.86
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.38	0.86
1:G:563:MET:CE	1:G:635:PRO:HG3	2.06	0.85
2:D:324:ASN:HD22	2:D:324:ASN:N	1.72	0.85
1:C:728:VAL:CG1	1:C:733:ASP:HB3	2.04	0.85
1:A:59[B]:GLU:CG	1:A:60:MET:HE2	2.08	0.84
1:A:698:ILE:H	1:A:698:ILE:HD12	1.42	0.84
2:H:286:MET:HE3	2:H:289:GLY:HA2	1.60	0.84
2:H:324:ASN:N	2:H:324:ASN:HD22	1.73	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.14	0.83
1:A:339:ILE:HD12	1:A:530:ASP:HA	1.59	0.83
2:B:261:THR:HG22	2:B:263:ILE:N	1.94	0.82
2:D:324:ASN:H	2:D:324:ASN:ND2	1.77	0.82
1:G:828:VAL:HG13	1:G:842:VAL:HG22	1.61	0.82
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.94	0.82
1:E:698:ILE:H	1:E:698:ILE:HD12	1.41	0.82
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.15	0.82
2:F:261:THR:CG2	2:F:263:ILE:HG13	2.09	0.82
2:H:236:ILE:HB	2:H:265:VAL:CG2	2.10	0.82
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.61	0.81
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.16	0.81
1:G:784:GLN:H	1:G:784:GLN:HE21	1.28	0.81
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.11	0.81
1:G:726:GLU:HG3	1:G:727:ILE:N	1.95	0.81
1:E:806:GLN:HA	1:E:809:MET:HE3	1.63	0.80
2:F:324:ASN:H	2:F:324:ASN:HD22	1.29	0.80
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.64	0.80
1:C:1:MET:HE3	1:C:2:PRO:HD2	1.63	0.80
1:E:343:ARG:HG3	1:E:344:THR:HG23	1.62	0.80
2:F:354:PRO:HB3	2:F:363:ALA:CB	2.12	0.80
1:G:831:ALA:HB2	1:G:840:ILE:HD11	1.62	0.80
1:A:726:GLU:HG3	1:A:727:ILE:N	1.97	0.79
2:F:170:TRP:HB3	2:F:216:LEU:HD12	1.62	0.79
1:G:479:VAL:CG2	1:G:483:GLY:HA3	2.12	0.79
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.63	0.79
1:C:1:MET:HB2	1:C:224:LYS:CE	2.11	0.79
1:G:686:LYS:O	1:G:687:LEU:HD23	1.82	0.78
1:E:38:ARG:HH11	1:E:38:ARG:HG3	1.48	0.78
2:H:234:ASP:OD1	2:H:378:ARG:HD2	1.82	0.78
2:D:261:THR:CG2	2:D:263:ILE:H	1.95	0.78
1:C:726:GLU:HG3	1:C:727:ILE:N	1.98	0.78
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.65	0.78
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.65	0.78
2:B:226:GLU:O	2:B:230:LYS:HG3	1.84	0.77
1:E:698:ILE:O	1:E:702:VAL:HG23	1.84	0.77
1:E:559:ARG:HG3	1:E:559:ARG:HH21	1.49	0.77
2:F:354:PRO:HB3	2:F:363:ALA:HB2	1.66	0.77
2:H:228:VAL:O	2:H:231:MET:HG3	1.84	0.77
1:A:710:TYR:HA	1:A:712:LEU:HD13	1.66	0.77
1:C:59:GLU:CG	1:C:60:MET:HE2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:563[A]:MET:CE	1:E:635:PRO:HG3	2.15	0.77
1:E:103:GLU:HG3	1:E:104:ARG:N	2.00	0.77
1:C:772:MET:SD	1:C:880:THR:HG22	2.25	0.77
2:H:227:ASP:HA	2:H:230[B]:LYS:HD3	1.67	0.76
2:B:201:ALA:HB2	2:B:239:SER:CB	2.16	0.76
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.67	0.76
1:C:698:ILE:H	1:C:698:ILE:HD12	1.50	0.76
2:H:201:ALA:HB2	2:H:239:SER:CB	2.16	0.76
2:H:291:HIS:HA	2:H:310:GLN:O	1.85	0.76
2:H:150:PHE:CD2	2:H:151:PRO:HD2	2.20	0.76
2:B:196:ALA:HB3	2:B:218:ILE:HD12	1.66	0.76
1:C:822:VAL:O	1:C:823:ARG:HD3	1.86	0.76
2:H:324:ASN:O	2:H:342:ARG:HD2	1.86	0.76
2:B:345:LYS:HB3	2:B:346:PRO:HD2	1.68	0.75
1:A:946:LEU:C	1:A:947:LEU:HD12	2.10	0.75
2:F:306:MET:HE1	2:F:329:HIS:CD2	2.21	0.75
2:B:357:SER:HB3	2:B:358:PRO:C	2.11	0.75
1:G:339:ILE:HD12	1:G:530:ASP:HA	1.68	0.75
1:C:963:LYS:HA	1:C:966:LYS:HE3	1.68	0.75
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.02	0.75
2:F:261:THR:HG22	2:F:263:ILE:H	1.51	0.75
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.68	0.75
1:C:675:ARG:H	1:C:675:ARG:CD	2.01	0.74
1:G:130:ARG:O	1:G:134:VAL:HG23	1.86	0.74
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.69	0.74
2:F:228:VAL:HA	2:F:231:MET:HE2	1.69	0.74
2:H:259:LEU:HD13	2:H:342:ARG:NH1	2.01	0.74
1:E:941:LYS:NZ	10:E:2769:HOH:O	2.21	0.74
1:G:343:ARG:HG2	1:G:344:THR:HG23	1.69	0.74
2:D:71:GLU:O	2:D:203:ARG:HG3	1.88	0.74
2:F:272:HIS:HB2	2:F:349:SER:HB2	1.69	0.74
1:A:959:ASP:O	1:A:963:LYS:HG3	1.86	0.74
1:A:489:LEU:HD22	1:A:516:LEU:HD23	1.69	0.74
1:A:944:ARG:N	10:A:4490:HOH:O	2.20	0.74
1:C:973:ALA:O	1:C:991:VAL:HG12	1.88	0.74
1:A:1:MET:HB2	1:A:224:LYS:HE3	1.70	0.74
2:B:357:SER:H	2:B:358:PRO:HA	1.52	0.74
2:F:196:ALA:HB3	2:F:218:ILE:CD1	2.16	0.74
2:H:261:THR:CG2	2:H:263:ILE:HG13	2.18	0.74
1:E:646:THR:HB	1:E:647:PRO:HD3	1.70	0.73
2:F:334:ASP:OD2	2:F:336:THR:HG23	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.00	0.73
2:B:187:GLU:CG	2:B:215:ARG:HD2	2.16	0.73
1:C:950:ARG:HD2	1:C:1018:SER:HB2	1.67	0.73
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.88	0.73
1:G:872:LYS:HD3	1:G:877:GLN:HG2	1.70	0.73
1:G:873:SER:O	1:G:877:GLN:HG3	1.88	0.73
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.71	0.73
2:F:261:THR:CG2	2:F:263:ILE:H	2.01	0.73
2:F:364:ALA:HB3	2:F:365:PRO:HD3	1.71	0.73
2:B:232:ASN:N	2:B:233:PRO:HD3	2.03	0.73
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.04	0.73
1:A:804:GLU:HB2	10:A:4642:HOH:O	1.88	0.73
2:F:306:MET:HE1	2:F:329:HIS:HD2	1.52	0.73
1:G:525:VAL:HG22	1:G:548:GLU:H	1.53	0.73
2:B:324:ASN:O	2:B:342:ARG:HD2	1.89	0.72
2:F:228:VAL:O	2:F:231:MET:HG3	1.89	0.72
1:C:772:MET:CE	1:C:880:THR:HG22	2.19	0.72
1:A:697:ALA:O	1:A:700:MET:HB3	1.90	0.72
1:E:873:SER:O	1:E:877:GLN:HG3	1.89	0.72
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.70	0.72
2:B:139:ASP:OD2	2:B:142:LEU:HB2	1.88	0.72
2:D:357:SER:N	2:D:358:PRO:HA	2.04	0.72
2:H:236:ILE:HB	2:H:265:VAL:HG23	1.71	0.72
1:E:710:TYR:HB3	1:E:711:PRO:HA	1.71	0.72
2:F:228:VAL:HA	2:F:231:MET:CE	2.18	0.72
1:G:679:GLN:O	1:G:683:GLU:HG3	1.90	0.71
1:G:698:ILE:H	1:G:698:ILE:CD1	2.02	0.71
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.24	0.71
1:C:679:GLN:O	1:C:683:GLU:HG3	1.91	0.71
2:B:354:PRO:HB3	2:B:363:ALA:HA	1.71	0.71
1:E:726:GLU:HG3	1:E:727:ILE:N	2.05	0.71
1:G:343:ARG:CG	1:G:344:THR:HG23	2.19	0.71
2:H:376:GLN:HA	2:H:379:LYS:NZ	2.04	0.71
1:E:889:SER:HB3	1:E:918:MET:HE3	1.73	0.71
1:E:930:LYS:HE3	10:E:1236:HOH:O	1.91	0.71
2:F:194:VAL:HG13	2:F:235:GLY:O	1.90	0.71
1:E:1:MET:HB2	1:E:224:LYS:NZ	2.05	0.71
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.25	0.71
2:B:376:GLN:HA	2:B:379:LYS:NZ	2.04	0.70
2:D:170:TRP:HA	5:D:4043:CL:CL	2.27	0.70
2:B:228:VAL:HG11	2:B:258:PHE:CE1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8[B]:LYS:HD3	1:E:84:ASP:OD1	1.91	0.70
2:D:255:ILE:HA	2:D:258:PHE:CD2	2.26	0.70
1:G:318:PRO:HG3	1:G:610:TYR:OH	1.91	0.70
2:B:354:PRO:HG2	2:B:367:PHE:HE2	1.56	0.70
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.74	0.70
2:B:376:GLN:HG2	2:B:377:TYR:N	2.04	0.70
2:D:150:PHE:CD2	2:D:151:PRO:HD2	2.26	0.70
1:C:702:VAL:HG11	1:C:735:ARG:HH21	1.57	0.70
1:C:784:GLN:HE21	1:C:784:GLN:H	1.37	0.70
2:H:196:ALA:HA	2:H:237:PHE:O	1.91	0.70
2:B:286:MET:HE3	2:B:289:GLY:HA2	1.71	0.70
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.74	0.70
1:G:517:ARG:HB3	1:G:522:LEU:HB3	1.72	0.70
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.19	0.70
1:G:930:LYS:HE3	10:G:4146:HOH:O	1.91	0.69
2:D:201:ALA:HB2	2:D:239:SER:CB	2.23	0.69
1:G:495:LYS:NZ	10:G:4624:HOH:O	2.25	0.69
1:A:675:ARG:H	1:A:675:ARG:CD	2.01	0.69
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.74	0.69
2:H:251:ALA:O	2:H:255:ILE:HG13	1.93	0.69
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.21	0.69
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.40	0.69
1:A:65:TYR:OH	1:A:80:LYS:HE3	1.91	0.69
1:G:763:ASP:HB3	1:G:779:MET:HE3	1.75	0.69
1:A:130:ARG:HB2	1:A:148:ILE:HG13	1.73	0.69
1:A:273:ARG:HD2	10:A:4130:HOH:O	1.93	0.69
2:B:357:SER:N	2:B:358:PRO:HA	2.05	0.69
2:D:2:ILE:HG23	10:D:2901:HOH:O	1.92	0.69
2:H:254:ALA:O	2:H:257:LYS:HB2	1.93	0.69
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.75	0.69
2:H:106:ASN:C	2:H:107:ILE:HD13	2.17	0.69
2:F:204:ASN:ND2	2:F:205:ILE:HG12	2.08	0.69
1:A:675:ARG:O	1:A:679:GLN:HG3	1.93	0.68
2:B:259:LEU:O	2:B:345:LYS:HD2	1.93	0.68
1:C:804:GLU:O	1:C:808:VAL:HG23	1.93	0.68
1:E:680:HIS:O	1:E:683:GLU:HB2	1.94	0.68
1:C:946:LEU:C	1:C:947:LEU:HD12	2.19	0.68
2:B:202:LYS:HE2	2:B:204:ASN:HD21	1.59	0.68
1:C:1061:LYS:HD3	10:C:4615:HOH:O	1.93	0.68
2:F:357:SER:N	2:F:358:PRO:HA	2.08	0.68
2:H:272:HIS:CB	2:H:349:SER:HB2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ILE:CD1	1:A:530:ASP:HA	2.24	0.68
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.12	0.68
2:H:306:MET:HE2	2:H:329:HIS:HD2	1.59	0.68
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.76	0.67
1:C:953:ASP:HB3	1:C:1044:LEU:HD22	1.73	0.67
2:H:306:MET:HE1	2:H:350:PHE:CE1	2.29	0.67
1:C:1064:SER:O	1:C:1068:MET:HG3	1.94	0.67
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.58	0.67
1:G:951:GLU:OE1	1:G:954:LYS:HD2	1.94	0.67
9:A:4012:NET:H42	9:A:4012:NET:H22	1.77	0.67
2:D:298:LYS:HB2	2:D:332:LEU:HD11	1.76	0.67
1:E:222:ARG:NH1	1:E:278[B]:GLU:HG2	2.09	0.67
1:A:1020:ARG:O	1:A:1024:GLU:HG3	1.93	0.67
1:E:76:LYS:HE3	10:E:2548:HOH:O	1.94	0.67
2:F:199:PHE:O	2:F:241:GLY:HA3	1.94	0.67
2:H:357:SER:N	2:H:358:PRO:HA	2.09	0.67
2:H:273:GLN:O	2:H:276:ALA:HB3	1.94	0.67
1:A:772[B]:MET:HE3	10:A:4465:HOH:O	1.95	0.67
2:H:370:PHE:O	2:H:373:LEU:HB2	1.93	0.67
1:A:59[B]:GLU:HG3	1:A:60:MET:HE2	1.77	0.67
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.59	0.67
2:H:199:PHE:O	2:H:241:GLY:HA3	1.94	0.67
1:C:4:ARG:HD3	1:C:7:ILE:CD1	2.21	0.66
2:D:81:VAL:HG22	2:D:110:ILE:CG2	2.25	0.66
2:D:199:PHE:O	2:D:241:GLY:HA3	1.94	0.66
1:E:730:ASP:OD2	1:E:733:ASP:HB2	1.95	0.66
1:E:738:PHE:O	1:E:741:ALA:HB3	1.95	0.66
2:H:354:PRO:HB3	2:H:363:ALA:CB	2.24	0.66
2:H:133:ILE:HD12	2:H:143:ALA:CB	2.18	0.66
1:A:166:CYS:C	1:A:167:ILE:HD12	2.19	0.66
2:B:286:MET:HE1	2:B:312:HIS:ND1	2.11	0.66
1:C:32:GLN:OE1	1:C:320:ALA:HB3	1.96	0.66
1:A:58:PRO:HD2	1:A:59[A]:GLU:OE2	1.96	0.66
2:H:170:TRP:HA	10:H:3185:HOH:O	1.96	0.66
1:E:222:ARG:CZ	1:E:278[B]:GLU:HG2	2.26	0.66
1:E:417:ASP:OD1	1:E:423:LYS:NZ	2.29	0.66
1:E:784:GLN:HE21	1:E:784:GLN:N	1.81	0.66
1:A:930:LYS:HE3	10:A:4080:HOH:O	1.96	0.66
2:B:375:GLU:O	2:B:376:GLN:C	2.38	0.66
2:F:224:SER:OG	2:F:227:ASP:HB2	1.95	0.66
1:C:902:GLY:O	1:C:1027:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.96	0.66
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.78	0.66
1:C:38:ARG:HG3	1:C:38:ARG:NH1	1.99	0.66
1:C:1020:ARG:O	1:C:1024:GLU:HG3	1.95	0.66
1:A:1069:HIS:HA	1:A:1072:ILE:HD12	1.78	0.65
2:B:219:VAL:HG23	2:B:220:PRO:O	1.95	0.65
2:F:324:ASN:HD22	2:F:324:ASN:N	1.94	0.65
1:C:772:MET:HE1	1:C:880:THR:CB	2.25	0.65
2:H:164:THR:HG21	2:H:168:TYR:HE1	1.61	0.65
1:A:1073:LYS:N	1:A:1073:LYS:HD3	2.12	0.65
2:B:71:GLU:O	2:B:203:ARG:HG3	1.95	0.65
2:F:261:THR:HG21	2:F:263:ILE:HG13	1.76	0.65
2:H:274:LEU:HD23	2:H:277:LEU:HD12	1.79	0.65
1:A:715:ARG:NH2	7:A:4007:ADP:O1A	2.30	0.65
2:B:187:GLU:HG2	2:B:215:ARG:CD	2.17	0.65
2:D:120:ARG:HB2	10:D:1026:HOH:O	1.96	0.65
2:D:286:MET:HE2	2:D:314:PHE:C	2.21	0.65
1:E:845:ARG:NH1	1:E:846:ALA:O	2.30	0.65
2:D:274:LEU:O	2:D:275:LEU:C	2.37	0.65
2:D:357:SER:H	2:D:358:PRO:HA	1.61	0.65
2:F:154:ASN:HD22	2:F:155:GLY:N	1.94	0.65
2:F:258:PHE:O	2:F:261:THR:HB	1.97	0.65
2:F:133:ILE:HD12	2:F:143:ALA:HB2	1.78	0.65
1:G:735:ARG:O	1:G:738:PHE:N	2.30	0.65
2:B:201:ALA:HB2	2:B:239:SER:OG	1.97	0.65
1:C:726:GLU:HG3	1:C:727:ILE:H	1.61	0.65
2:H:218:ILE:N	2:H:218:ILE:HD13	2.12	0.65
1:E:4:ARG:HD3	1:E:7:ILE:HD12	1.79	0.64
2:B:168:TYR:O	2:B:218:ILE:N	2.29	0.64
2:D:152:GLY:O	2:D:156:MET:HE3	1.96	0.64
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.79	0.64
2:H:298:LYS:NZ	10:H:3040:HOH:O	2.30	0.64
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.32	0.64
1:A:735:ARG:O	1:A:738:PHE:N	2.30	0.64
2:F:205:ILE:HG22	2:F:367:PHE:HZ	1.62	0.64
2:H:324:ASN:HA	2:H:343:THR:OG1	1.97	0.64
2:H:324:ASN:HB2	2:H:344:ASP:OD2	1.94	0.64
2:B:205:ILE:O	2:B:208:MET:HB2	1.96	0.64
1:C:79:GLU:HA	1:C:111:PHE:CE2	2.33	0.64
2:D:290:HIS:HB3	2:D:310:GLN:HB3	1.80	0.64
2:F:363:ALA:O	2:F:366:LEU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:ILE:CD1	1:G:530:ASP:HA	2.27	0.64
1:G:709:GLY:O	1:G:754:HIS:ND1	2.29	0.64
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.97	0.64
1:G:704:LYS:O	1:G:707:GLU:HB2	1.97	0.64
2:H:261:THR:HG21	2:H:263:ILE:HG13	1.78	0.64
2:B:135:GLY:O	2:B:138:PRO:HD3	1.98	0.64
2:D:277:LEU:HD21	2:D:283:THR:HG23	1.79	0.64
2:H:160:LYS:HE3	2:H:161:GLU:OE2	1.97	0.64
1:E:688:LYS:HD3	1:E:838:TYR:CE1	2.32	0.64
1:E:698:ILE:HD12	1:E:698:ILE:N	2.13	0.64
2:H:258:PHE:O	2:H:261:THR:HB	1.97	0.64
2:H:103:LYS:O	2:H:106:ASN:N	2.30	0.64
2:H:195:VAL:HG22	2:H:217:THR:HB	1.79	0.64
2:H:324:ASN:HD22	2:H:324:ASN:H	1.45	0.64
1:A:563:MET:CE	1:A:635:PRO:HG3	2.27	0.64
2:D:255:ILE:HA	2:D:258:PHE:HD2	1.62	0.64
2:F:223:THR:HG22	2:F:228:VAL:HG23	1.80	0.64
1:C:698:ILE:H	1:C:698:ILE:CD1	2.11	0.64
1:C:734:LEU:HD22	1:C:738:PHE:CD2	2.32	0.64
1:C:1037:LYS:HA	10:C:4613:HOH:O	1.98	0.64
2:F:318:GLU:O	2:F:321:LEU:HB2	1.98	0.64
1:G:1014:ILE:HD12	1:G:1015:ASN:N	2.13	0.64
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.44	0.63
2:D:228:VAL:HG12	2:D:229:LEU:N	2.13	0.63
1:E:315:THR:O	1:E:531:THR:HG22	1.98	0.63
1:E:686:LYS:O	1:E:687:LEU:HD23	1.97	0.63
1:G:1061:LYS:NZ	10:G:4665:HOH:O	2.31	0.63
2:H:274:LEU:O	2:H:275:LEU:C	2.39	0.63
2:D:251:ALA:O	2:D:255:ILE:HG13	1.99	0.63
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.16	0.63
1:E:563[A]:MET:HE3	1:E:635:PRO:HG3	1.79	0.63
1:E:1017:THR:HG21	1:E:1023:ILE:HA	1.80	0.63
1:G:100:LEU:N	1:G:100:LEU:HD12	2.14	0.63
1:G:527:LYS:HD2	2:H:116:ARG:HD3	1.80	0.63
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.34	0.63
1:G:667:ASP:OD2	1:G:677:ARG:NH2	2.30	0.63
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.81	0.63
1:E:726:GLU:OE1	1:E:1020:ARG:NE	2.29	0.63
1:G:475:LYS:HD3	1:G:488:PHE:CZ	2.33	0.63
1:G:490:ARG:NH2	10:G:4419:HOH:O	2.31	0.63
2:B:157:ASP:OD1	2:B:160:LYS:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:THR:O	1:G:343:ARG:NE	2.29	0.63
1:G:734:LEU:HD22	1:G:738:PHE:CE2	2.33	0.63
2:H:83:ARG:HD2	2:H:83:ARG:O	1.99	0.63
1:C:509:ARG:HD3	10:C:4385:HOH:O	1.99	0.62
1:G:702:VAL:O	1:G:706:LYS:HD3	1.98	0.62
2:H:133:ILE:HG22	2:H:138:PRO:HB3	1.80	0.62
2:B:378:ARG:C	2:B:380:THR:H	2.06	0.62
1:E:930:LYS:NZ	1:E:1058:ALA:O	2.33	0.62
1:G:588:ALA:O	1:G:591:GLU:HB3	1.98	0.62
1:A:947:LEU:HD12	1:A:947:LEU:N	2.14	0.62
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.45	0.62
2:H:364:ALA:N	2:H:365:PRO:HD2	2.14	0.62
2:F:196:ALA:CB	2:F:218:ILE:HD12	2.28	0.62
1:G:695:VAL:HG22	1:G:700:MET:HG2	1.82	0.62
2:H:357:SER:H	2:H:358:PRO:HA	1.62	0.62
2:B:78:GLN:NE2	2:B:78:GLN:HA	2.15	0.62
1:C:681:ALA:O	1:C:684:ARG:HB3	1.99	0.62
1:E:645:GLN:HG3	1:E:649:LYS:HE3	1.82	0.62
1:E:806:GLN:HA	1:E:809:MET:CE	2.30	0.62
2:F:298:LYS:NZ	10:F:2619:HOH:O	2.32	0.62
1:G:668:ALA:O	1:G:671:ARG:HB2	2.00	0.62
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.80	0.62
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.82	0.62
1:C:947:LEU:HD12	1:C:947:LEU:N	2.15	0.62
1:E:340:THR:O	1:E:343:ARG:NE	2.31	0.62
2:H:345:LYS:HB3	2:H:346:PRO:HD2	1.80	0.62
2:B:6:LEU:HD12	2:B:7:LEU:N	2.15	0.62
2:B:186:LYS:O	2:B:189:GLU:HB2	2.00	0.62
1:C:906:LEU:HD13	1:C:1030:ARG:NE	2.14	0.62
2:B:218:ILE:N	2:B:218:ILE:HD13	2.15	0.62
1:C:715:ARG:NH2	7:C:4027:ADP:O1A	2.29	0.62
1:E:478:GLU:HB3	1:E:479:VAL:HG13	1.81	0.62
2:F:187:GLU:HG2	2:F:215:ARG:HD3	1.81	0.62
1:A:43:ARG:NH2	1:A:81:GLU:OE2	2.30	0.61
1:E:959:ASP:O	1:E:963:LYS:HG3	2.00	0.61
2:F:376:GLN:HA	2:F:379[A]:LYS:NZ	2.15	0.61
1:G:905:PRO:HB2	1:G:1040:TYR:OH	2.00	0.61
2:F:74:GLN:NE2	10:F:3611:HOH:O	2.32	0.61
2:H:364:ALA:O	2:H:368:ASP:N	2.30	0.61
1:C:998:ARG:HG3	1:C:999:PRO:HA	1.81	0.61
1:E:59:GLU:CD	1:E:59:GLU:H	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:SER:OG	1:E:302:PRO:HA	2.00	0.61
1:C:959:ASP:O	1:C:962:ALA:HB3	2.01	0.61
1:E:267:ALA:O	1:E:271:VAL:HG23	2.01	0.61
1:G:1000:HIS:NE2	1:G:1003:ASP:OD1	2.33	0.61
1:C:259:LYS:HD3	2:D:175:TRP:CE3	2.36	0.61
2:F:306:MET:CE	2:F:329:HIS:HD2	2.14	0.61
1:G:874:LEU:HB3	1:G:879:VAL:O	2.01	0.61
2:F:232:ASN:N	2:F:233:PRO:HD3	2.15	0.61
1:A:734:LEU:HD22	1:A:738:PHE:CE2	2.35	0.61
2:B:375:GLU:O	2:B:377:TYR:N	2.34	0.61
1:C:671:ARG:HG2	1:C:677:ARG:HD2	1.83	0.61
1:C:772:MET:HE1	1:C:880:THR:CA	2.31	0.61
2:F:225:ALA:O	2:F:229:LEU:HG	2.01	0.61
1:G:680:HIS:O	1:G:683:GLU:HB2	2.01	0.61
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.66	0.61
2:H:232:ASN:N	2:H:233:PRO:HD3	2.15	0.61
1:A:784:GLN:HE21	1:A:784:GLN:N	1.79	0.60
1:C:321:LYS:NZ	1:C:611:ASP:OD1	2.29	0.60
2:H:376:GLN:HA	2:H:379:LYS:HZ2	1.66	0.60
2:F:300:VAL:HG22	2:F:328:THR:O	2.01	0.60
1:G:1017:THR:HG22	1:G:1023:ILE:HG13	1.82	0.60
2:H:199:PHE:HB3	2:H:270:LEU:HD23	1.83	0.60
1:C:951:GLU:O	1:C:954:LYS:HB2	2.00	0.60
2:F:342:ARG:NH2	2:F:344:ASP:OD1	2.32	0.60
2:F:364:ALA:HB3	2:F:365:PRO:CD	2.31	0.60
2:B:116:ARG:O	2:B:120:ARG:HG3	2.01	0.60
1:C:950:ARG:HG2	1:C:1016:THR:OG1	2.01	0.60
1:G:64:THR:O	1:G:1065:VAL:HG23	2.01	0.60
1:G:784:GLN:HE21	1:G:784:GLN:N	1.98	0.60
1:A:709:GLY:O	1:A:754:HIS:ND1	2.29	0.60
1:C:751:LEU:O	1:C:752:LEU:HD12	2.02	0.60
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.83	0.60
2:F:253:THR:O	2:F:256:GLN:HB2	2.02	0.60
1:E:714:VAL:HG13	1:E:752:LEU:CD1	2.32	0.60
2:H:225:ALA:HB3	2:H:257:LYS:HG2	1.83	0.60
2:B:261:THR:HG21	2:B:263:ILE:HD12	1.84	0.60
1:C:772:MET:HE1	1:C:880:THR:HG22	1.83	0.60
1:E:679:GLN:HG3	1:E:689:GLN:HE22	1.66	0.60
2:F:261:THR:HG23	2:F:263:ILE:HG13	1.84	0.60
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.28	0.60
2:H:107:ILE:HD13	2:H:107:ILE:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:227:ASP:O	2:H:230[A]:LYS:HB2	2.02	0.60
1:A:583:VAL:O	1:A:587:LEU:HG	2.01	0.60
2:B:172:GLN:O	2:B:207:ARG:HA	2.02	0.60
2:B:324:ASN:HA	2:B:343:THR:OG1	2.02	0.60
2:B:345:LYS:HB3	2:B:346:PRO:CD	2.32	0.60
1:E:1:MET:HE3	1:E:2:PRO:HD2	1.82	0.60
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.15	0.60
1:A:730:ASP:OD2	1:A:733:ASP:HB2	2.02	0.60
1:C:907:LEU:HD11	8:C:4031:ORN:HD3	1.83	0.60
2:D:26:ALA:O	2:D:131:CYS:HA	2.02	0.60
2:D:364:ALA:N	2:D:365:PRO:HD3	2.17	0.60
1:A:150:HIS:N	1:A:154:GLU:OE1	2.30	0.59
1:A:504[B]:LYS:HB3	10:A:4325:HOH:O	2.01	0.59
1:E:591:GLU:HG3	1:E:591:GLU:O	2.02	0.59
1:G:646:THR:HB	1:G:647:PRO:HD3	1.84	0.59
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.84	0.59
1:G:711:PRO:HG2	1:G:755:PHE:HD2	1.66	0.59
1:E:478:GLU:HA	10:E:1520:HOH:O	2.00	0.59
1:A:65:TYR:CG	1:A:77:ILE:HD13	2.38	0.59
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.51	0.59
2:B:63:VAL:O	2:B:94:ASN:HB2	2.02	0.59
2:B:183:GLN:HA	2:B:183:GLN:HE21	1.68	0.59
2:H:23:THR:HG23	2:H:134:ALA:O	2.01	0.59
2:H:306:MET:HE2	2:H:329:HIS:CD2	2.36	0.59
1:A:1026:SER:HB2	1:A:1030:ARG:HH12	1.67	0.59
1:G:147:GLY:O	1:G:205:LEU:HD12	2.01	0.59
1:G:419:GLU:HB2	1:G:423:LYS:HE3	1.83	0.59
1:G:586:SER:O	1:G:587:LEU:C	2.45	0.59
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.37	0.59
1:C:672:ALA:HB3	1:C:844:PRO:HG3	1.84	0.59
1:G:946:LEU:HB3	1:G:1013:ILE:HG12	1.83	0.59
1:G:973:ALA:O	1:G:990:LEU:HD12	2.02	0.59
1:A:420:ALA:HA	1:A:423:LYS:HD2	1.83	0.59
2:F:334:ASP:CG	2:F:336:THR:HG23	2.28	0.59
1:E:734:LEU:HD22	1:E:738:PHE:CD2	2.38	0.59
2:H:184:ALA:N	10:H:2978:HOH:O	2.31	0.59
1:A:698:ILE:H	1:A:698:ILE:CD1	2.13	0.59
2:B:258:PHE:O	2:B:261:THR:HB	2.02	0.59
1:C:858:GLY:HA2	1:C:1069:HIS:NE2	2.17	0.59
1:G:726:GLU:HG3	1:G:727:ILE:H	1.68	0.59
2:H:142:LEU:O	2:H:146:LYS:HG3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:244:ASP:OD2	2:F:245:PRO:HD2	2.03	0.59
2:B:363:ALA:O	2:B:366:LEU:HB2	2.03	0.59
1:E:209:SER:OG	1:E:211:ILE:HG13	2.01	0.59
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.33	0.59
1:A:477:ALA:HB3	10:A:4355:HOH:O	2.01	0.58
1:C:698:ILE:HD12	1:C:698:ILE:N	2.15	0.58
1:E:59:GLU:OE1	10:E:1581:HOH:O	2.16	0.58
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.38	0.58
1:C:967:GLN:HG2	1:C:1054:LEU:HD13	1.84	0.58
2:H:48:TYR:HA	2:H:51:GLN:NE2	2.18	0.58
1:A:698:ILE:O	1:A:701:ALA:HB3	2.04	0.58
1:A:1000:HIS:O	1:A:1003:ASP:HB2	2.04	0.58
2:F:254:ALA:O	2:F:257:LYS:HB2	2.03	0.58
2:H:193:HIS:N	2:H:234:ASP:OD2	2.37	0.58
1:C:710:TYR:HB3	1:C:711:PRO:HA	1.85	0.58
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.85	0.58
1:G:678:PHE:O	1:G:682:VAL:HG23	2.03	0.58
1:G:901:PRO:HD2	5:G:4083:CL:CL	2.39	0.58
1:A:1061:LYS:NZ	10:A:4658:HOH:O	2.35	0.58
2:B:228:VAL:HG12	2:B:229:LEU:N	2.19	0.58
1:G:150:HIS:N	1:G:154:GLU:OE1	2.35	0.58
1:G:803:GLN:HG3	1:G:807:ASP:OD1	2.03	0.58
1:C:873:SER:O	1:C:877:GLN:HG3	2.04	0.58
1:G:1041:ASP:HA	8:G:4076:ORN:O	2.03	0.58
1:C:421:LEU:HB3	1:G:421:LEU:HB3	1.84	0.58
1:E:139:ILE:HD11	1:E:141:LEU:HD12	1.86	0.58
2:D:196:ALA:HA	2:D:237:PHE:O	2.03	0.58
2:D:298:LYS:HB2	2:D:332:LEU:CD1	2.33	0.58
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.39	0.58
1:A:710:TYR:HA	1:A:712:LEU:CD1	2.33	0.58
2:B:160:LYS:HE3	2:B:161:GLU:OE2	2.04	0.58
1:C:906:LEU:HD13	1:C:1030:ARG:CD	2.33	0.58
1:C:953:ASP:CB	1:C:1044:LEU:HD22	2.34	0.58
2:D:228:VAL:O	2:D:231:MET:HG3	2.04	0.58
1:C:677:ARG:O	1:C:680:HIS:HB2	2.04	0.58
1:C:993:LYS:HD2	1:C:996:GLU:OE2	2.03	0.58
1:G:101:GLU:OE2	1:G:104:ARG:NH2	2.30	0.58
1:G:872:LYS:O	1:G:877:GLN:NE2	2.29	0.58
1:A:737:TYR:CE1	1:A:741:ALA:HB2	2.39	0.57
1:G:561:LYS:HE2	10:G:4453:HOH:O	2.03	0.57
1:C:9:SER:O	1:C:84:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:GLU:O	1:C:706:LYS:HB2	2.04	0.57
2:F:117:LYS:HE3	10:F:1560:HOH:O	2.03	0.57
1:G:427:GLU:HG3	1:G:438:TYR:CE1	2.39	0.57
1:A:904:ASP:OD2	1:A:905:PRO:HD2	2.04	0.57
1:A:1031:ARG:HB2	10:A:4508:HOH:O	2.04	0.57
1:C:781:HIS:HE1	1:C:789:SER:HB3	1.70	0.57
2:H:139:ASP:OD2	2:H:142:LEU:HB2	2.03	0.57
2:H:318:GLU:HA	2:H:321:LEU:HD13	1.86	0.57
1:E:976:GLY:O	1:E:980:VAL:HG23	2.04	0.57
1:G:224:LYS:HE2	1:G:329:GLY:O	2.05	0.57
2:D:6:LEU:O	2:D:133:ILE:N	2.35	0.57
1:G:223:ASP:CG	1:G:227:ASN:HB2	2.28	0.57
1:G:426:ARG:C	1:G:426:ARG:HD3	2.29	0.57
2:H:255:ILE:HA	2:H:258:PHE:CD2	2.40	0.57
2:B:170:TRP:HA	10:B:4092:HOH:O	2.03	0.57
1:E:27:ASP:OD2	1:E:55:MET:HB3	2.05	0.57
1:E:144:ALA:HB1	1:E:208:GLU:HG2	1.85	0.57
1:E:783:GLU:OE1	8:E:4054:ORN:NE	2.38	0.57
1:E:831:ALA:HB2	1:E:840:ILE:HD11	1.84	0.57
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.22	0.57
1:G:663:GLY:O	1:G:664:THR:C	2.47	0.57
1:G:686:LYS:C	1:G:687:LEU:HD23	2.30	0.57
1:G:697:ALA:O	1:G:700:MET:HB3	2.05	0.57
1:C:1067:GLU:O	1:C:1070:ALA:HB3	2.05	0.57
2:D:222:GLN:O	2:D:223:THR:C	2.45	0.57
1:E:27:ASP:OD2	1:E:53:THR:HB	2.04	0.57
1:E:998:ARG:HA	1:E:999:PRO:C	2.27	0.57
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.12	0.57
2:H:253:THR:O	2:H:256:GLN:HB2	2.04	0.57
2:H:369:HIS:O	2:H:370:PHE:C	2.45	0.57
1:E:736:ARG:O	1:E:739:GLN:HB3	2.04	0.57
1:G:1:MET:HB3	1:G:2:PRO:HD2	1.86	0.57
1:G:118:ALA:HA	10:G:4315:HOH:O	2.04	0.57
1:G:868:VAL:HG23	1:G:877:GLN:HE22	1.69	0.57
1:C:784:GLN:H	1:C:784:GLN:NE2	2.02	0.57
1:E:503:ALA:HB1	1:E:508:VAL:O	2.05	0.57
1:E:714:VAL:HG13	1:E:752:LEU:HD11	1.87	0.57
2:D:6:LEU:HD12	2:D:7:LEU:H	1.69	0.57
1:E:695:VAL:HA	1:E:700:MET:HE2	1.87	0.57
2:F:223:THR:CG2	2:F:228:VAL:HG23	2.35	0.57
2:H:254:ALA:O	2:H:255:ILE:C	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:MET:O	2:D:211:ASP:HB2	2.04	0.56
2:F:279:SER:HB2	2:F:325:LEU:HD11	1.86	0.56
2:H:286:MET:HB2	2:H:313:GLY:O	2.05	0.56
1:A:70:HIS:O	1:A:74:VAL:HG23	2.05	0.56
1:C:482:THR:HG22	10:C:4369:HOH:O	2.04	0.56
2:D:375:GLU:O	2:D:376:GLN:C	2.48	0.56
2:H:190:LEU:HD23	2:H:213:GLY:HA2	1.87	0.56
1:A:89:THR:O	1:A:304:VAL:HG22	2.05	0.56
1:A:392:GLN:OE1	1:A:495:LYS:HD3	2.06	0.56
1:A:467:GLU:O	1:A:471:ARG:HG2	2.05	0.56
1:A:951:GLU:OE1	1:A:951:GLU:HA	2.04	0.56
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.86	0.56
1:C:622:THR:O	1:C:626:VAL:HG23	2.04	0.56
1:E:110:GLU:HG2	1:E:111:PHE:CE1	2.40	0.56
1:E:258:ASP:O	1:E:262:GLN:HG2	2.04	0.56
2:F:354:PRO:CB	2:F:363:ALA:HB2	2.34	0.56
2:H:246:ALA:HB3	2:H:247:PRO:HD3	1.86	0.56
1:A:252:PRO:O	1:A:254:GLN:NE2	2.38	0.56
1:A:831:ALA:HB2	1:A:840:ILE:HD11	1.88	0.56
1:G:712:LEU:HD23	1:G:752:LEU:HG	1.86	0.56
1:G:891:LYS:HG2	1:G:892:GLU:N	2.16	0.56
1:A:728:VAL:HG11	1:A:734:LEU:HA	1.88	0.56
2:B:144:LEU:O	2:B:148:ARG:HG3	2.06	0.56
2:B:234:ASP:OD1	2:B:378:ARG:HD2	2.05	0.56
1:E:349:GLU:O	2:F:294:ASN:HB2	2.06	0.56
1:A:728:VAL:HG12	1:A:733:ASP:HB3	1.84	0.56
1:A:972:ASP:OD1	1:A:989:ARG:HB3	2.05	0.56
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.04	0.56
1:G:65:TYR:CG	1:G:77:ILE:HD13	2.40	0.56
1:G:481:ILE:HD12	1:G:508:VAL:HG11	1.88	0.56
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.38	0.56
2:D:259:LEU:O	2:D:345:LYS:HE3	2.05	0.56
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.86	0.56
1:A:223:ASP:CG	1:A:227:ASN:HB2	2.31	0.56
1:A:426:ARG:C	1:A:426:ARG:HD3	2.31	0.56
1:E:1026:SER:CB	1:E:1030:ARG:HH12	2.18	0.56
1:G:1014:ILE:HD12	1:G:1014:ILE:C	2.31	0.56
1:C:4:ARG:CD	1:C:7:ILE:HD12	2.23	0.56
2:H:261:THR:HG22	2:H:263:ILE:N	2.13	0.56
2:H:324:ASN:ND2	2:H:324:ASN:N	2.45	0.56
1:C:343:ARG:HG3	1:C:344:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:PHE:HA	1:E:165:PRO:C	2.30	0.56
1:G:974:THR:O	1:G:975:HIS:C	2.49	0.56
1:A:816:LEU:HD11	1:A:839:LEU:HD21	1.87	0.55
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.40	0.55
1:C:417:ASP:OD2	1:C:419:GLU:HB2	2.05	0.55
2:F:322:PRO:HD2	2:F:325:LEU:HD12	1.88	0.55
1:G:470:VAL:O	1:G:474:GLU:HG3	2.06	0.55
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.38	0.55
2:H:261:THR:HG22	2:H:262:ASP:N	2.20	0.55
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.30	0.55
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.88	0.55
1:C:770:GLY:HA3	1:C:823:ARG:CZ	2.36	0.55
2:D:174:SER:O	2:D:182:PRO:HD3	2.05	0.55
2:B:104:ARG:HG2	2:B:105:HIS:CD2	2.40	0.55
1:C:860:PRO:HB2	1:C:863:LYS:HB2	1.87	0.55
1:G:412:LYS:HE3	1:G:434:ASP:OD2	2.07	0.55
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.42	0.55
1:E:1026:SER:O	1:E:1027:ARG:C	2.47	0.55
1:A:805:ILE:HD12	1:A:835:ASN:ND2	2.21	0.55
1:E:146:SER:HB2	1:E:206:ILE:O	2.07	0.55
1:G:995:HIS:H	1:G:995:HIS:CD2	2.24	0.55
1:C:142:GLU:HG2	1:C:296:ILE:HG12	1.89	0.55
1:E:667:ASP:OD2	1:E:677:ARG:NH2	2.30	0.55
2:H:286:MET:CE	2:H:289:GLY:HA2	2.36	0.55
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.37	0.55
1:A:958:VAL:HG22	1:A:981:LEU:HD23	1.88	0.55
2:B:334:ASP:CG	2:B:336:THR:HG23	2.32	0.55
2:D:286:MET:HE3	2:D:313:GLY:C	2.31	0.55
1:E:761:GLU:HB3	1:E:781:HIS:ND1	2.21	0.55
1:E:967[A]:GLN:HG3	1:E:1054:LEU:HB3	1.89	0.55
1:G:148:ILE:HD13	1:G:204:LEU:O	2.07	0.55
1:C:904:ASP:HB2	1:C:1027:ARG:NH1	2.22	0.55
1:E:688:LYS:HD3	1:E:838:TYR:CZ	2.42	0.55
2:F:317:ASP:OD1	2:F:320:THR:HG23	2.06	0.55
1:A:479:VAL:HB	1:A:483:GLY:HA3	1.88	0.55
1:C:158:VAL:O	1:C:161:ASP:HB3	2.07	0.55
2:D:48:TYR:HA	2:D:51:GLN:NE2	2.22	0.55
2:D:285:LYS:HB2	2:D:314:PHE:CE1	2.41	0.55
2:F:324:ASN:HA	2:F:343:THR:OG1	2.06	0.55
2:B:41:GLU:HG3	2:B:69:ASP:O	2.08	0.54
2:B:290:HIS:HB2	2:B:312:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:VAL:HG21	1:C:728:VAL:HG21	1.88	0.54
2:D:6:LEU:HD12	2:D:15:PHE:O	2.07	0.54
1:G:384:VAL:HG22	1:G:385:MET:N	2.22	0.54
1:A:523:HIS:HB3	1:A:524:PRO:HD2	1.89	0.54
1:C:734:LEU:HD22	1:C:738:PHE:CE2	2.43	0.54
1:E:1026:SER:HB2	1:E:1030:ARG:HH12	1.73	0.54
1:G:79:GLU:HG2	1:G:111:PHE:CE2	2.42	0.54
2:B:334:ASP:OD2	2:B:336:THR:HG23	2.08	0.54
1:A:220:VAL:O	1:A:281:GLY:HA2	2.07	0.54
1:G:738:PHE:O	1:G:739:GLN:C	2.50	0.54
2:B:175:TRP:HA	2:B:180:GLY:O	2.07	0.54
2:B:202:LYS:HE2	2:B:204:ASN:ND2	2.22	0.54
1:C:939:MET:HE3	1:C:1054:LEU:HD21	1.90	0.54
1:E:906:LEU:CD2	1:E:1023:ILE:HG23	2.38	0.54
2:F:286[A]:MET:HE2	2:F:313:GLY:C	2.33	0.54
1:G:164:PHE:HB3	1:G:165:PRO:HA	1.89	0.54
2:H:201:ALA:HB2	2:H:239:SER:HB2	1.89	0.54
1:E:479:VAL:CG2	1:E:483:GLY:HA3	2.37	0.54
1:A:79:GLU:HB2	1:A:111:PHE:CZ	2.43	0.54
2:D:212:ARG:HH21	2:D:364:ALA:CB	2.21	0.54
1:E:726:GLU:OE2	1:E:736:ARG:NH2	2.41	0.54
1:C:58:PRO:HD2	1:C:59:GLU:OE2	2.08	0.54
2:F:234:ASP:HB3	2:F:374:ILE:CG2	2.38	0.54
1:G:738:PHE:O	1:G:741:ALA:HB3	2.08	0.54
2:H:133:ILE:CD1	2:H:143:ALA:HB2	2.18	0.54
1:G:672:ALA:HB3	1:G:844:PRO:HG3	1.90	0.54
2:H:345:LYS:HB3	2:H:346:PRO:CD	2.38	0.54
2:B:249:ASP:OD1	2:B:250:TYR:N	2.40	0.54
2:D:290:HIS:HB2	2:D:312:HIS:CD2	2.44	0.54
2:D:318:GLU:O	2:D:321:LEU:HB2	2.08	0.54
1:E:110:GLU:HG2	1:E:111:PHE:CD1	2.43	0.54
1:E:998:ARG:CB	1:E:999:PRO:HA	2.38	0.54
2:F:46:PRO:O	2:F:242:PRO:HG3	2.08	0.54
2:F:376:GLN:HA	2:F:379[A]:LYS:HZ2	1.71	0.54
1:G:479:VAL:HG23	1:G:483:GLY:HA3	1.86	0.54
1:G:892:GLU:OE1	8:G:4076:ORN:NE	2.41	0.54
2:H:297:VAL:CG1	2:H:306:MET:HE3	2.38	0.54
2:H:297:VAL:HG11	2:H:306:MET:HE3	1.90	0.54
1:A:710:TYR:OH	1:A:734:LEU:HD12	2.08	0.53
2:B:272:HIS:HB2	2:B:349:SER:HB2	1.89	0.53
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:SER:O	1:C:666:PRO:C	2.51	0.53
1:E:679:GLN:O	1:E:683:GLU:HG3	2.09	0.53
1:G:73:VAL:O	1:G:77:ILE:HG13	2.08	0.53
1:G:1017:THR:CG2	1:G:1023:ILE:HG13	2.37	0.53
1:E:702:VAL:HG13	1:E:731:GLU:HG2	1.89	0.53
2:F:139:ASP:HB3	2:F:142:LEU:HB3	1.90	0.53
1:G:728:VAL:HG11	1:G:734:LEU:CA	2.34	0.53
1:G:1001:ILE:HG22	1:G:1002:GLN:N	2.24	0.53
2:B:39:TYR:CZ	2:B:61:GLY:HA2	2.44	0.53
1:E:59:GLU:OE2	1:E:59:GLU:N	2.40	0.53
1:E:417:ASP:HB3	1:E:420:ALA:CB	2.39	0.53
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.08	0.53
2:B:191:PRO:HD2	2:B:213:GLY:O	2.08	0.53
2:D:286:MET:HE2	2:D:314:PHE:O	2.07	0.53
2:F:251:ALA:O	2:F:252:ILE:C	2.49	0.53
1:G:645[B]:GLN:HG3	1:G:649:LYS:HE3	1.91	0.53
1:G:685:LEU:HD13	1:G:815:LYS:HB3	1.90	0.53
2:H:259:LEU:HD13	2:H:342:ARG:HH12	1.72	0.53
2:F:193:HIS:N	2:F:234:ASP:OD2	2.30	0.53
2:F:203:ARG:NH2	10:F:3236:HOH:O	2.28	0.53
2:F:252:ILE:HG23	2:F:278:ALA:HA	1.89	0.53
1:G:29:SER:HB3	1:G:304:VAL:HG21	1.91	0.53
1:G:806:GLN:HA	1:G:809:MET:HE2	1.91	0.53
2:B:45:ASP:O	2:B:76:HIS:HB2	2.08	0.53
2:B:46:PRO:O	2:B:242:PRO:HG3	2.08	0.53
2:F:272:HIS:CB	2:F:349:SER:HB2	2.37	0.53
1:G:693:ALA:HB3	1:G:708:ILE:HD11	1.91	0.53
1:A:734:LEU:HD22	1:A:738:PHE:HE2	1.72	0.53
1:A:1072:ILE:C	1:A:1073:LYS:HD3	2.34	0.53
2:B:86:PRO:HA	10:B:4038:HOH:O	2.09	0.53
1:G:796:LEU:HD23	1:G:796:LEU:C	2.34	0.53
2:H:323:ALA:C	2:H:325:LEU:H	2.17	0.53
1:A:59[A]:GLU:HG3	1:A:60:MET:HE2	1.89	0.53
2:B:222:GLN:HE21	2:B:222:GLN:H	1.55	0.53
2:B:364:ALA:O	2:B:365:PRO:C	2.52	0.53
1:C:511:ALA:O	1:C:515:LYS:HG3	2.08	0.53
1:E:158:VAL:HG11	1:E:206:ILE:HB	1.90	0.53
2:F:125:LYS:HD3	10:F:3194:HOH:O	2.09	0.53
2:H:34:THR:HA	2:H:56:THR:OG1	2.08	0.53
2:H:277:LEU:HD21	2:H:283:THR:HG23	1.89	0.53
1:A:59[B]:GLU:HG2	1:A:60:MET:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:526:TYR:CE1	1:E:545:SER:HB3	2.43	0.53
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.43	0.53
2:H:363:ALA:O	2:H:367:PHE:N	2.39	0.53
1:A:417:ASP:OD2	1:A:418:PRO:HD2	2.08	0.52
1:C:11:LEU:HA	1:C:45:ILE:O	2.09	0.52
1:A:128:ASP:CG	1:A:131:ARG:HG3	2.34	0.52
1:A:421:LEU:HB3	1:E:421:LEU:HB3	1.91	0.52
1:C:561:LYS:O	1:C:562:ILE:HD13	2.09	0.52
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.38	0.52
1:E:967[B]:GLN:OE1	1:E:1055:ASN:ND2	2.43	0.52
1:G:768:CYS:HB2	1:G:773:VAL:HG22	1.90	0.52
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.92	0.52
1:A:1027:ARG:HA	1:A:1030:ARG:NH2	2.24	0.52
1:C:1031:ARG:NH2	10:C:4611:HOH:O	2.43	0.52
1:E:967[B]:GLN:HG2	1:E:1054:LEU:HB3	1.91	0.52
1:G:579:ASP:O	1:G:583:VAL:HG23	2.10	0.52
1:A:103:GLU:HG3	1:A:104:ARG:N	2.16	0.52
1:C:78:ILE:O	1:C:82:ARG:N	2.31	0.52
1:E:912:ARG:NH2	10:E:3602:HOH:O	2.38	0.52
2:F:259:LEU:O	2:F:345:LYS:HD2	2.10	0.52
2:H:366:LEU:O	2:H:369:HIS:HB3	2.09	0.52
1:C:809:MET:O	1:C:813:VAL:HG23	2.09	0.52
1:G:223:ASP:OD2	1:G:227:ASN:HB2	2.09	0.52
1:G:343:ARG:HG3	1:G:344:THR:HG23	1.88	0.52
1:G:972:ASP:OD1	1:G:989:ARG:HB3	2.09	0.52
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.15	0.52
1:A:702:VAL:HG13	1:A:731:GLU:HG2	1.91	0.52
2:B:284:VAL:O	2:B:314:PHE:HB3	2.10	0.52
1:C:126:ALA:HB3	1:C:302:PRO:HG3	1.92	0.52
1:C:571:ARG:HD3	1:C:574:GLN:HB2	1.92	0.52
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.39	0.52
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.75	0.52
1:G:164:PHE:CB	1:G:165:PRO:HA	2.38	0.52
1:G:308:SER:HB3	10:G:4280:HOH:O	2.09	0.52
1:A:1006:LYS:O	1:A:1006:LYS:HG3	2.09	0.52
2:B:327:VAL:HG13	2:B:337:LEU:CD1	2.39	0.52
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.91	0.52
1:E:130:ARG:O	1:E:134:VAL:HG23	2.10	0.52
2:F:246:ALA:N	2:F:247:PRO:HD2	2.24	0.52
2:H:272:HIS:HA	2:H:349:SER:CB	2.39	0.52
1:A:1063:ILE:HD13	1:A:1068:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:THR:HG23	2:D:262:ASP:N	2.24	0.52
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.39	0.52
1:G:679:GLN:HG3	1:G:689:GLN:HE22	1.75	0.52
1:C:763:ASP:HB3	1:C:779:MET:HE3	1.91	0.52
1:E:726:GLU:HG3	1:E:727:ILE:H	1.70	0.52
1:G:690:PRO:HG3	1:G:756:LEU:HD11	1.91	0.52
2:H:173:GLY:O	2:H:207:ARG:HG2	2.10	0.52
2:H:324:ASN:ND2	2:H:324:ASN:H	2.06	0.52
2:B:157:ASP:CG	2:B:160:LYS:HG2	2.34	0.52
1:C:224:LYS:HE2	1:C:329:GLY:O	2.10	0.52
1:C:796:LEU:HD23	1:C:796:LEU:C	2.35	0.52
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.45	0.52
1:E:944:ARG:HG2	1:E:1010:TYR:HD1	1.74	0.52
1:G:828:VAL:HG13	1:G:842:VAL:CG2	2.37	0.52
1:G:954:LYS:O	1:G:980:VAL:HG11	2.10	0.52
2:H:226:GLU:O	2:H:230[A]:LYS:HG3	2.09	0.52
2:B:249:ASP:HA	2:B:252:ILE:HG13	1.91	0.51
1:G:69:ILE:O	1:G:69:ILE:HG22	2.11	0.51
1:G:98:CYS:O	1:G:99:ALA:C	2.51	0.51
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.75	0.51
2:H:45:ASP:CG	2:H:202:LYS:HD2	2.36	0.51
1:A:675:ARG:H	1:A:675:ARG:HD3	1.74	0.51
2:B:254:ALA:O	2:B:257[B]:LYS:HB2	2.09	0.51
1:E:648:LEU:CD2	1:E:845:ARG:HD3	2.40	0.51
1:E:734:LEU:HD22	1:E:738:PHE:CE2	2.44	0.51
1:G:1063:ILE:HG13	1:G:1067:GLU:OE2	2.11	0.51
2:H:71:GLU:O	2:H:203:ARG:HG3	2.10	0.51
2:H:369:HIS:CE1	2:H:373:LEU:HG	2.45	0.51
9:A:4012:NET:H42	9:A:4012:NET:C2	2.40	0.51
1:C:674:ASP:OD2	1:C:677:ARG:HB2	2.11	0.51
1:E:101:GLU:OE2	1:E:104:ARG:NH2	2.30	0.51
1:G:358:LYS:HG2	1:G:359:ILE:N	2.22	0.51
2:H:201:ALA:HB2	2:H:239:SER:HG	1.75	0.51
1:G:950:ARG:HG3	1:G:1016:THR:OG1	2.09	0.51
2:B:51:GLN:O	2:B:78:GLN:N	2.42	0.51
1:C:500:ALA:O	1:C:504:LYS:HG3	2.09	0.51
1:G:710:TYR:HA	1:G:711:PRO:C	2.34	0.51
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.93	0.51
2:H:265:VAL:O	2:H:347:ALA:HA	2.10	0.51
1:C:772:MET:HE1	1:C:880:THR:CG2	2.40	0.51
1:G:784:GLN:HE22	1:G:1043:THR:HB	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:VAL:HG22	1:A:548:GLU:H	1.76	0.51
1:A:733:ASP:O	1:A:736:ARG:HB3	2.10	0.51
2:B:228:VAL:O	2:B:231:MET:HG3	2.10	0.51
2:B:317:ASP:O	2:B:321:LEU:HD13	2.09	0.51
1:E:509:ARG:HH11	1:E:512:GLU:HG3	1.75	0.51
1:G:561:LYS:O	1:G:562:ILE:HD13	2.11	0.51
1:G:735:ARG:O	1:G:736:ARG:C	2.54	0.51
2:H:214:CYS:SG	2:H:371:ILE:HD11	2.50	0.51
2:H:222:GLN:O	2:H:223:THR:O	2.29	0.51
2:F:218:ILE:HD13	2:F:218:ILE:N	2.25	0.51
1:G:333:ASP:OD1	1:G:333:ASP:N	2.43	0.51
2:H:169:SER:HA	2:H:216:LEU:O	2.11	0.51
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.91	0.51
1:E:464:VAL:HG11	2:F:88:ILE:HD13	1.93	0.51
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.26	0.51
1:G:947:LEU:HA	1:G:1014:ILE:CG2	2.41	0.51
1:A:780:GLU:OE2	1:A:798:ALA:HB1	2.10	0.51
2:B:10:GLU:HG3	2:B:129:ASN:O	2.11	0.51
1:E:475:LYS:HD3	1:E:488:PHE:CZ	2.46	0.51
1:G:24:CYS:O	1:G:25:GLU:C	2.51	0.51
1:A:737:TYR:CZ	1:A:741:ALA:HB2	2.46	0.50
2:B:13:THR:HG22	2:B:15:PHE:CE2	2.46	0.50
1:E:6:ASP:OD2	1:E:6:ASP:N	2.44	0.50
1:E:1021:ARG:O	1:E:1025:ASP:OD2	2.29	0.50
1:C:57:ASP:HB2	1:C:60:MET:HG2	1.93	0.50
1:E:840:ILE:O	1:E:841:GLU:HB3	2.11	0.50
1:A:504[A]:LYS:HB3	10:A:4325:HOH:O	2.11	0.50
1:G:135:ALA:HB1	1:G:274:GLU:HG3	1.93	0.50
1:G:757:ASP:O	1:G:758:ASP:C	2.55	0.50
1:G:1026:SER:CB	1:G:1030:ARG:HH12	2.24	0.50
1:A:361:ARG:CZ	1:A:404:VAL:HG12	2.41	0.50
2:B:236:ILE:HB	2:B:265:VAL:HG22	1.94	0.50
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.11	0.50
1:E:755:PHE:CE1	7:E:4050:ADP:C2	2.99	0.50
1:G:713:VAL:O	1:G:713:VAL:HG12	2.11	0.50
1:G:734:LEU:HD22	1:G:738:PHE:CD2	2.46	0.50
1:G:947:LEU:HG	1:G:1014:ILE:CG2	2.40	0.50
1:A:775:ILE:HG13	1:A:810:ARG:HG2	1.94	0.50
1:C:340:THR:O	1:C:343:ARG:HG2	2.12	0.50
1:E:8[A]:LYS:NZ	10:E:2527:HOH:O	2.43	0.50
2:F:234:ASP:HB3	2:F:374:ILE:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:235:GLY:HA2	2:H:264:PRO:HD2	1.93	0.50
1:A:165:PRO:HA	1:A:182:ALA:O	2.12	0.50
1:A:167:ILE:HD12	1:A:167:ILE:N	2.25	0.50
2:B:224:SER:O	2:B:225:ALA:C	2.54	0.50
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.11	0.50
1:G:711:PRO:O	1:G:712:LEU:HD12	2.11	0.50
2:B:173:GLY:C	2:B:207:ARG:HB3	2.36	0.50
2:B:231:MET:O	2:B:232:ASN:O	2.30	0.50
2:B:255:ILE:HG22	2:B:278:ALA:CB	2.42	0.50
2:D:286:MET:HE1	2:D:312:HIS:CE1	2.46	0.50
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.47	0.50
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.29	0.50
1:G:731:GLU:O	1:G:735:ARG:HG3	2.12	0.50
1:A:99:ALA:HB1	1:A:115:MET:HE2	1.93	0.50
2:B:245:PRO:C	2:B:247:PRO:HD2	2.37	0.50
1:C:343:ARG:HD2	1:C:536:PHE:HB3	1.93	0.50
1:G:220:VAL:O	1:G:281:GLY:HA2	2.11	0.50
1:G:941:LYS:NZ	1:G:1056:ALA:O	2.34	0.50
2:B:222:GLN:HG3	2:B:250:TYR:CD1	2.47	0.49
2:B:254:ALA:O	2:B:257[A]:LYS:HB2	2.11	0.49
1:C:130:ARG:HD2	10:C:4522:HOH:O	2.11	0.49
1:E:563[A]:MET:HE1	1:E:635:PRO:HG3	1.92	0.49
2:F:286[A]:MET:CE	2:F:289:GLY:HA2	2.35	0.49
1:G:461:TRP:O	1:G:465:GLN:HG3	2.11	0.49
1:G:695:VAL:HG21	1:G:701:ALA:CA	2.36	0.49
1:A:751:LEU:O	1:A:752:LEU:HD12	2.12	0.49
2:B:176:THR:O	2:B:180:GLY:N	2.37	0.49
2:B:222:GLN:O	2:B:223:THR:C	2.55	0.49
2:B:324:ASN:HB2	2:B:342:ARG:HE	1.77	0.49
1:C:475:LYS:O	1:C:479:VAL:HG22	2.13	0.49
1:E:686:LYS:C	1:E:687:LEU:HD23	2.37	0.49
1:E:809:MET:O	1:E:813:VAL:HG23	2.12	0.49
1:G:597:ILE:HG12	1:G:615:ARG:HB2	1.93	0.49
1:G:802:SER:OG	1:G:805:ILE:HB	2.12	0.49
1:G:873:SER:OG	1:G:876:GLU:HG3	2.12	0.49
10:G:4302:HOH:O	2:H:37:THR:HG22	2.13	0.49
2:B:158:LEU:HD12	2:B:243:GLY:CA	2.42	0.49
2:H:251:ALA:O	2:H:252:ILE:C	2.55	0.49
1:A:331:THR:OG1	1:A:334:GLU:HG3	2.12	0.49
1:A:560:GLU:OE1	1:A:636:LYS:HE3	2.11	0.49
1:C:145[B]:ARG:HB3	1:C:208:GLU:CD	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:CG	1:C:227:ASN:HB2	2.37	0.49
1:E:442:ALA:O	1:E:447:LEU:HB2	2.13	0.49
1:G:757:ASP:O	1:G:833:LYS:HE3	2.11	0.49
1:A:548:GLU:OE2	2:B:83:ARG:NE	2.43	0.49
1:A:993:LYS:HB2	1:A:996:GLU:OE1	2.12	0.49
1:C:262:GLN:OE1	1:C:262:GLN:HA	2.11	0.49
1:C:344:THR:HB	1:C:345:PRO:HD2	1.95	0.49
1:E:339:ILE:HD11	1:E:531:THR:HG23	1.94	0.49
2:F:154:ASN:HD22	2:F:154:ASN:C	2.19	0.49
2:H:201:ALA:HB2	2:H:239:SER:OG	2.12	0.49
2:F:46:PRO:HA	2:F:76:HIS:CG	2.47	0.49
1:G:79:GLU:HG2	1:G:111:PHE:CZ	2.48	0.49
1:G:471:ARG:HH21	1:G:474:GLU:CD	2.21	0.49
1:G:965:LEU:HG	1:G:971:LEU:HD11	1.95	0.49
2:H:184:ALA:O	2:H:185:LYS:O	2.29	0.49
2:H:227:ASP:O	2:H:230[B]:LYS:HB2	2.11	0.49
1:A:11:LEU:HA	1:A:45:ILE:O	2.13	0.49
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.47	0.49
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.42	0.49
1:C:324:ALA:O	1:C:327:ALA:HB3	2.12	0.49
1:C:420:ALA:O	1:C:421:LEU:C	2.55	0.49
1:C:554:ASN:N	1:C:555:PRO:HD3	2.27	0.49
1:G:563:MET:HE1	1:G:635:PRO:HG3	1.92	0.49
1:G:651:ALA:O	1:G:652:ARG:C	2.54	0.49
1:A:698:ILE:HD12	1:A:698:ILE:N	2.19	0.49
1:A:814:GLN:NE2	10:A:4443:HOH:O	2.45	0.49
1:A:957:VAL:O	1:A:958:VAL:C	2.52	0.49
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.94	0.49
2:D:290:HIS:HB3	2:D:310:GLN:CB	2.42	0.49
2:D:290:HIS:HB2	2:D:312:HIS:NE2	2.28	0.49
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.48	0.49
2:H:186:LYS:O	2:H:189:GLU:HB2	2.13	0.49
2:B:263:ILE:HG23	2:B:264:PRO:HD2	1.93	0.49
1:E:18:ILE:HD12	1:E:23:ALA:HA	1.95	0.49
1:E:808:VAL:HA	10:E:1628:HOH:O	2.13	0.49
2:F:350:PHE:HB2	2:F:366:LEU:HD13	1.94	0.49
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.94	0.49
2:H:63:VAL:HG12	2:H:91:ASN:HB2	1.94	0.49
2:H:350:PHE:CG	2:H:366:LEU:HD11	2.48	0.49
1:A:501:ARG:NH1	10:A:4325:HOH:O	2.43	0.49
2:B:231:MET:O	2:B:232:ASN:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:O	1:E:329:GLY:O	2.30	0.49
2:F:125:LYS:HB2	10:F:3196:HOH:O	2.12	0.49
1:G:698:ILE:O	1:G:701:ALA:HB3	2.13	0.49
1:A:696:THR:OG1	1:A:700:MET:HE1	2.13	0.48
1:A:943:GLY:C	10:A:4490:HOH:O	2.56	0.48
1:A:954:LYS:O	1:A:957:VAL:HG12	2.13	0.48
1:C:180:GLY:HA2	1:C:376:THR:OG1	2.13	0.48
1:E:224:LYS:HE2	1:E:329:GLY:O	2.14	0.48
1:E:708:ILE:HD12	1:E:752:LEU:HB3	1.94	0.48
1:E:944:ARG:HG2	1:E:1010:TYR:CD1	2.46	0.48
2:H:264:PRO:HA	2:H:346:PRO:O	2.14	0.48
1:A:534:ALA:O	2:B:123:ARG:NH1	2.36	0.48
1:A:692:ASN:HA	1:A:752:LEU:O	2.13	0.48
2:B:371:ILE:O	2:B:374:ILE:N	2.46	0.48
2:F:195:VAL:HG23	2:F:233:PRO:HB3	1.94	0.48
1:G:1:MET:O	1:G:334:GLU:OE1	2.31	0.48
1:G:167:ILE:HD12	1:G:167:ILE:N	2.28	0.48
2:H:25:SER:HB2	2:H:133:ILE:HG12	1.95	0.48
2:B:166:GLU:O	2:B:167:ALA:O	2.32	0.48
2:B:285:LYS:HB2	2:B:314:PHE:CD1	2.49	0.48
1:C:615:ARG:NE	1:C:633:GLU:OE1	2.45	0.48
2:H:131:CYS:SG	2:H:133:ILE:HG13	2.53	0.48
1:A:222:ARG:HD3	1:A:277:VAL:O	2.13	0.48
1:A:503:ALA:HB2	1:A:510:GLU:HA	1.94	0.48
2:B:249:ASP:CA	2:B:252:ILE:HG13	2.44	0.48
2:B:285:LYS:HG3	2:B:314:PHE:CD1	2.48	0.48
2:B:341:HIS:CG	2:B:348:PHE:HB3	2.49	0.48
1:C:145[A]:ARG:HB3	1:C:208:GLU:HG2	1.96	0.48
1:C:953:ASP:OD1	1:C:1016:THR:OG1	2.29	0.48
1:E:343:ARG:HD2	1:E:536:PHE:HB3	1.95	0.48
1:E:417:ASP:OD2	1:E:418:PRO:HD2	2.13	0.48
2:F:363:ALA:C	2:F:365:PRO:HD2	2.38	0.48
1:G:710:TYR:HB3	1:G:711:PRO:HA	1.96	0.48
2:H:150:PHE:CG	2:H:151:PRO:HD2	2.48	0.48
1:A:863:LYS:NZ	10:A:4411:HOH:O	2.45	0.48
2:B:203:ARG:O	2:B:207:ARG:HG3	2.14	0.48
1:C:712:LEU:O	1:C:727:ILE:HA	2.12	0.48
1:C:1017[B]:THR:HG21	1:C:1023:ILE:HA	1.95	0.48
1:G:257:THR:O	1:G:258:ASP:C	2.56	0.48
1:G:598:MET:HG3	1:G:599:VAL:N	2.27	0.48
2:H:23:THR:HG22	2:H:24:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLU:HG2	1:A:497:PHE:CE1	2.48	0.48
1:A:735:ARG:O	1:A:736:ARG:C	2.56	0.48
2:B:174:SER:O	2:B:182:PRO:HD3	2.13	0.48
1:C:950:ARG:CD	1:C:1018:SER:HB2	2.40	0.48
1:E:698:ILE:H	1:E:698:ILE:CD1	2.14	0.48
1:E:750:VAL:HG12	1:E:752:LEU:HD13	1.95	0.48
1:E:1017:THR:HG21	1:E:1023:ILE:CA	2.44	0.48
2:F:324:ASN:ND2	2:F:324:ASN:H	2.05	0.48
2:F:363:ALA:O	2:F:364:ALA:C	2.57	0.48
1:G:336:MET:HB3	1:G:342:GLY:HA2	1.96	0.48
1:G:805:ILE:HD13	1:G:832:VAL:HG11	1.96	0.48
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.48	0.48
2:H:255:ILE:HA	2:H:258:PHE:HD2	1.77	0.48
1:A:133:ASP:HB2	10:A:4119:HOH:O	2.13	0.48
1:A:142:GLU:OE2	1:A:294:ARG:NH2	2.46	0.48
1:A:315:THR:O	1:A:531:THR:HG22	2.13	0.48
2:B:298:LYS:HE2	2:B:303:ASN:OD1	2.14	0.48
1:G:814[B]:GLN:HG2	1:G:818:PHE:CE2	2.49	0.48
2:H:286:MET:HE1	2:H:312:HIS:ND1	2.29	0.48
1:A:704:LYS:O	1:A:707:GLU:HB2	2.14	0.48
1:A:951:GLU:HA	1:A:954:LYS:HD2	1.95	0.48
2:B:6:LEU:HD23	2:B:138:PRO:HB2	1.96	0.48
2:B:350:PHE:CG	2:B:366:LEU:HD11	2.48	0.48
1:C:145[A]:ARG:HB3	1:C:208:GLU:CD	2.38	0.48
1:C:697:ALA:O	1:C:700:MET:HB3	2.14	0.48
2:D:206:LEU:O	2:D:210:VAL:HG23	2.12	0.48
2:F:272:HIS:HA	2:F:349:SER:HB2	1.96	0.48
2:F:354:PRO:HB3	2:F:363:ALA:HB1	1.90	0.48
1:G:6:ASP:OD2	1:G:6:ASP:N	2.45	0.48
1:A:143:THR:HA	1:A:296:ILE:HG23	1.96	0.48
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.41	0.48
9:A:4012:NET:H22	9:A:4012:NET:C4	2.41	0.48
1:C:946:LEU:HB3	1:C:1013:ILE:HG12	1.96	0.48
2:H:324:ASN:O	2:H:342:ARG:HA	2.14	0.48
1:A:101:GLU:HA	1:A:101:GLU:OE2	2.13	0.47
1:C:1052:MET:HG3	10:C:4606:HOH:O	2.13	0.47
2:H:272:HIS:HA	2:H:349:SER:HB2	1.95	0.47
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.67	0.47
1:A:947:LEU:HG	1:A:1014:ILE:CG2	2.44	0.47
1:C:710:TYR:HA	1:C:712:LEU:CD1	2.44	0.47
2:D:172:GLN:HG2	2:D:173:GLY:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:726:GLU:CD	1:E:736:ARG:HH22	2.21	0.47
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.50	0.47
1:A:528:ARG:HG2	1:A:543:MET:HG2	1.96	0.47
1:A:710:TYR:CB	1:A:711:PRO:HA	2.43	0.47
1:A:730:ASP:H	1:A:733:ASP:HB2	1.79	0.47
2:D:185:LYS:HD3	2:D:190:LEU:HD21	1.95	0.47
1:G:734:LEU:HD22	1:G:738:PHE:HE2	1.77	0.47
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.96	0.47
2:F:228:VAL:HA	2:F:231:MET:HE3	1.93	0.47
1:G:1017:THR:HG21	1:G:1023:ILE:CA	2.40	0.47
2:H:225:ALA:CB	2:H:257:LYS:HG2	2.44	0.47
1:A:101:GLU:OE2	1:A:104:ARG:NH1	2.43	0.47
1:A:972:ASP:HA	1:A:989:ARG:O	2.14	0.47
2:B:331:SER:O	2:B:335:GLY:N	2.46	0.47
1:C:526:TYR:CE1	1:C:545:SER:HB3	2.50	0.47
2:D:116:ARG:O	2:D:120:ARG:HG3	2.15	0.47
1:E:692:ASN:HA	1:E:752:LEU:O	2.13	0.47
1:E:779:MET:HA	1:E:795:SER:O	2.14	0.47
2:F:244:ASP:O	2:F:247:PRO:HD2	2.14	0.47
1:G:936:ASN:HB2	10:G:4102:HOH:O	2.13	0.47
2:H:46:PRO:HA	2:H:76:HIS:CG	2.49	0.47
1:A:703:GLU:O	1:A:704:LYS:C	2.57	0.47
2:B:75:VAL:HG11	2:B:107:ILE:HG13	1.96	0.47
2:B:290:HIS:HB3	2:B:310:GLN:HB3	1.96	0.47
1:C:3:LYS:HB3	1:C:330:TYR:CZ	2.50	0.47
2:D:6:LEU:O	2:D:132:ILE:HA	2.14	0.47
2:D:71:GLU:C	2:D:203:ARG:HG3	2.39	0.47
2:D:261:THR:CG2	2:D:263:ILE:HG13	2.45	0.47
1:E:1067:GLU:O	1:E:1068:MET:C	2.56	0.47
1:G:479:VAL:HB	1:G:483:GLY:HA3	1.95	0.47
1:G:646:THR:HB	1:G:647:PRO:CD	2.44	0.47
1:G:860:PRO:O	1:G:861:LEU:C	2.57	0.47
1:G:892:GLU:HG3	1:G:893:VAL:N	2.29	0.47
1:A:731:GLU:O	1:A:735:ARG:HG3	2.14	0.47
1:A:755:PHE:CE1	7:A:4007:ADP:C2	3.03	0.47
1:A:812:GLN:NE2	10:A:4621:HOH:O	2.30	0.47
2:B:137:ASN:O	2:B:138:PRO:C	2.57	0.47
2:B:201:ALA:HA	2:B:240:ASN:OD1	2.14	0.47
1:C:358:LYS:HE3	10:C:4075:HOH:O	2.14	0.47
2:D:317:ASP:OD1	2:D:320:THR:HG23	2.14	0.47
1:E:400:ARG:HD3	10:E:1472:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:646:THR:HB	1:E:647:PRO:CD	2.42	0.47
2:F:201:ALA:HB2	2:F:239:SER:CB	2.44	0.47
1:G:170:PRO:HA	1:G:204:LEU:HD23	1.97	0.47
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.15	0.47
2:H:198:ASP:C	2:H:200:GLY:H	2.23	0.47
1:A:337:ASN:N	1:A:344:THR:O	2.32	0.47
1:C:167:ILE:N	1:C:167:ILE:HD12	2.30	0.47
1:E:534:ALA:O	2:F:123:ARG:HD3	2.15	0.47
1:G:29:SER:CB	1:G:304:VAL:HG21	2.45	0.47
1:G:702:VAL:HG11	1:G:735:ARG:NH2	2.30	0.47
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.39	0.47
1:C:953:ASP:CG	1:C:1044:LEU:HD22	2.40	0.47
1:E:157:ALA:O	1:E:160:ALA:HB3	2.15	0.47
1:E:648:LEU:HD22	1:E:845:ARG:HD3	1.97	0.47
2:F:170:TRP:CH2	2:F:203:ARG:HG2	2.50	0.47
2:H:254:ALA:O	2:H:257:LYS:N	2.45	0.47
2:H:320:THR:O	2:H:320:THR:OG1	2.29	0.47
1:C:358:LYS:HG2	1:C:359:ILE:N	2.29	0.47
1:C:479:VAL:HB	1:C:483:GLY:HA3	1.96	0.47
1:C:683:GLU:O	1:C:686:LYS:N	2.42	0.47
1:C:802:SER:O	1:C:805:ILE:HG22	2.15	0.47
2:D:228:VAL:O	2:D:229:LEU:C	2.57	0.47
1:E:1049:ALA:HA	1:E:1052:MET:HE3	1.97	0.47
1:G:688:LYS:HZ2	1:G:836:GLU:CD	2.23	0.47
2:H:133:ILE:CG2	2:H:138:PRO:HB3	2.45	0.47
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.78	0.47
1:E:676:GLU:O	1:E:680:HIS:ND1	2.48	0.46
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.97	0.46
2:F:50:ARG:HD2	2:F:50:ARG:HA	1.57	0.46
2:F:324:ASN:O	2:F:343:THR:N	2.39	0.46
1:G:3:LYS:HG3	1:G:3:LYS:O	2.13	0.46
2:B:71:GLU:C	2:B:203:ARG:HG3	2.39	0.46
1:C:891:LYS:HE2	1:C:891:LYS:HB3	1.76	0.46
1:E:54:ILE:O	1:E:57:ASP:HB2	2.15	0.46
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.80	0.46
2:F:160:LYS:HG3	2:F:161:GLU:HG2	1.96	0.46
1:G:70:HIS:HE1	1:G:72:GLU:HG3	1.80	0.46
1:G:222:ARG:CZ	1:G:273:ARG:HG2	2.46	0.46
1:G:642:TYR:OH	1:G:865:ALA:HB3	2.15	0.46
2:H:181:LEU:HA	2:H:181:LEU:HD23	1.74	0.46
2:B:57:TYR:CE1	2:B:58:PRO:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:TYR:HA	2:B:219:VAL:HG22	1.97	0.46
2:B:268:ILE:HD13	2:B:268:ILE:HA	1.73	0.46
2:B:273:GLN:O	2:B:276:ALA:HB3	2.14	0.46
2:B:290:HIS:NE2	2:B:334:ASP:OD1	2.44	0.46
1:C:424:ILE:O	1:C:425:ARG:C	2.56	0.46
1:E:51:PRO:HG3	1:E:918:MET:HB2	1.97	0.46
2:F:322:PRO:HG2	2:F:325:LEU:HD12	1.96	0.46
1:G:28:TYR:O	1:G:32:GLN:HG3	2.15	0.46
1:G:1030:ARG:HG3	1:G:1030:ARG:NH1	2.30	0.46
2:H:222:GLN:O	2:H:223:THR:C	2.58	0.46
2:H:252:ILE:O	2:H:253:THR:C	2.58	0.46
2:H:331:SER:O	2:H:335:GLY:N	2.46	0.46
1:A:680:HIS:O	1:A:683:GLU:HB2	2.15	0.46
2:B:285:LYS:HB2	2:B:314:PHE:CE1	2.50	0.46
1:C:940:LYS:HG3	1:C:1011:THR:HB	1.98	0.46
2:D:286:MET:HB2	2:D:313:GLY:O	2.15	0.46
2:D:324:ASN:O	2:D:342:ARG:HA	2.15	0.46
1:E:950:ARG:HD3	10:E:1679:HOH:O	2.15	0.46
2:F:35:SER:HB3	2:F:37:THR:O	2.15	0.46
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.50	0.46
1:G:139:ILE:HG21	1:G:274:GLU:HB2	1.98	0.46
1:G:419:GLU:CB	1:G:423:LYS:HE3	2.46	0.46
1:G:807:ASP:HA	1:G:810:ARG:HG3	1.97	0.46
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.97	0.46
2:H:286:MET:N	2:H:313:GLY:O	2.42	0.46
1:A:278:GLU:HG2	10:A:4221:HOH:O	2.16	0.46
1:A:471:ARG:HH21	1:A:474:GLU:CD	2.22	0.46
2:B:46:PRO:HA	2:B:76:HIS:CG	2.51	0.46
1:C:75:ARG:HD3	10:C:4110:HOH:O	2.14	0.46
1:C:698:ILE:O	1:C:702:VAL:HG23	2.15	0.46
1:C:737:TYR:O	1:C:739:GLN:N	2.48	0.46
2:F:227:ASP:O	2:F:230:LYS:HB2	2.14	0.46
2:F:236:ILE:HD13	2:F:258:PHE:CG	2.50	0.46
2:F:272:HIS:HA	2:F:349:SER:CB	2.45	0.46
1:G:472:LEU:O	1:G:473:GLU:C	2.55	0.46
1:G:955:GLU:HB2	10:G:4683:HOH:O	2.15	0.46
1:A:154:GLU:HA	10:A:4721:HOH:O	2.15	0.46
1:C:644:GLY:O	1:C:647:PRO:HD2	2.16	0.46
1:C:772:MET:CE	1:C:880:THR:HA	2.46	0.46
2:F:286[A]:MET:HE1	2:F:312:HIS:O	2.16	0.46
1:G:231:VAL:HG11	1:G:319:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:LYS:HE2	2:H:69:ASP:OD2	2.16	0.46
1:G:818:PHE:O	1:G:819:GLU:C	2.57	0.46
2:H:268:ILE:O	2:H:269:CYS:HB3	2.15	0.46
1:A:146:SER:HB2	1:A:206:ILE:O	2.15	0.46
2:B:192:PHE:HZ	2:B:375:GLU:OE2	1.99	0.46
2:B:296:PRO:HB2	2:B:332:LEU:HB2	1.97	0.46
2:F:59:HIS:ND1	2:F:84:ASP:OD2	2.44	0.46
1:G:479:VAL:CB	1:G:483:GLY:HA3	2.46	0.46
1:G:647:PRO:O	1:G:648:LEU:C	2.58	0.46
1:G:994:VAL:HG22	1:G:1000:HIS:CG	2.51	0.46
1:A:654:LEU:O	1:A:659:VAL:HG23	2.16	0.46
2:B:221:ALA:HB1	2:B:250:TYR:HE1	1.80	0.46
1:C:764:VAL:HG11	1:C:813:VAL:HG21	1.97	0.46
2:D:187:GLU:CG	2:D:215:ARG:HD2	2.18	0.46
1:E:18:ILE:HD12	1:E:23:ALA:C	2.40	0.46
1:E:953:ASP:O	1:E:955:GLU:N	2.49	0.46
1:G:344:THR:HB	1:G:345:PRO:HD2	1.98	0.46
2:B:34:THR:HA	2:B:56:THR:OG1	2.16	0.46
2:B:46:PRO:O	2:B:47:SER:C	2.58	0.46
1:C:6:ASP:OD2	1:C:6:ASP:N	2.45	0.46
1:C:119:THR:O	1:C:123:ILE:HG13	2.15	0.46
1:C:166:CYS:C	1:C:167:ILE:HD12	2.41	0.46
1:C:475:LYS:O	1:C:476:VAL:C	2.58	0.46
2:D:81:VAL:HG22	2:D:110:ILE:HG22	1.97	0.46
2:D:364:ALA:N	2:D:365:PRO:CD	2.79	0.46
1:E:735:ARG:O	1:E:736:ARG:C	2.58	0.46
1:G:479:VAL:HG21	1:G:483:GLY:HA3	1.96	0.46
1:G:493:LYS:HD2	1:G:493:LYS:HA	1.73	0.46
1:G:516:LEU:HD12	1:G:516:LEU:HA	1.68	0.46
1:G:698:ILE:HD12	1:G:698:ILE:N	2.14	0.46
2:H:25:SER:HA	2:H:132:ILE:O	2.15	0.46
2:H:299:ASP:OD2	2:H:301:GLU:HB2	2.16	0.46
2:B:6:LEU:HD11	2:B:8:VAL:CG2	2.46	0.46
2:B:255:ILE:HG22	2:B:278:ALA:HB1	1.98	0.46
1:C:145[B]:ARG:HB3	1:C:208:GLU:HG2	1.98	0.46
1:C:343:ARG:HG3	1:C:344:THR:CG2	2.45	0.46
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.96	0.46
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.80	0.46
2:D:158:LEU:HD23	2:D:158:LEU:HA	1.76	0.46
2:H:364:ALA:N	2:H:365:PRO:CD	2.79	0.46
1:A:29[B]:SER:OG	1:A:30:GLY:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:THR:O	1:E:343:ARG:HG2	2.15	0.45
1:G:954:LYS:O	1:G:957:VAL:HG12	2.15	0.45
2:H:261:THR:CG2	2:H:262:ASP:N	2.79	0.45
1:A:509:ARG:O	1:A:510:GLU:C	2.57	0.45
1:A:642:TYR:OH	1:A:865:ALA:HB3	2.15	0.45
2:B:332:LEU:HD12	2:B:332:LEU:HA	1.69	0.45
1:C:315:THR:O	1:C:531:THR:HG22	2.16	0.45
1:C:734:LEU:CD2	1:C:738:PHE:CE2	2.99	0.45
2:D:144:LEU:O	2:D:145:GLU:C	2.56	0.45
2:D:222:GLN:HG3	2:D:250:TYR:CD1	2.51	0.45
1:E:1028:VAL:O	1:E:1032:SER:HB2	2.15	0.45
1:G:247:SER:O	1:G:358:LYS:HE2	2.17	0.45
1:G:619:GLU:HB3	1:G:620:PRO:HD2	1.97	0.45
1:G:702:VAL:O	1:G:705:ALA:HB3	2.16	0.45
2:H:85:LEU:HD12	2:H:86:PRO:HD2	1.99	0.45
2:B:273:GLN:O	2:B:277:LEU:HG	2.17	0.45
2:B:306:MET:CE	2:B:350:PHE:CZ	3.00	0.45
2:D:23:THR:HG22	2:D:24:GLY:N	2.30	0.45
2:F:252:ILE:CG2	2:F:278:ALA:HA	2.47	0.45
1:G:730:ASP:OD2	1:G:733:ASP:HB2	2.17	0.45
1:G:865:ALA:O	1:G:869:MET:HG3	2.17	0.45
1:G:956:ARG:HB2	1:G:1044:LEU:CD2	2.47	0.45
2:B:57:TYR:O	2:B:60:ILE:HD11	2.16	0.45
2:B:167:ALA:HA	2:B:218:ILE:O	2.15	0.45
2:B:270:LEU:HD12	2:B:273:GLN:OE1	2.16	0.45
2:B:366:LEU:HD23	2:B:366:LEU:HA	1.86	0.45
2:D:227:ASP:O	2:D:230:LYS:HB2	2.17	0.45
1:E:157:ALA:HA	10:E:1310:HOH:O	2.15	0.45
1:E:695:VAL:CG1	1:E:696:THR:N	2.79	0.45
1:E:765:ASP:O	1:E:776:GLY:N	2.49	0.45
2:F:274:LEU:HD23	2:F:274:LEU:HA	1.81	0.45
2:F:285:LYS:HB2	2:F:314:PHE:CE1	2.52	0.45
1:G:293:GLY:O	1:G:294:ARG:C	2.57	0.45
2:B:285:LYS:CG	2:B:314:PHE:CE1	2.99	0.45
1:C:101:GLU:O	1:C:105:GLN:HG2	2.16	0.45
1:C:554:ASN:N	1:C:555:PRO:CD	2.80	0.45
1:C:701:ALA:O	1:C:705:ALA:HB2	2.16	0.45
2:F:324:ASN:O	2:F:342:ARG:HA	2.16	0.45
1:G:782:ILE:HD12	1:G:782:ILE:N	2.31	0.45
2:H:227:ASP:HA	2:H:230[A]:LYS:HD2	1.98	0.45
1:A:479:VAL:HG23	1:A:480:GLY:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ASP:CG	2:B:378:ARG:HD2	2.42	0.45
2:B:261:THR:CG2	2:B:263:ILE:HG13	2.47	0.45
1:C:314:ALA:HB1	1:C:356:VAL:HG21	1.97	0.45
1:C:499:ASP:HA	1:C:513:ILE:HG21	1.99	0.45
1:C:867:ARG:O	1:C:868:VAL:C	2.54	0.45
2:D:153:LEU:N	2:D:153:LEU:CD1	2.80	0.45
2:D:257:LYS:O	2:D:258:PHE:C	2.59	0.45
1:E:353:ASP:OD1	2:F:116:ARG:HD2	2.17	0.45
1:E:1026:SER:HB2	1:E:1030:ARG:NH1	2.30	0.45
2:F:157:ASP:HB2	2:F:247:PRO:HB2	1.99	0.45
2:F:269:CYS:SG	2:F:270:LEU:N	2.90	0.45
2:F:379[B]:LYS:NZ	10:F:3308:HOH:O	2.49	0.45
1:G:738:PHE:O	1:G:739:GLN:O	2.35	0.45
1:G:1021:ARG:O	1:G:1022:ALA:C	2.60	0.45
1:A:947:LEU:N	1:A:947:LEU:CD1	2.80	0.45
2:B:199:PHE:O	2:B:241:GLY:HA3	2.17	0.45
2:B:228:VAL:CG1	2:B:258:PHE:CE1	3.00	0.45
2:B:229:LEU:HA	2:B:229:LEU:HD23	1.67	0.45
1:E:403:GLU:OE1	1:E:646:THR:HG23	2.16	0.45
1:E:854:SER:O	1:E:858:GLY:N	2.48	0.45
1:G:156:LEU:HB3	10:G:4217:HOH:O	2.16	0.45
1:G:622:THR:O	1:G:623:LEU:C	2.59	0.45
1:G:704:LYS:HD2	1:G:704:LYS:HA	1.63	0.45
1:A:734:LEU:CD2	1:A:738:PHE:HE2	2.30	0.45
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.77	0.45
1:C:237:PHE:HB3	1:C:248:ILE:O	2.16	0.45
1:C:516:LEU:HD12	1:C:516:LEU:HA	1.73	0.45
1:G:903:VAL:HG12	1:G:904:ASP:N	2.30	0.45
2:H:164:THR:HG21	2:H:168:TYR:CE1	2.47	0.45
2:H:186:LYS:O	2:H:189:GLU:N	2.41	0.45
1:A:358:LYS:HE3	10:A:4053:HOH:O	2.15	0.45
1:A:734:LEU:CD2	1:A:738:PHE:CE2	3.00	0.45
1:A:740:THR:H	1:A:740:THR:HG23	1.41	0.45
2:B:120:ARG:HH21	2:B:120:ARG:HD3	1.61	0.45
2:B:246:ALA:N	2:B:247:PRO:CD	2.80	0.45
1:C:704:LYS:O	1:C:707:GLU:HB2	2.17	0.45
1:C:729:TYR:N	1:C:729:TYR:CD1	2.85	0.45
1:C:734:LEU:HD22	1:C:738:PHE:HD2	1.80	0.45
2:D:285:LYS:HB2	2:D:314:PHE:CD1	2.52	0.45
2:D:291:HIS:HA	2:D:310:GLN:O	2.17	0.45
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:PRO:HB3	1:E:183:TYR:CD1	2.51	0.45
1:E:436:ILE:CG2	1:E:437:TRP:CE3	3.00	0.45
1:E:698:ILE:HG23	1:E:738:PHE:CD2	2.51	0.45
2:F:261:THR:CG2	2:F:262:ASP:N	2.80	0.45
1:G:264:MET:HE2	1:G:295:LEU:HD11	1.99	0.45
1:G:472:LEU:O	1:G:476:VAL:HG23	2.16	0.45
2:B:48:TYR:O	2:B:49:SER:C	2.59	0.45
2:B:300:VAL:HG23	2:B:301:GLU:N	2.32	0.45
1:C:447:LEU:HA	1:C:447:LEU:HD23	1.70	0.45
1:E:259:LYS:HD3	2:F:175:TRP:CE3	2.52	0.45
1:E:331:THR:OG1	1:E:333:ASP:OD1	2.30	0.45
1:G:734:LEU:CD2	1:G:738:PHE:CE2	2.99	0.45
1:C:1020:ARG:O	1:C:1020:ARG:HG3	2.16	0.44
2:D:154:ASN:HD22	2:D:154:ASN:HA	1.38	0.44
1:E:246:ASP:OD1	1:E:379:LYS:N	2.42	0.44
2:F:279:SER:O	2:F:322:PRO:HG3	2.17	0.44
1:G:168:ILE:CG2	1:G:204:LEU:HD22	2.46	0.44
2:H:326:ARG:O	2:H:340:ILE:HA	2.16	0.44
2:H:357:SER:N	2:H:358:PRO:CA	2.79	0.44
1:A:341:GLY:C	1:A:343:ARG:H	2.25	0.44
1:A:347:SER:O	2:B:296:PRO:HB3	2.17	0.44
2:B:71:GLU:HG3	2:B:202:LYS:HE3	1.98	0.44
2:B:226:GLU:H	2:B:226:GLU:HG2	1.52	0.44
1:C:974:THR:O	1:C:975:HIS:C	2.57	0.44
2:D:261:THR:CG2	2:D:262:ASP:N	2.80	0.44
1:E:998:ARG:HB3	1:E:999:PRO:HA	2.00	0.44
1:G:471:ARG:O	1:G:472:LEU:C	2.60	0.44
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.99	0.44
2:H:259:LEU:HD23	2:H:259:LEU:HA	1.84	0.44
1:A:167:ILE:N	1:A:167:ILE:CD1	2.80	0.44
2:B:228:VAL:HG11	2:B:258:PHE:HE1	1.81	0.44
2:B:285:LYS:CB	2:B:314:PHE:CD1	3.00	0.44
2:B:286:MET:CE	2:B:312:HIS:ND1	2.80	0.44
2:B:375:GLU:O	2:B:378:ARG:N	2.44	0.44
2:D:268:ILE:HD13	2:D:268:ILE:HA	1.44	0.44
1:E:67:GLU:HB3	1:E:68:PRO:HD2	1.99	0.44
2:F:291:HIS:HA	2:F:310:GLN:O	2.17	0.44
2:H:277:LEU:O	2:H:280:GLY:N	2.37	0.44
2:H:295:HIS:HA	2:H:296:PRO:HD3	1.94	0.44
1:A:990:LEU:HD23	1:G:979:ILE:CG1	2.41	0.44
1:C:59:GLU:HG3	1:C:60:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:O	1:C:79:GLU:C	2.60	0.44
1:C:235:GLU:HB2	1:C:253:ALA:HA	1.98	0.44
1:C:772:MET:HE1	1:C:880:THR:HA	2.00	0.44
2:D:254:ALA:O	2:D:257:LYS:HB2	2.18	0.44
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.66	0.44
1:E:936:ASN:HB2	10:E:1189:HOH:O	2.17	0.44
2:F:12:GLY:HA2	2:F:144:LEU:HD13	1.98	0.44
2:F:204:ASN:ND2	2:F:205:ILE:N	2.65	0.44
1:G:710:TYR:HB3	1:G:729:TYR:O	2.16	0.44
1:A:896:PRO:HG3	1:A:914:THR:HG23	1.99	0.44
1:C:503:ALA:HB1	1:C:508:VAL:O	2.17	0.44
1:C:645:GLN:HG3	1:C:649:LYS:NZ	2.33	0.44
1:C:912:ARG:NH1	10:C:4459:HOH:O	2.51	0.44
2:D:6:LEU:HD12	2:D:7:LEU:N	2.32	0.44
1:E:289:ASN:O	1:E:293:GLY:N	2.46	0.44
1:E:680:HIS:C	1:E:683:GLU:HB2	2.42	0.44
1:E:956:ARG:HA	10:E:2746:HOH:O	2.17	0.44
2:F:222[A]:GLN:HG2	2:F:250:TYR:CG	2.52	0.44
1:G:5:THR:C	1:G:7:ILE:H	2.25	0.44
1:G:65:TYR:OH	1:G:80:LYS:HE3	2.17	0.44
2:B:249:ASP:O	2:B:252:ILE:HG13	2.17	0.44
1:C:18:ILE:HG23	1:C:23:ALA:HA	1.99	0.44
1:C:229:ILE:O	1:C:229:ILE:HG13	2.18	0.44
1:E:1032:SER:O	1:E:1036:TYR:HD1	2.00	0.44
1:G:294:ARG:NH1	10:G:4546:HOH:O	2.47	0.44
1:G:475:LYS:CD	1:G:488:PHE:CZ	3.00	0.44
1:G:834:ASN:O	1:G:835:ASN:C	2.61	0.44
1:G:905:PRO:HG2	1:G:1030:ARG:HB3	1.99	0.44
2:H:306:MET:CE	2:H:329:HIS:CD2	3.00	0.44
2:B:201:ALA:HB2	2:B:239:SER:HB2	1.94	0.44
2:B:228:VAL:CG1	2:B:258:PHE:HE1	2.31	0.44
1:E:150:HIS:N	1:E:154:GLU:OE1	2.48	0.44
1:E:756:LEU:HD23	1:E:756:LEU:HA	1.81	0.44
1:E:796:LEU:HD23	1:E:796:LEU:C	2.42	0.44
2:F:25:SER:HA	2:F:132:ILE:O	2.18	0.44
1:G:780:GLU:HB3	1:G:798:ALA:HA	1.98	0.44
2:H:325:LEU:HA	2:H:325:LEU:HD23	1.36	0.44
1:A:223:ASP:OD1	1:A:227:ASN:HB2	2.18	0.44
1:A:704:LYS:HD2	1:A:704:LYS:HA	1.66	0.44
1:A:992:ASN:HB2	1:A:999:PRO:O	2.17	0.44
2:B:208:MET:O	2:B:211:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:GLN:O	1:C:784:GLN:HG2	2.18	0.44
1:C:992:ASN:ND2	1:E:975:HIS:NE2	2.66	0.44
1:E:559:ARG:HG3	1:E:559:ARG:NH2	2.26	0.44
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.99	0.44
1:E:993:LYS:O	1:E:994:VAL:C	2.57	0.44
1:E:1001:ILE:HG21	1:E:1029:ILE:HG12	2.00	0.44
2:F:268:ILE:O	2:F:269:CYS:HB3	2.18	0.44
1:G:272:LEU:HD12	1:G:272:LEU:N	2.31	0.44
1:G:729:TYR:N	1:G:729:TYR:CD1	2.86	0.44
1:G:833:LYS:O	1:G:834:ASN:C	2.58	0.44
2:H:223:THR:CG2	2:H:228:VAL:HG23	2.47	0.44
1:A:267:ALA:O	1:A:271:VAL:HG23	2.17	0.44
1:A:419:GLU:HG3	10:A:4778:HOH:O	2.18	0.44
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.18	0.44
1:C:57:ASP:HB3	1:C:59:GLU:OE1	2.18	0.44
1:E:456:THR:O	1:E:457:ASN:HB2	2.18	0.44
1:G:202:LYS:O	1:G:202:LYS:HG2	2.17	0.44
2:B:354:PRO:HB3	2:B:363:ALA:CA	2.46	0.43
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.88	0.43
2:D:23:THR:CG2	2:D:24:GLY:N	2.81	0.43
2:D:193:HIS:ND1	2:D:215:ARG:NH2	2.66	0.43
2:D:226:GLU:O	2:D:230:LYS:HG3	2.17	0.43
1:E:981:LEU:HD12	1:E:988:PRO:HG3	2.00	0.43
2:F:263:ILE:HG12	2:F:377:TYR:OH	2.17	0.43
2:B:225:ALA:O	2:B:226:GLU:C	2.60	0.43
1:C:622:THR:OG1	1:C:625:ASP:OD1	2.30	0.43
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.18	0.43
1:E:623:LEU:HD11	1:E:627:LEU:HD11	2.00	0.43
1:E:641:GLN:OE1	1:E:641:GLN:N	2.51	0.43
1:E:704:LYS:O	1:E:707:GLU:N	2.50	0.43
1:G:803:GLN:O	1:G:804:GLU:C	2.59	0.43
1:G:1030:ARG:HG3	1:G:1030:ARG:HH11	1.83	0.43
1:A:85:ALA:HA	1:A:114:THR:O	2.18	0.43
2:B:367:PHE:O	2:B:368:ASP:C	2.55	0.43
1:C:75:ARG:O	1:C:76:LYS:C	2.59	0.43
1:C:1065:VAL:O	1:C:1069:HIS:HB2	2.18	0.43
1:G:597:ILE:HA	1:G:615:ARG:O	2.18	0.43
1:G:967:GLN:HG3	1:G:1054:LEU:HB3	1.99	0.43
1:G:986:ILE:HG22	1:G:988:PRO:HD3	2.00	0.43
1:A:159:ALA:HB2	1:A:188:PHE:CZ	2.54	0.43
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LYS:O	1:C:542:TYR:OH	2.30	0.43
1:C:351:SER:HA	2:D:36:MET:HE2	2.01	0.43
1:E:87:LEU:HA	1:E:88:PRO:HD3	1.84	0.43
2:F:205:ILE:HG12	2:F:205:ILE:H	1.40	0.43
2:F:263:ILE:HG23	2:F:264:PRO:HD2	1.99	0.43
1:G:301:ASN:HA	1:G:302:PRO:HD3	1.84	0.43
1:G:417:ASP:OD2	1:G:418:PRO:HD2	2.18	0.43
2:H:102:LEU:HD23	2:H:102:LEU:HA	1.84	0.43
2:H:107:ILE:N	2:H:107:ILE:CD1	2.82	0.43
2:H:175:TRP:HA	2:H:180:GLY:O	2.17	0.43
2:H:222:GLN:HE21	2:H:222:GLN:H	1.64	0.43
2:H:273:GLN:NE2	2:H:351:GLN:HE22	2.17	0.43
2:H:351:GLN:NE2	10:H:3174:HOH:O	2.34	0.43
2:B:297:VAL:O	2:B:306:MET:HG3	2.18	0.43
1:C:590:ARG:O	1:C:591:GLU:C	2.59	0.43
1:C:698:ILE:CD1	1:C:698:ILE:N	2.80	0.43
1:C:991:VAL:HB	1:C:1004[B]:ARG:NH1	2.33	0.43
1:E:669:ILE:HA	1:E:844:PRO:HG2	2.00	0.43
1:E:940:LYS:HG3	1:E:1011:THR:HB	2.01	0.43
1:G:9:SER:OG	1:G:83:PRO:HA	2.17	0.43
1:G:148:ILE:CG2	1:G:149:ALA:N	2.80	0.43
1:G:347:SER:O	2:H:296:PRO:HB3	2.18	0.43
1:G:727:ILE:HD12	1:G:909:PRO:HG3	1.99	0.43
1:G:950:ARG:HG3	1:G:950:ARG:H	1.58	0.43
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.19	0.43
1:C:70:HIS:O	1:C:71:TRP:C	2.61	0.43
1:C:604:GLU:HG2	10:C:4550:HOH:O	2.18	0.43
1:C:947:LEU:N	1:C:947:LEU:CD1	2.81	0.43
1:E:434:ASP:O	1:E:435:ARG:C	2.60	0.43
1:E:693:ALA:N	1:E:708:ILE:HD11	2.33	0.43
1:G:166:CYS:C	1:G:167:ILE:HD12	2.43	0.43
1:G:645[A]:GLN:HG3	1:G:649:LYS:HE3	2.00	0.43
2:H:137:ASN:O	2:H:138:PRO:C	2.60	0.43
2:H:186:LYS:O	2:H:187:GLU:C	2.61	0.43
2:H:364:ALA:O	2:H:365:PRO:C	2.61	0.43
2:H:365:PRO:O	2:H:366:LEU:C	2.59	0.43
1:A:710:TYR:HA	1:A:711:PRO:C	2.42	0.43
1:E:726:GLU:CG	1:E:727:ILE:N	2.79	0.43
1:E:885:PRO:HA	1:E:886:PRO:HD3	1.65	0.43
1:G:3:LYS:HB3	1:G:330:TYR:CE1	2.54	0.43
1:G:58:PRO:HD2	1:G:59:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:PHE:HB3	1:G:248:ILE:HB	2.01	0.43
1:G:992:ASN:HB2	1:G:999:PRO:O	2.18	0.43
2:H:261:THR:HG21	2:H:263:ILE:CG1	2.48	0.43
1:A:59[A]:GLU:CG	1:A:60:MET:HE2	2.48	0.43
1:A:679:GLN:HG2	10:A:4614:HOH:O	2.17	0.43
2:B:49:SER:HA	2:B:76:HIS:O	2.18	0.43
2:B:365:PRO:O	2:B:366:LEU:C	2.62	0.43
2:B:371:ILE:O	2:B:372:GLU:C	2.57	0.43
1:C:503:ALA:HB2	1:C:510:GLU:HA	2.00	0.43
1:C:892:GLU:OE1	8:C:4031:ORN:NE	2.52	0.43
1:E:676:GLU:O	1:E:677:ARG:C	2.62	0.43
2:F:116:ARG:O	2:F:120:ARG:HG3	2.19	0.43
2:F:252:ILE:HG23	2:F:278:ALA:CA	2.48	0.43
1:G:158:VAL:HG11	1:G:206:ILE:HB	2.01	0.43
1:G:321:LYS:NZ	1:G:611:ASP:OD1	2.44	0.43
1:G:423:LYS:HB3	10:G:4377:HOH:O	2.19	0.43
1:G:735:ARG:O	1:G:738:PHE:HB2	2.18	0.43
1:G:973:ALA:O	1:G:990:LEU:HA	2.18	0.43
2:H:344:ASP:C	2:H:345:LYS:HG2	2.43	0.43
1:A:141:LEU:HB3	1:A:297:VAL:CG2	2.49	0.43
1:A:409:PHE:CE1	1:A:469:LEU:HD12	2.54	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.84	0.43
2:B:300:VAL:HG22	2:B:328:THR:O	2.19	0.43
2:B:371:ILE:HD13	2:B:371:ILE:HA	1.81	0.43
1:C:735:ARG:O	1:C:736:ARG:C	2.61	0.43
1:E:220:VAL:O	1:E:281:GLY:HA2	2.19	0.43
2:F:204:ASN:HD21	2:F:205:ILE:CD1	2.31	0.43
1:G:420:ALA:HA	1:G:423:LYS:HD2	2.00	0.43
1:G:534:ALA:O	2:H:123:ARG:HD3	2.19	0.43
1:G:625:ASP:O	1:G:629:ILE:HG13	2.18	0.43
2:H:201:ALA:CB	2:H:239:SER:HB2	2.49	0.43
1:A:9:SER:OG	1:A:83:PRO:HA	2.19	0.43
1:A:726:GLU:HG3	1:A:727:ILE:H	1.81	0.43
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.83	0.43
1:C:294:ARG:HD2	5:C:4038:CL:CL	2.56	0.43
2:D:194:VAL:HB	2:D:216:LEU:HD23	2.01	0.43
1:E:711:PRO:HG2	1:E:755:PHE:HD2	1.84	0.43
1:E:773[A]:VAL:HG21	1:E:814:GLN:HA	2.00	0.43
1:E:803:GLN:O	1:E:804:GLU:C	2.60	0.43
1:E:805:ILE:HD12	1:E:832:VAL:HG11	2.01	0.43
2:F:48:TYR:HA	2:F:51:GLN:NE2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1063:ILE:HG12	1:G:1064:SER:N	2.33	0.43
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.92	0.42
1:A:692:ASN:HB3	1:A:753:ASP:CG	2.44	0.42
2:B:261:THR:CG2	2:B:262:ASP:N	2.81	0.42
1:C:385:MET:HE2	1:C:618:PHE:CE1	2.54	0.42
1:C:456:THR:O	1:C:457:ASN:HB2	2.18	0.42
1:C:563:MET:CE	1:C:635:PRO:HG3	2.49	0.42
1:E:730:ASP:O	1:E:731:GLU:C	2.62	0.42
2:F:236:ILE:HB	2:F:265:VAL:HG22	2.01	0.42
1:G:417:ASP:HB3	1:G:420:ALA:HB2	2.00	0.42
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.23	0.42
2:H:209:LEU:O	2:H:212:ARG:N	2.52	0.42
1:A:1026:SER:O	1:A:1027:ARG:C	2.59	0.42
2:B:190:LEU:HB2	2:B:215:ARG:HB2	2.02	0.42
2:B:259:LEU:HD23	2:B:259:LEU:HA	1.77	0.42
1:C:71:TRP:O	1:C:72:GLU:C	2.61	0.42
1:C:306:ARG:HG2	1:C:306:ARG:NH1	2.33	0.42
1:C:375:THR:OG1	1:C:376:THR:N	2.51	0.42
1:C:561:LYS:HE2	10:C:4424:HOH:O	2.19	0.42
1:C:839:LEU:HD12	1:C:839:LEU:HA	1.81	0.42
1:E:213:TRP:CH2	1:E:289:ASN:HB2	2.54	0.42
1:E:331:THR:OG1	1:E:334:GLU:HG3	2.18	0.42
1:E:479:VAL:HG23	1:E:483:GLY:HA3	2.00	0.42
1:E:568:GLY:O	1:E:602:ASN:HB2	2.18	0.42
2:F:172:GLN:HG2	2:F:173:GLY:N	2.33	0.42
2:F:378:ARG:NH2	10:F:3310:HOH:O	2.51	0.42
1:G:343:ARG:HG3	1:G:344:THR:CG2	2.49	0.42
1:G:690:PRO:O	1:G:691:ALA:C	2.60	0.42
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.53	0.42
2:H:221:ALA:O	2:H:222:GLN:C	2.62	0.42
2:H:236:ILE:O	2:H:265:VAL:HG22	2.19	0.42
1:A:10:ILE:HD13	1:A:37:LEU:HD13	2.01	0.42
1:A:452:VAL:O	1:A:453:PHE:C	2.61	0.42
1:A:936:ASN:HB2	10:A:4034:HOH:O	2.18	0.42
2:B:144:LEU:HD11	2:B:148:ARG:NE	2.34	0.42
1:C:523:HIS:HB3	1:C:524:PRO:HD2	2.01	0.42
1:C:704:LYS:HD2	1:C:707:GLU:OE2	2.19	0.42
1:C:930:LYS:NZ	1:C:1058:ALA:O	2.45	0.42
2:D:258:PHE:O	2:D:261:THR:HB	2.19	0.42
1:E:339:ILE:HD13	1:E:339:ILE:HG21	1.83	0.42
1:E:403:GLU:CD	1:E:646:THR:HG23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:286[A]:MET:HE2	2:F:314:PHE:N	2.34	0.42
2:F:345:LYS:HB3	2:F:346:PRO:CD	2.43	0.42
2:H:132:ILE:HG22	2:H:133:ILE:N	2.33	0.42
2:H:150:PHE:CE1	2:H:152:GLY:HA2	2.54	0.42
1:E:563[A]:MET:HE2	1:E:563[A]:MET:HB2	1.78	0.42
2:F:194:VAL:HG13	2:F:235:GLY:C	2.44	0.42
2:F:206:LEU:O	2:F:209:LEU:N	2.48	0.42
2:F:214:CYS:SG	2:F:371:ILE:HD11	2.60	0.42
1:G:854:SER:HA	1:G:859:VAL:O	2.19	0.42
1:G:938:THR:HB	10:G:4673:HOH:O	2.18	0.42
1:A:76:LYS:HA	1:A:76:LYS:HD2	1.70	0.42
1:A:139:ILE:HG13	1:A:141:LEU:HG	2.00	0.42
1:A:472:LEU:O	1:A:473:GLU:C	2.61	0.42
2:B:48:TYR:HA	2:B:51:GLN:NE2	2.34	0.42
2:B:162:VAL:HG21	2:B:200:GLY:HA3	2.01	0.42
1:C:671:ARG:NH2	1:C:819:GLU:O	2.52	0.42
1:E:714:VAL:HG13	1:E:752:LEU:HD12	2.00	0.42
1:E:766:ALA:HB1	1:E:774:LEU:O	2.19	0.42
1:E:773[B]:VAL:HG12	1:E:818:PHE:CZ	2.55	0.42
1:E:904:ASP:O	1:E:906:LEU:N	2.48	0.42
2:F:328:THR:HG21	2:F:341:HIS:HB2	2.02	0.42
1:G:85:ALA:HB1	1:G:114:THR:O	2.19	0.42
1:G:514:ARG:HD3	10:G:4409:HOH:O	2.20	0.42
2:H:64:GLY:C	2:H:65:THR:HG23	2.44	0.42
1:A:17:PRO:HB2	1:A:894:VAL:HG21	2.01	0.42
1:A:577:GLU:H	1:A:577:GLU:CD	2.28	0.42
1:A:820:LEU:O	1:A:821:GLN:HB2	2.19	0.42
1:A:946:LEU:HB3	1:A:1013:ILE:HG12	2.01	0.42
1:C:529:VAL:HB	1:C:542:TYR:CD2	2.54	0.42
2:F:63:VAL:O	2:F:94:ASN:HB2	2.19	0.42
2:F:357:SER:N	2:F:358:PRO:CA	2.79	0.42
1:G:669:ILE:HA	1:G:844:PRO:HG2	2.02	0.42
1:A:358:LYS:HG2	1:A:359:ILE:N	2.33	0.42
2:B:261:THR:HG21	2:B:263:ILE:CD1	2.49	0.42
2:B:279:SER:HB2	2:B:325:LEU:HD11	2.02	0.42
1:C:363:ASN:ND2	1:C:365:GLU:OE1	2.40	0.42
1:C:711:PRO:C	1:C:712:LEU:HD12	2.44	0.42
2:D:224:SER:OG	2:D:227:ASP:HB2	2.20	0.42
2:D:267:GLY:O	2:D:349:SER:HB2	2.19	0.42
1:E:796:LEU:HA	1:E:797:PRO:HA	1.79	0.42
2:F:78:GLN:NE2	10:F:3227:HOH:O	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:891:LYS:HE3	1:G:893:VAL:HG12	2.01	0.42
2:H:46:PRO:C	2:H:48:TYR:H	2.27	0.42
2:H:170:TRP:HB3	2:H:216:LEU:HD12	2.01	0.42
2:H:342:ARG:HD2	2:H:342:ARG:HA	1.85	0.42
1:A:1021:ARG:O	1:A:1025:ASP:OD2	2.37	0.42
2:B:339:GLY:C	2:B:340:ILE:HG23	2.44	0.42
1:C:375:THR:HG23	1:C:377:GLN:H	1.84	0.42
1:C:470:VAL:O	1:C:474:GLU:HG3	2.20	0.42
1:C:675:ARG:H	1:C:675:ARG:HD3	1.83	0.42
2:D:158:LEU:O	2:D:161:GLU:HB2	2.20	0.42
1:E:109:GLU:O	1:E:110:GLU:C	2.57	0.42
1:E:208:GLU:O	1:E:208:GLU:HG3	2.18	0.42
1:E:503:ALA:HB2	1:E:510:GLU:HA	2.01	0.42
1:E:734:LEU:HD23	1:E:734:LEU:HA	1.82	0.42
2:F:208:MET:HE1	2:F:363:ALA:HB1	2.01	0.42
1:G:764:VAL:O	1:G:827:ASN:HA	2.19	0.42
1:G:820:LEU:O	1:G:821:GLN:C	2.62	0.42
1:G:1031:ARG:HE	1:G:1031:ARG:HB3	1.41	0.42
2:H:219:VAL:HG23	2:H:220:PRO:O	2.20	0.42
1:A:59[B]:GLU:CD	1:A:60:MET:HE2	2.44	0.42
1:A:237:PHE:HB3	1:A:248:ILE:O	2.19	0.42
1:A:353:ASP:OD1	2:B:116:ARG:HD2	2.19	0.42
2:B:298:LYS:O	2:B:329:HIS:HA	2.19	0.42
1:C:695:VAL:HG12	1:C:696:THR:N	2.35	0.42
1:C:905:PRO:HB2	1:C:1040:TYR:HH	1.83	0.42
1:E:471:ARG:O	1:E:474:GLU:HB2	2.20	0.42
1:E:883:VAL:C	1:E:884:ILE:HG12	2.43	0.42
1:G:407:THR:HG21	1:G:504:LYS:HE3	2.00	0.42
2:H:60:ILE:O	2:H:86:PRO:HD2	2.19	0.42
2:H:194:VAL:HG13	2:H:195:VAL:N	2.34	0.42
2:B:169:SER:HA	2:B:216:LEU:O	2.20	0.42
2:B:209:LEU:O	2:B:214:CYS:HB2	2.19	0.42
2:B:221:ALA:HB1	2:B:250:TYR:CE1	2.55	0.42
2:B:335:GLY:O	2:B:336:THR:C	2.63	0.42
2:B:348:PHE:HE1	2:B:366:LEU:HD22	1.84	0.42
1:C:145[A]:ARG:HB3	1:C:208:GLU:CG	2.50	0.42
9:C:4032:NET:H63	9:C:4032:NET:H31	1.90	0.42
2:D:188:ASP:OD2	2:D:188:ASP:N	2.29	0.42
1:E:196:LEU:HG	1:E:204:LEU:CD1	2.50	0.42
1:E:246:ASP:CG	1:E:379:LYS:H	2.27	0.42
1:E:308:SER:HB3	10:E:1376:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:286[B]:MET:HE1	2:F:290:HIS:NE2	2.34	0.42
1:G:560:GLU:HB3	1:G:636:LYS:HD2	2.00	0.42
1:A:435:ARG:O	1:A:439:ILE:HG13	2.20	0.41
1:A:504[B]:LYS:HG2	10:A:4325:HOH:O	2.19	0.41
2:B:33:ASN:HB3	2:B:55:LEU:CD2	2.50	0.41
2:B:166:GLU:O	2:B:167:ALA:C	2.62	0.41
2:B:187:GLU:C	2:B:189:GLU:H	2.28	0.41
1:C:1041:ASP:OD1	1:C:1047:GLY:HA2	2.20	0.41
1:E:781:HIS:CE1	1:E:789:SER:HA	2.55	0.41
1:G:275:ILE:HA	1:G:275:ILE:HD12	1.74	0.41
1:G:1063:ILE:O	1:G:1063:ILE:HG23	2.20	0.41
2:H:231:MET:O	2:H:232:ASN:C	2.63	0.41
2:H:274:LEU:HD23	2:H:274:LEU:HA	1.74	0.41
1:A:154:GLU:O	1:A:155:ALA:C	2.61	0.41
1:A:701:ALA:O	1:A:705:ALA:N	2.32	0.41
2:B:138:PRO:HA	10:B:4125:HOH:O	2.19	0.41
2:B:286:MET:CE	2:B:289:GLY:HA2	2.47	0.41
1:C:242:ILE:O	1:C:243:HIS:C	2.62	0.41
1:E:275:ILE:HD12	1:E:275:ILE:HA	1.82	0.41
1:E:750:VAL:HG12	1:E:750:VAL:O	2.19	0.41
1:A:136:MET:HA	1:A:139:ILE:HG12	2.02	0.41
1:A:843:ASN:HA	1:A:844:PRO:HD3	1.76	0.41
2:B:274:LEU:O	2:B:275:LEU:C	2.61	0.41
2:B:340:ILE:O	2:B:340:ILE:HG13	2.18	0.41
2:D:6:LEU:N	2:D:133:ILE:O	2.47	0.41
1:E:58:PRO:HD2	1:E:59:GLU:OE2	2.19	0.41
1:E:648:LEU:HD13	10:E:1595:HOH:O	2.20	0.41
1:E:734:LEU:CD2	1:E:738:PHE:CE2	3.03	0.41
1:E:805:ILE:HD12	1:E:832:VAL:CG1	2.51	0.41
1:G:3:LYS:HB3	1:G:330:TYR:CZ	2.54	0.41
1:G:734:LEU:HA	1:G:734:LEU:HD23	1.80	0.41
2:H:363:ALA:O	2:H:366:LEU:HB2	2.20	0.41
1:A:534:ALA:HB2	2:B:116:ARG:NH1	2.35	0.41
2:B:342:ARG:HD2	2:B:342:ARG:HA	1.88	0.41
1:C:421:LEU:HA	1:C:421:LEU:HD23	1.84	0.41
1:E:417:ASP:OD2	1:E:419:GLU:N	2.47	0.41
1:E:781:HIS:HE1	1:E:789:SER:HB3	1.85	0.41
2:F:154:ASN:HD22	2:F:155:GLY:H	1.69	0.41
1:G:423:LYS:H	1:G:423:LYS:HG3	1.68	0.41
1:G:1051:ALA:HA	1:G:1054:LEU:HD12	2.01	0.41
2:B:144:LEU:O	2:B:147:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.90	0.41
1:C:710:TYR:HA	1:C:711:PRO:C	2.45	0.41
1:E:101:GLU:OE2	1:E:101:GLU:HA	2.20	0.41
1:E:516:LEU:HD12	1:E:516:LEU:HA	1.85	0.41
1:E:628:GLU:O	1:E:631:ARG:HB3	2.21	0.41
1:E:710:TYR:CB	1:E:711:PRO:HA	2.43	0.41
1:E:1061:LYS:HD3	10:E:3549:HOH:O	2.20	0.41
2:F:150:PHE:CG	2:F:151:PRO:HD2	2.52	0.41
2:F:255:ILE:HA	2:F:258:PHE:HD2	1.86	0.41
1:G:4:ARG:HD3	1:G:7:ILE:HD12	2.00	0.41
1:G:11:LEU:O	1:G:86:VAL:HA	2.19	0.41
1:G:421:LEU:HD23	1:G:421:LEU:HA	1.89	0.41
1:G:752:LEU:HD12	1:G:752:LEU:HA	1.68	0.41
1:G:947:LEU:HD12	1:G:947:LEU:N	2.34	0.41
1:A:318:PRO:HB2	1:A:321:LYS:HB2	2.02	0.41
2:B:256:GLN:O	2:B:259:LEU:HB2	2.21	0.41
2:B:321:LEU:HD12	2:B:321:LEU:HA	1.67	0.41
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.09	0.41
1:E:186:GLU:HB2	10:E:1334:HOH:O	2.21	0.41
2:F:207:ARG:NH2	10:F:3234:HOH:O	2.54	0.41
1:G:259:LYS:HD3	2:H:175:TRP:CD2	2.56	0.41
1:G:734:LEU:CD2	1:G:738:PHE:HE2	2.32	0.41
1:G:1044:LEU:HD12	1:G:1044:LEU:HA	1.87	0.41
2:H:263:ILE:HG23	2:H:264:PRO:HD2	2.03	0.41
2:H:267:GLY:O	2:H:268:ILE:HD13	2.21	0.41
1:A:223:ASP:OD2	1:A:227:ASN:HB2	2.21	0.41
1:A:534:ALA:O	2:B:123:ARG:HD3	2.21	0.41
2:B:283:THR:HA	2:B:315:ALA:O	2.20	0.41
2:B:344:ASP:C	2:B:345:LYS:HG2	2.45	0.41
1:C:187:GLU:O	1:C:188:PHE:C	2.61	0.41
1:C:1071:GLN:HE21	1:C:1071:GLN:HB3	1.54	0.41
2:F:321:LEU:HD12	2:F:321:LEU:HA	1.82	0.41
2:F:364:ALA:O	2:F:365:PRO:C	2.61	0.41
1:G:596:THR:O	1:G:614:ASP:HB2	2.21	0.41
1:G:1057:ASP:HB3	1:G:1060:GLU:HB2	2.02	0.41
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.56	0.41
1:A:367:PHE:CE1	1:A:912:ARG:HG2	2.56	0.41
1:A:860:PRO:O	1:A:864:VAL:HG23	2.21	0.41
2:B:6:LEU:HD11	2:B:8:VAL:HG22	2.02	0.41
2:B:153:LEU:O	2:B:156:MET:HB2	2.20	0.41
2:B:265:VAL:O	2:B:347:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ARG:HG3	1:C:148:ILE:HG13	2.03	0.41
1:C:525:VAL:HG12	1:C:551:CYS:HB2	2.01	0.41
1:C:783:GLU:OE2	1:C:783:GLU:N	2.51	0.41
1:C:992:ASN:O	1:C:1000:HIS:HB2	2.20	0.41
1:C:1001:ILE:HG22	1:C:1002:GLN:N	2.34	0.41
2:D:153:LEU:N	2:D:153:LEU:HD12	2.34	0.41
1:E:809:MET:HG2	1:E:830:PHE:CD2	2.55	0.41
1:G:51:PRO:C	1:G:53:THR:H	2.28	0.41
1:G:194:ARG:HH11	1:G:194:ARG:HD3	1.76	0.41
1:G:847:ALA:C	1:G:849:THR:H	2.29	0.41
2:H:66:ASN:OD1	2:H:68:ALA:N	2.54	0.41
2:H:83:ARG:HD2	2:H:83:ARG:C	2.45	0.41
1:A:322:VAL:O	1:A:326:LEU:HD13	2.21	0.41
1:A:527:LYS:HB2	1:A:544:TYR:CE2	2.55	0.41
1:A:689:GLN:HG2	1:A:690:PRO:HD2	2.03	0.41
1:A:806:GLN:HA	1:A:809:MET:HE3	2.03	0.41
2:B:33:ASN:HB3	2:B:55:LEU:HD23	2.03	0.41
2:B:373:LEU:HA	2:B:373:LEU:HD23	1.64	0.41
1:C:427:GLU:HG3	1:C:438:TYR:CE1	2.56	0.41
1:C:695:VAL:CG1	1:C:696:THR:N	2.83	0.41
1:C:732:ALA:O	1:C:733:ASP:C	2.62	0.41
2:D:189:GLU:C	2:D:190:LEU:HG	2.46	0.41
2:D:191:PRO:HD2	2:D:213:GLY:O	2.21	0.41
1:E:509:ARG:NH1	1:E:515:LYS:NZ	2.68	0.41
1:E:681:ALA:O	1:E:682:VAL:C	2.60	0.41
1:E:695:VAL:HG13	1:E:696:THR:N	2.36	0.41
1:E:854:SER:HA	1:E:859:VAL:O	2.20	0.41
1:E:891:LYS:HE2	1:E:891:LYS:HB3	1.71	0.41
1:E:948:SER:O	1:E:1015:ASN:HA	2.21	0.41
1:E:974:THR:O	1:E:975:HIS:C	2.63	0.41
1:E:1073:LYS:HD3	1:E:1073:LYS:N	2.36	0.41
2:F:299:ASP:O	2:F:303:ASN:N	2.47	0.41
1:G:392:GLN:O	1:G:396:GLN:HG3	2.21	0.41
1:G:671:ARG:HH22	1:G:819:GLU:HG3	1.84	0.41
1:G:981:LEU:CD1	1:G:988:PRO:HG3	2.42	0.41
1:G:1034:LEU:HD12	1:G:1034:LEU:HA	1.85	0.41
2:H:376:GLN:HA	2:H:379:LYS:HZ3	1.82	0.41
1:A:259:LYS:HD3	2:B:175:TRP:CZ3	2.57	0.41
1:A:425:ARG:HG2	10:A:4337:HOH:O	2.20	0.41
1:A:441:ASP:OD2	1:A:444:ARG:NH1	2.49	0.41
1:C:1000:HIS:CD2	1:C:1000:HIS:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:LYS:HB2	1:E:42:TYR:OH	2.21	0.41
1:E:65:TYR:OH	1:E:81:GLU:OE1	2.30	0.41
1:E:141:LEU:HD23	1:E:141:LEU:HA	1.82	0.41
1:E:236:ASN:HA	1:E:249:THR:HG22	2.03	0.41
1:E:490:ARG:HA	1:E:522:LEU:HD21	2.02	0.41
1:E:731:GLU:O	1:E:735:ARG:HG3	2.21	0.41
2:F:303:ASN:C	2:F:304:VAL:HG13	2.44	0.41
1:G:100:LEU:O	1:G:104:ARG:HB2	2.21	0.41
1:G:427:GLU:HG3	1:G:438:TYR:CD1	2.56	0.41
1:G:472:LEU:HD23	1:G:472:LEU:HA	1.90	0.41
1:G:475:LYS:HG2	1:G:488:PHE:CZ	2.56	0.41
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.56	0.41
1:G:1000:HIS:CD2	1:G:1000:HIS:C	2.99	0.41
2:H:8:VAL:HG12	2:H:9:LEU:N	2.35	0.41
2:H:199:PHE:HE2	2:H:238:LEU:HB3	1.86	0.41
2:H:378:ARG:C	2:H:380:THR:N	2.79	0.41
1:A:57:ASP:HA	1:A:58:PRO:HD3	1.67	0.40
1:A:701:ALA:O	1:A:702:VAL:C	2.65	0.40
1:A:1044:LEU:HD12	1:A:1044:LEU:HA	1.70	0.40
2:B:73:SER:HA	2:B:203:ARG:NH2	2.36	0.40
1:C:553:ALA:HB3	10:C:4403:HOH:O	2.21	0.40
1:C:737:TYR:O	1:C:738:PHE:C	2.64	0.40
2:D:266:PHE:HB2	2:D:370:PHE:CE1	2.56	0.40
1:E:704:LYS:O	1:E:705:ALA:C	2.64	0.40
1:E:735:ARG:O	1:E:738:PHE:N	2.53	0.40
2:F:249:ASP:OD1	2:F:250:TYR:N	2.52	0.40
1:G:9:SER:HA	1:G:43:ARG:O	2.21	0.40
1:G:40:GLU:HG2	1:G:325:LYS:HE2	2.02	0.40
1:G:223:ASP:OD1	1:G:227:ASN:HB2	2.21	0.40
1:G:674:ASP:HB3	1:G:677:ARG:CB	2.35	0.40
1:G:795:SER:OG	1:G:797:PRO:O	2.39	0.40
2:H:33:ASN:OD1	2:H:292:GLY:HA2	2.21	0.40
2:H:45:ASP:OD1	2:H:202:LYS:HD2	2.19	0.40
2:H:153:LEU:HD12	2:H:153:LEU:HA	1.66	0.40
2:H:153:LEU:HD12	2:H:156:MET:SD	2.60	0.40
2:H:261:THR:HG22	2:H:263:ILE:HG13	2.00	0.40
2:H:371:ILE:HD13	2:H:371:ILE:HA	1.92	0.40
1:A:163:GLY:O	1:A:166:CYS:HB3	2.22	0.40
1:A:246:ASP:CG	1:A:379:LYS:H	2.28	0.40
2:B:81:VAL:HG22	2:B:110:ILE:CG2	2.51	0.40
2:B:181:LEU:HD23	2:B:181:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:VAL:O	2:B:211:ASP:C	2.63	0.40
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.51	0.40
1:C:502:LEU:O	1:C:503:ALA:C	2.64	0.40
2:D:261:THR:HG21	2:D:263:ILE:HG13	2.03	0.40
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.21	0.40
1:G:24:CYS:C	1:G:26:PHE:N	2.79	0.40
1:G:262:GLN:OE1	1:G:262:GLN:HA	2.19	0.40
1:G:349:GLU:O	2:H:294:ASN:HB2	2.21	0.40
1:G:480:GLY:O	1:G:481:ILE:C	2.65	0.40
2:H:46:PRO:O	2:H:48:TYR:N	2.53	0.40
2:B:191:PRO:HD2	2:B:213:GLY:CA	2.52	0.40
1:C:43:ARG:HH11	1:C:43:ARG:HD2	1.73	0.40
1:C:562:ILE:HD13	1:C:562:ILE:HA	1.92	0.40
1:E:8[A]:LYS:HG3	10:E:2527:HOH:O	2.21	0.40
1:E:884:ILE:HA	1:E:885:PRO:HD3	1.65	0.40
2:F:268:ILE:HD13	2:F:268:ILE:HA	1.82	0.40
1:G:141:LEU:HD23	1:G:141:LEU:HA	1.90	0.40
1:G:168:ILE:HG22	1:G:204:LEU:HD22	2.03	0.40
1:G:770:GLY:CA	1:G:823:ARG:CZ	2.99	0.40
1:G:1073:LYS:HA	1:G:1073:LYS:HD3	1.65	0.40
2:H:264:PRO:HA	2:H:346:PRO:HB2	2.02	0.40
1:A:240:MET:HE3	7:A:4001:ADP:C4	2.55	0.40
1:A:757:ASP:O	1:A:758:ASP:C	2.65	0.40
1:A:797:PRO:O	1:A:798:ALA:C	2.61	0.40
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.77	0.40
1:A:998:ARG:HA	1:A:999:PRO:HA	1.68	0.40
2:B:164:THR:HG23	2:B:220:PRO:HG3	2.04	0.40
2:B:166:GLU:C	2:B:167:ALA:O	2.63	0.40
2:B:326:ARG:CZ	2:B:341:HIS:HB3	2.51	0.40
1:C:85:ALA:HB1	1:C:114:THR:O	2.21	0.40
2:D:195:VAL:HG21	2:D:231:MET:HE3	2.03	0.40
2:D:374:ILE:O	2:D:377:TYR:HB3	2.21	0.40
1:E:47:VAL:HA	1:E:65:TYR:O	2.22	0.40
1:E:979:ILE:O	1:E:983:GLU:HG3	2.21	0.40
2:F:273:GLN:NE2	2:F:314:PHE:O	2.54	0.40
2:F:364:ALA:N	2:F:365:PRO:HD2	2.35	0.40
2:F:376:GLN:HA	2:F:379[A]:LYS:HZ3	1.87	0.40
1:G:671:ARG:NH2	1:G:819:GLU:O	2.54	0.40
1:G:819:GLU:O	1:G:821:GLN:HG2	2.21	0.40
1:G:839:LEU:HA	1:G:839:LEU:HD12	1.76	0.40
1:G:978:ALA:O	1:G:979:ILE:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:289:GLY:N	10:H:3157:HOH:O	2.47	0.40
2:H:354:PRO:CB	2:H:363:ALA:CB	2.98	0.40
1:A:86:VAL:O	1:A:86:VAL:HG13	2.20	0.40
1:A:420:ALA:O	1:A:421:LEU:C	2.63	0.40
2:B:249:ASP:O	2:B:250:TYR:C	2.65	0.40
1:C:780:GLU:HB3	1:C:798:ALA:HA	2.02	0.40
2:D:228:VAL:C	2:D:230:LYS:N	2.79	0.40
1:E:358:LYS:HG2	1:E:359:ILE:N	2.36	0.40
1:E:712:LEU:N	1:E:728:VAL:O	2.42	0.40
1:E:1049:ALA:O	1:E:1050:THR:C	2.62	0.40
1:G:165:PRO:HA	1:G:182:ALA:O	2.22	0.40
2:H:33:ASN:HA	2:H:291:HIS:O	2.22	0.40
2:H:283:THR:OG1	10:H:3162:HOH:O	2.22	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	1059/1073 (99%)	993 (94%)	63 (6%)	3 (0%)	36	36
1	C	1060/1073 (99%)	997 (94%)	59 (6%)	4 (0%)	30	28
1	E	1059/1073 (99%)	1008 (95%)	46 (4%)	5 (0%)	24	22
1	G	1060/1073 (99%)	989 (93%)	64 (6%)	7 (1%)	18	15
2	B	372/382 (97%)	334 (90%)	31 (8%)	7 (2%)	6	3
2	D	373/382 (98%)	351 (94%)	21 (6%)	1 (0%)	36	36
2	F	374/382 (98%)	360 (96%)	11 (3%)	3 (1%)	16	12
2	H	372/382 (97%)	324 (87%)	40 (11%)	8 (2%)	5	2
All	All	5729/5820 (98%)	5356 (94%)	335 (6%)	38 (1%)	21	15

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	167	ALA
1	G	558	ASP
1	G	739	GLN
2	H	185	LYS
2	H	223	THR
2	B	336	THR
1	C	738	PHE
1	C	739	GLN
1	E	954	LYS
2	B	127	ALA
2	B	376	GLN
1	E	478	GLU
1	E	975	HIS
2	H	47	SER
2	H	253	THR
1	A	342	GLY
1	A	716	PRO
1	A	975	HIS
2	B	145	GLU
1	C	1020	ARG
1	E	675	ARG
2	F	165	ALA
2	F	364	ALA
1	G	586	SER
1	G	736	ARG
1	G	975	HIS
2	D	364	ALA
2	F	243	GLY
1	G	740	THR
2	H	230[A]	LYS
2	H	230[B]	LYS
2	H	366	LEU
1	G	652	ARG
2	B	191	PRO
2	B	233	PRO
1	C	2	PRO
1	E	2	PRO
2	H	138	PRO

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%)	806 (92%)	65 (8%)	12	10
1	C	872/878 (99%)	799 (92%)	73 (8%)	10	7
1	E	871/878 (99%)	793 (91%)	78 (9%)	9	6
1	G	872/878 (99%)	794 (91%)	78 (9%)	9	6
2	B	306/311 (98%)	257 (84%)	49 (16%)	2	1
2	D	307/311 (99%)	283 (92%)	24 (8%)	11	9
2	F	308/311 (99%)	274 (89%)	34 (11%)	6	3
2	H	306/311 (98%)	268 (88%)	38 (12%)	4	2
All	All	4713/4756 (99%)	4274 (91%)	439 (9%)	8	6

All (439) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	8	LYS
1	A	38	ARG
1	A	55	MET
1	A	103	GLU
1	A	113	VAL
1	A	137	LYS
1	A	174	MET
1	A	185	ARG
1	A	202	LYS
1	A	220	VAL
1	A	275	ILE
1	A	297	VAL
1	A	336	MET
1	A	338	ASP
1	A	343	ARG
1	A	358	LYS
1	A	363	ASN
1	A	412	LYS

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Mol	Chain	Res	Type
1	A	416	ASP
1	A	426	ARG
1	A	429	LYS
1	A	471	ARG
1	A	481	ILE
1	A	542	TYR
1	A	548	GLU
1	A	559	ARG
1	A	562	ILE
1	A	591	GLU
1	A	636	LYS
1	A	645	GLN
1	A	671	ARG
1	A	675	ARG
1	A	696	THR
1	A	704	LYS
1	A	706	LYS
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	752	LEU
1	A	763	ASP
1	A	784	GLN
1	A	805	ILE
1	A	835	ASN
1	A	839	LEU
1	A	849	THR
1	A	855	LYS
1	A	884	ILE
1	A	912	ARG
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	955	GLU
1	A	963	LYS
1	A	966	LYS
1	A	967	GLN
1	A	992	ASN
1	A	1006	LYS
1	A	1014	ILE
1	A	1018	SER
1	A	1020	ARG

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Mol	Chain	Res	Type
1	A	1026	SER
1	A	1028	VAL
1	A	1032	SER
1	A	1063	ILE
2	B	6	LEU
2	B	7	LEU
2	B	18	ARG
2	B	20	ILE
2	B	25	SER
2	B	49	SER
2	B	78	GLN
2	B	87	LEU
2	B	104	ARG
2	B	113	ILE
2	B	118	LEU
2	B	128	GLN
2	B	153	LEU
2	B	154	ASN
2	B	156	MET
2	B	166	GLU
2	B	169	SER
2	B	186	LYS
2	B	192	PHE
2	B	195	VAL
2	B	204	ASN
2	B	205	ILE
2	B	215	ARG
2	B	218	ILE
2	B	219	VAL
2	B	222	GLN
2	B	226	GLU
2	B	228	VAL
2	B	231	MET
2	B	252	ILE
2	B	255	ILE
2	B	257[A]	LYS
2	B	257[B]	LYS
2	B	268	ILE
2	B	282	LYS
2	B	284	VAL
2	B	304	VAL
2	B	306	MET

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Mol	Chain	Res	Type
2	B	321	LEU
2	B	324	ASN
2	B	326	ARG
2	B	332	LEU
2	B	333	PHE
2	B	336	THR
2	B	345	LYS
2	B	373	LEU
2	B	376	GLN
2	B	379	LYS
2	B	380	THR
1	C	4	ARG
1	C	5[A]	THR
1	C	5[B]	THR
1	C	5[C]	THR
1	C	8	LYS
1	C	38	ARG
1	C	44	VAL
1	C	46	ASN
1	C	76	LYS
1	C	145[A]	ARG
1	C	145[B]	ARG
1	C	174	MET
1	C	185	ARG
1	C	275	ILE
1	C	279	THR
1	C	297	VAL
1	C	344	THR
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	416	ASP
1	C	419	GLU
1	C	422	THR
1	C	482	THR
1	C	519	GLN
1	C	559	ARG
1	C	571	ARG
1	C	591	GLU
1	C	645	GLN
1	C	655	GLU
1	C	665	SER

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Mol	Chain	Res	Type
1	C	671	ARG
1	C	675	ARG
1	C	677	ARG
1	C	680	HIS
1	C	688	LYS
1	C	696	THR
1	C	698	ILE
1	C	704	LYS
1	C	706	LYS
1	C	707	GLU
1	C	714	VAL
1	C	728	VAL
1	C	733	ASP
1	C	734	LEU
1	C	735	ARG
1	C	751	LEU
1	C	752	LEU
1	C	763	ASP
1	C	772	MET
1	C	784	GLN
1	C	803	GLN
1	C	805	ILE
1	C	811	GLN
1	C	821	GLN
1	C	835	ASN
1	C	845	ARG
1	C	849	THR
1	C	855	LYS
1	C	880	THR
1	C	912	ARG
1	C	936	ASN
1	C	940	LYS
1	C	951	GLU
1	C	955	GLU
1	C	998	ARG
1	C	1006	LYS
1	C	1014	ILE
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1028	VAL
1	C	1031	ARG

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Mol	Chain	Res	Type
2	D	18	ARG
2	D	27	VAL
2	D	104	ARG
2	D	142	LEU
2	D	154	ASN
2	D	166	GLU
2	D	169	SER
2	D	185	LYS
2	D	190	LEU
2	D	204	ASN
2	D	222	GLN
2	D	228	VAL
2	D	257	LYS
2	D	261	THR
2	D	263	ILE
2	D	268	ILE
2	D	306	MET
2	D	324	ASN
2	D	326	ARG
2	D	355	GLU
2	D	357	SER
2	D	372	GLU
2	D	376	GLN
2	D	379	LYS
1	E	5	THR
1	E	8[A]	LYS
1	E	8[B]	LYS
1	E	20	ILE
1	E	38	ARG
1	E	55	MET
1	E	59	GLU
1	E	103	GLU
1	E	119	THR
1	E	128	ASP
1	E	190	GLU
1	E	202	LYS
1	E	217	GLU
1	E	236	ASN
1	E	275	ILE
1	E	326	LEU
1	E	363	ASN
1	E	412	LYS

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Mol	Chain	Res	Type
1	E	414	SER
1	E	416	ASP
1	E	422	THR
1	E	478	GLU
1	E	479	VAL
1	E	509	ARG
1	E	515	LYS
1	E	518	ASP
1	E	548	GLU
1	E	556	SER
1	E	558	ASP
1	E	559	ARG
1	E	571	ARG
1	E	591	GLU
1	E	634	LYS
1	E	645	GLN
1	E	669	ILE
1	E	671	ARG
1	E	675	ARG
1	E	677	ARG
1	E	684	ARG
1	E	688	LYS
1	E	689	GLN
1	E	695	VAL
1	E	703	GLU
1	E	706	LYS
1	E	714	VAL
1	E	715	ARG
1	E	731	GLU
1	E	733	ASP
1	E	734	LEU
1	E	751	LEU
1	E	752	LEU
1	E	763	ASP
1	E	772	MET
1	E	774	LEU
1	E	784	GLN
1	E	795	SER
1	E	805	ILE
1	E	839	LEU
1	E	849	THR
1	E	855	LYS

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Mol	Chain	Res	Type
1	E	884	ILE
1	E	891	LYS
1	E	912	ARG
1	E	940	LYS
1	E	941	LYS
1	E	950	ARG
1	E	951	GLU
1	E	966	LYS
1	E	967[A]	GLN
1	E	967[B]	GLN
1	E	980	VAL
1	E	991	VAL
1	E	1006	LYS
1	E	1014	ILE
1	E	1018	SER
1	E	1020	ARG
1	E	1026	SER
1	E	1052	MET
2	F	6	LEU
2	F	10	GLU
2	F	18	ARG
2	F	73	SER
2	F	104	ARG
2	F	110	ILE
2	F	113	ILE
2	F	166	GLU
2	F	178	THR
2	F	186	LYS
2	F	192	PHE
2	F	204	ASN
2	F	205	ILE
2	F	215	ARG
2	F	216	LEU
2	F	226	GLU
2	F	231	MET
2	F	257	LYS
2	F	261	THR
2	F	268	ILE
2	F	282	LYS
2	F	321	LEU
2	F	324	ASN
2	F	332	LEU

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Mol	Chain	Res	Type
2	F	333	PHE
2	F	340	ILE
2	F	343	THR
2	F	354	PRO
2	F	355	GLU
2	F	372	GLU
2	F	376	GLN
2	F	379[A]	LYS
2	F	379[B]	LYS
2	F	380	THR
1	G	3	LYS
1	G	8	LYS
1	G	24	CYS
1	G	55	MET
1	G	77	ILE
1	G	79	GLU
1	G	103	GLU
1	G	148	ILE
1	G	162	VAL
1	G	174	MET
1	G	185	ARG
1	G	217	GLU
1	G	220	VAL
1	G	275	ILE
1	G	300	MET
1	G	321	LYS
1	G	326	LEU
1	G	331	THR
1	G	338	ASP
1	G	363	ASN
1	G	412	LYS
1	G	422	THR
1	G	426	ARG
1	G	428	LEU
1	G	475	LYS
1	G	479	VAL
1	G	509	ARG
1	G	515	LYS
1	G	519	GLN
1	G	548	GLU
1	G	558	ASP
1	G	559	ARG

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Mol	Chain	Res	Type
1	G	571	ARG
1	G	591	GLU
1	G	645[A]	GLN
1	G	645[B]	GLN
1	G	648	LEU
1	G	665	SER
1	G	670	ASP
1	G	675	ARG
1	G	692	ASN
1	G	704	LYS
1	G	706	LYS
1	G	713	VAL
1	G	714	VAL
1	G	726	GLU
1	G	728	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	774	LEU
1	G	780	GLU
1	G	784	GLN
1	G	795	SER
1	G	800	THR
1	G	811	GLN
1	G	815	LYS
1	G	836	GLU
1	G	849	THR
1	G	855	LYS
1	G	906	LEU
1	G	912	ARG
1	G	940	LYS
1	G	950	ARG
1	G	951	GLU
1	G	955	GLU
1	G	967	GLN
1	G	991	VAL
1	G	992	ASN
1	G	1001	ILE
1	G	1006	LYS

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Mol	Chain	Res	Type
1	G	1014	ILE
1	G	1018	SER
1	G	1020	ARG
1	G	1031	ARG
2	H	6	LEU
2	H	18	ARG
2	H	25	SER
2	H	73	SER
2	H	78	GLN
2	H	87	LEU
2	H	104	ARG
2	H	107	ILE
2	H	113	ILE
2	H	153	LEU
2	H	166	GLU
2	H	178	THR
2	H	192	PHE
2	H	194	VAL
2	H	205	ILE
2	H	216	LEU
2	H	218	ILE
2	H	222	GLN
2	H	226	GLU
2	H	231	MET
2	H	239	SER
2	H	252	ILE
2	H	265	VAL
2	H	268	ILE
2	H	272	HIS
2	H	279	SER
2	H	282	LYS
2	H	291	HIS
2	H	300	VAL
2	H	306	MET
2	H	324	ASN
2	H	326	ARG
2	H	332	LEU
2	H	355	GLU
2	H	372	GLU
2	H	374	ILE
2	H	376	GLN
2	H	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	105	GLN
1	A	266	ASN
1	A	679	GLN
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	814	GLN
1	A	827	ASN
1	A	834	ASN
1	A	835	ASN
1	A	843	ASN
1	A	936	ASN
1	A	942	HIS
1	A	967	GLN
1	A	987	ASN
1	A	992	ASN
1	A	995	HIS
1	A	1000	HIS
1	A	1007	ASN
1	A	1035	GLN
1	A	1039	HIS
1	A	1055	ASN
1	A	1071	GLN
2	B	16	HIS
2	B	51	GLN
2	B	78	GLN
2	B	154	ASN
2	B	183	GLN
2	B	193	HIS
2	B	204	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	46	ASN
1	C	105	GLN
1	C	266	ASN
1	C	457	ASN
1	C	784	GLN
1	C	803	GLN
1	C	811	GLN

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Mol	Chain	Res	Type
1	C	834	ASN
1	C	835	ASN
1	C	843	ASN
1	C	898	ASN
1	C	932	GLN
1	C	936	ASN
1	C	942	HIS
1	C	992	ASN
1	C	995	HIS
1	C	1000	HIS
1	C	1007	ASN
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	154	ASN
2	D	324	ASN
2	D	351	GLN
1	E	93	GLN
1	E	105	GLN
1	E	266	ASN
1	E	454	ASN
1	E	491	GLN
1	E	689	GLN
1	E	784	GLN
1	E	803	GLN
1	E	814	GLN
1	E	834	ASN
1	E	898	ASN
1	E	936	ASN
1	E	987	ASN
1	E	992	ASN
1	E	1007	ASN
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	14	GLN
2	F	16	HIS
2	F	51	GLN
2	F	78	GLN
2	F	105	HIS
2	F	154	ASN

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Mol	Chain	Res	Type
2	F	204	ASN
2	F	324	ASN
2	F	351	GLN
1	G	46	ASN
1	G	105	GLN
1	G	391	GLN
1	G	679	GLN
1	G	689	GLN
1	G	784	GLN
1	G	803	GLN
1	G	806	GLN
1	G	812	GLN
1	G	936	ASN
1	G	987	ASN
1	G	992	ASN
1	G	995	HIS
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN
1	G	1071	GLN
2	H	51	GLN
2	H	105	HIS
2	H	154	ASN
2	H	222	GLN
2	H	232	ASN
2	H	273	GLN
2	H	324	ASN
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 86 ligands modelled in this entry, 66 are monoatomic - leaving 20 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
8	ORN	E	4054	-	7,8,8	0.89	0	6,9,9	1.16	1 (16%)
7	ADP	E	4050	3,4	28,29,29	1.16	2 (7%)	43,45,45	0.83	2 (4%)
9	NET	G	4077	-	8,8,8	0.69	0	10,10,10	0.69	0
7	ADP	A	4001	3	28,29,29	1.40	6 (21%)	43,45,45	1.04	3 (6%)
7	ADP	C	4021	3	28,29,29	1.36	5 (17%)	43,45,45	0.95	3 (6%)
8	ORN	C	4031	-	7,8,8	0.99	0	6,9,9	0.80	0
6	PO4	G	4071	3	4,4,4	2.36	2 (50%)	6,6,6	1.14	0
9	NET	E	4055	-	8,8,8	0.68	0	10,10,10	0.65	0
6	PO4	E	4049	3	4,4,4	2.52	3 (75%)	6,6,6	0.79	0
7	ADP	G	4072	3,4	28,29,29	1.30	4 (14%)	43,45,45	0.92	0
6	PO4	C	4026	3	4,4,4	2.83	3 (75%)	6,6,6	1.08	0
8	ORN	A	4011	-	7,8,8	0.82	0	6,9,9	1.40	1 (16%)
9	NET	C	4032	-	8,8,8	0.60	0	10,10,10	0.73	0
7	ADP	G	4066	3	28,29,29	1.25	3 (10%)	43,45,45	1.28	5 (11%)
6	PO4	A	4006	3	4,4,4	2.16	2 (50%)	6,6,6	1.46	1 (16%)
7	ADP	C	4027	3,4	28,29,29	1.34	4 (14%)	43,45,45	1.14	3 (6%)
9	NET	A	4012	-	8,8,8	0.59	0	10,10,10	0.75	0
7	ADP	E	4044	3	28,29,29	1.50	1 (3%)	43,45,45	0.80	1 (2%)
8	ORN	G	4076	-	7,8,8	0.95	1 (14%)	6,9,9	0.91	0
7	ADP	A	4007	3,4	28,29,29	1.41	2 (7%)	43,45,45	0.91	1 (2%)

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
8	ORN	A	4011	-	-	3/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NET	E	4055	-	-	0/12/12/12	-
9	NET	C	4032	-	-	2/12/12/12	-
7	ADP	G	4066	3	-	2/16/32/32	0/3/3/3
8	ORN	E	4054	-	-	5/8/8/8	-
7	ADP	C	4027	3,4	-	0/16/32/32	0/3/3/3
7	ADP	E	4050	3,4	-	3/16/32/32	0/3/3/3
9	NET	A	4012	-	-	0/12/12/12	-
7	ADP	A	4001	3	-	1/16/32/32	0/3/3/3
7	ADP	C	4021	3	-	1/16/32/32	0/3/3/3
7	ADP	A	4007	3,4	-	0/16/32/32	0/3/3/3
7	ADP	E	4044	3	-	2/16/32/32	0/3/3/3
7	ADP	G	4072	3,4	-	0/16/32/32	0/3/3/3
8	ORN	G	4076	-	-	6/8/8/8	-
9	NET	G	4077	-	-	0/12/12/12	-
8	ORN	C	4031	-	-	6/8/8/8	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	4044	ADP	PA-O3A	-6.01	1.53	1.59
7	A	4007	ADP	PA-O3A	-5.14	1.54	1.59
7	A	4001	ADP	PA-O3A	-3.91	1.55	1.59
6	C	4026	PO4	P-O2	-3.88	1.43	1.54
7	C	4027	ADP	O2'-C2'	3.64	1.52	1.43
7	G	4072	ADP	O3'-C3'	3.45	1.51	1.43
6	G	4071	PO4	P-O2	-3.41	1.44	1.54
6	E	4049	PO4	P-O3	-3.33	1.44	1.54
7	C	4027	ADP	O3'-C3'	3.25	1.51	1.43
7	C	4021	ADP	O2'-C2'	3.17	1.50	1.43
6	A	4006	PO4	P-O2	-2.98	1.46	1.54
6	E	4049	PO4	P-O2	-2.87	1.46	1.54
6	C	4026	PO4	P-O3	-2.85	1.46	1.54
7	G	4066	ADP	O2'-C2'	2.78	1.49	1.43
6	C	4026	PO4	P-O4	-2.78	1.46	1.54
7	C	4021	ADP	C2-N1	2.76	1.38	1.33
7	G	4072	ADP	O2'-C2'	2.73	1.49	1.43
7	G	4066	ADP	C2-N1	2.72	1.38	1.33
7	C	4021	ADP	PA-O3A	-2.67	1.56	1.59
7	G	4066	ADP	O3'-C3'	2.56	1.49	1.43
7	E	4050	ADP	O2'-C2'	2.51	1.49	1.43
7	A	4001	ADP	O2'-C2'	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	4072	ADP	C2-N3	-2.42	1.29	1.33
7	C	4021	ADP	O3'-C3'	2.38	1.48	1.43
7	G	4072	ADP	O4'-C1'	-2.34	1.36	1.42
7	A	4001	ADP	C2-N3	-2.34	1.29	1.33
7	E	4050	ADP	PA-O3A	-2.32	1.57	1.59
6	G	4071	PO4	P-O3	-2.31	1.47	1.54
7	C	4027	ADP	PA-O3A	-2.20	1.57	1.59
7	A	4001	ADP	PB-O2B	-2.13	1.46	1.54
7	A	4001	ADP	O3'-C3'	2.13	1.48	1.43
7	C	4027	ADP	C2-N1	2.13	1.37	1.33
7	A	4007	ADP	C2-N1	2.11	1.37	1.33
7	A	4001	ADP	C2-N1	2.10	1.37	1.33
8	G	4076	ORN	O-C	2.09	1.28	1.22
6	A	4006	PO4	P-O4	-2.04	1.48	1.54
7	C	4021	ADP	O4'-C1'	-2.03	1.37	1.42
6	E	4049	PO4	P-O4	-2.00	1.48	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	4027	ADP	O2A-PA-O3A	3.50	116.74	107.27
7	G	4066	ADP	O3B-PB-O3A	-3.44	93.09	104.64
7	A	4001	ADP	C5-C6-N6	3.11	131.00	123.29
7	G	4066	ADP	O2'-C2'-C3'	2.91	121.14	111.82
7	G	4066	ADP	O4'-C1'-N9	-2.85	102.62	108.09
6	A	4006	PO4	O2-P-O1	-2.81	101.01	110.95
7	C	4027	ADP	O2'-C2'-C3'	2.80	120.81	111.82
7	C	4021	ADP	O3'-C3'-C2'	2.77	120.69	111.82
7	E	4050	ADP	O3'-C3'-C2'	2.53	119.94	111.82
7	G	4066	ADP	O3'-C3'-C2'	2.52	119.91	111.82
8	A	4011	ORN	CB-CA-C	-2.45	103.95	110.45
8	E	4054	ORN	OXT-C-O	-2.28	118.91	124.08
7	A	4001	ADP	O2A-PA-O3A	2.26	113.38	107.27
7	C	4021	ADP	O2'-C2'-C3'	2.24	119.01	111.82
7	C	4021	ADP	C5-C6-N6	2.20	128.72	123.29
7	G	4066	ADP	O2B-PB-O3A	2.19	111.99	104.64
7	E	4050	ADP	O2A-PA-O3A	2.14	113.06	107.27
7	E	4044	ADP	O3'-C3'-C2'	2.05	118.39	111.82
7	A	4001	ADP	N6-C6-N1	-2.03	113.86	118.38
7	A	4007	ADP	O2A-PA-O3A	2.02	112.72	107.27
7	C	4027	ADP	C2'-C3'-C4'	-2.01	98.73	102.61

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	4050	ADP	PA-O3A-PB-O3B
8	A	4011	ORN	N-CA-CB-CG
8	A	4011	ORN	C-CA-CB-CG
8	C	4031	ORN	N-CA-CB-CG
8	C	4031	ORN	C-CA-CB-CG
8	E	4054	ORN	N-CA-CB-CG
8	E	4054	ORN	C-CA-CB-CG
8	G	4076	ORN	N-CA-CB-CG
8	G	4076	ORN	C-CA-CB-CG
8	G	4076	ORN	O-C-CA-N
8	E	4054	ORN	OXT-C-CA-N
8	C	4031	ORN	CA-CB-CG-CD
8	G	4076	ORN	CA-CB-CG-CD
8	G	4076	ORN	OXT-C-CA-N
8	E	4054	ORN	O-C-CA-N
8	C	4031	ORN	OXT-C-CA-N
7	C	4021	ADP	PB-O3A-PA-O1A
7	E	4044	ADP	PB-O3A-PA-O1A
7	G	4066	ADP	PB-O3A-PA-O1A
7	G	4066	ADP	C5'-O5'-PA-O1A
7	E	4050	ADP	PB-O3A-PA-O2A
7	E	4050	ADP	PA-O3A-PB-O1B
8	C	4031	ORN	NE-CD-CG-CB
8	E	4054	ORN	NE-CD-CG-CB
8	G	4076	ORN	NE-CD-CG-CB
8	C	4031	ORN	O-C-CA-N
9	C	4032	NET	C4-C3-N1-C5
8	A	4011	ORN	OXT-C-CA-N
9	C	4032	NET	C4-C3-N1-C7
7	A	4001	ADP	PB-O3A-PA-O2A
7	E	4044	ADP	PB-O3A-PA-O2A

There are no ring outliers.

9 monomers are involved in 14 short contacts:

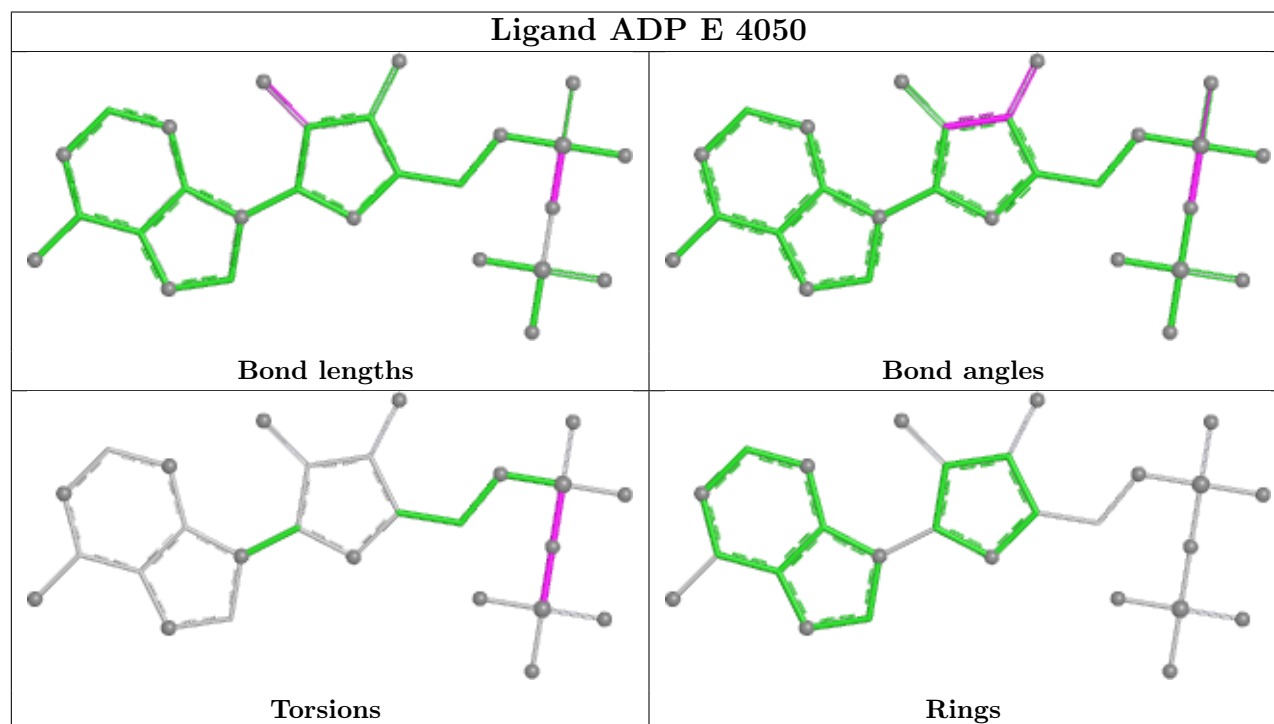
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	4054	ORN	1	0
7	E	4050	ADP	1	0
7	A	4001	ADP	1	0
8	C	4031	ORN	2	0

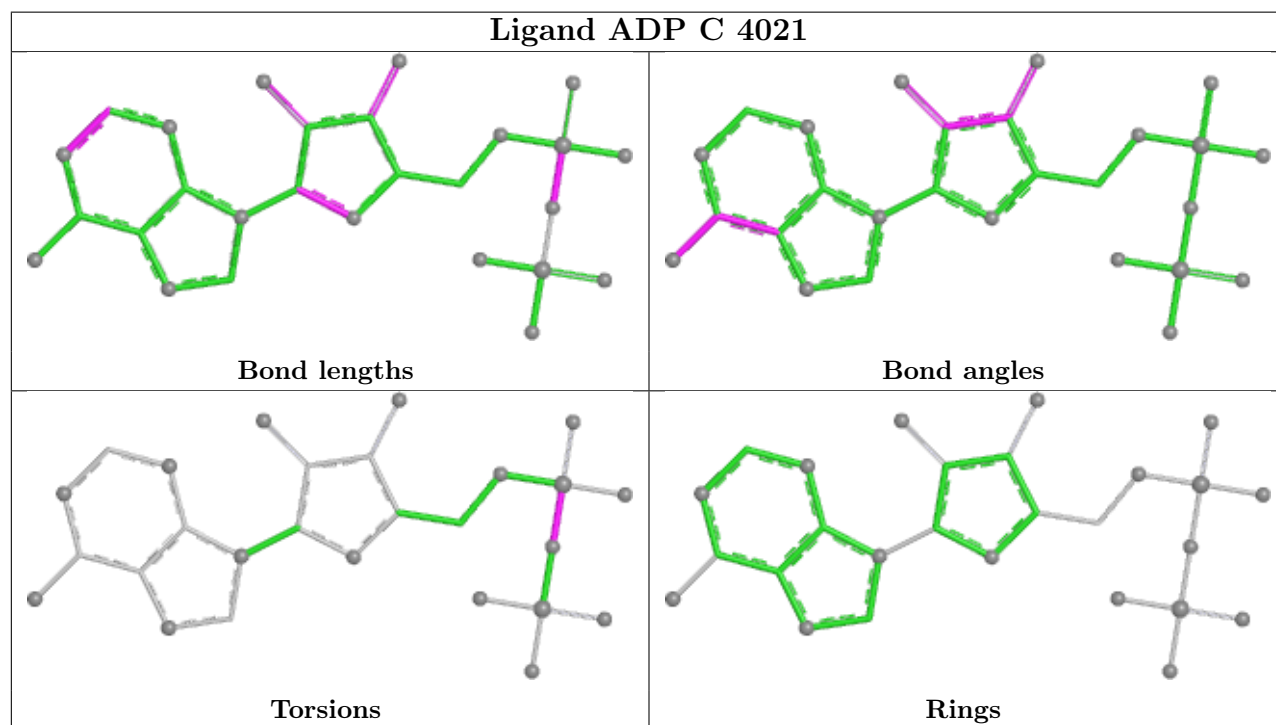
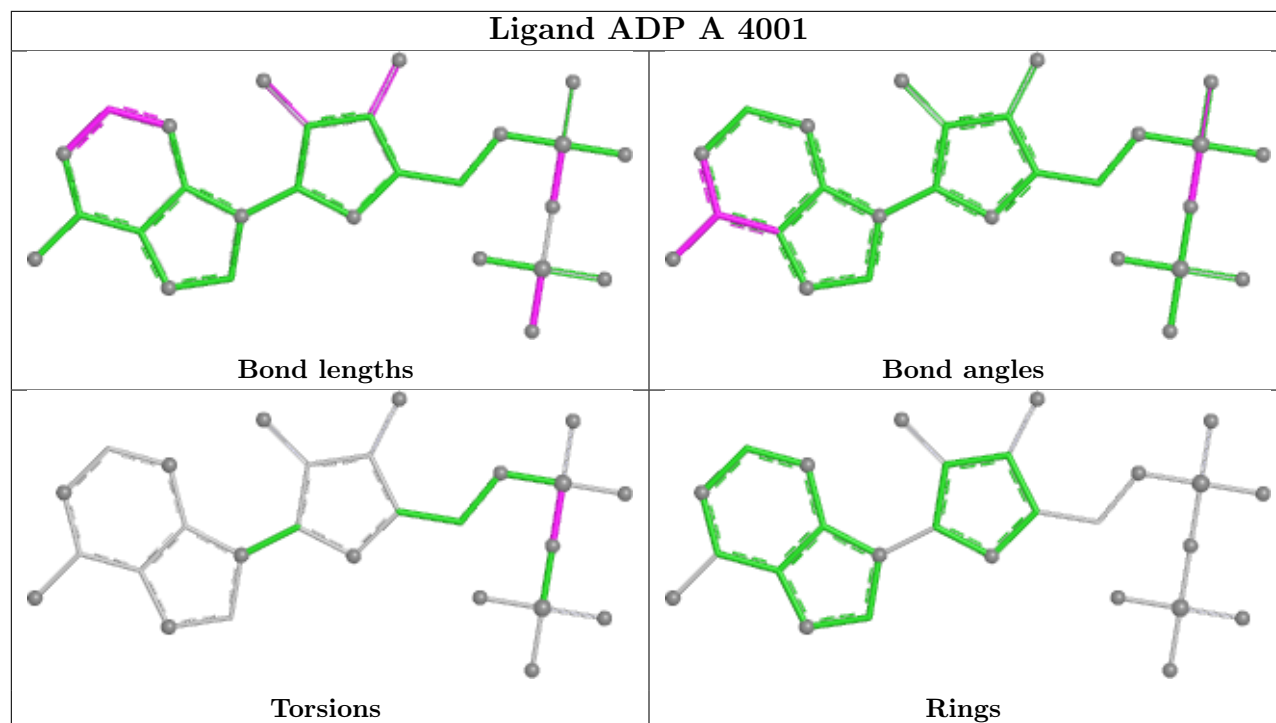
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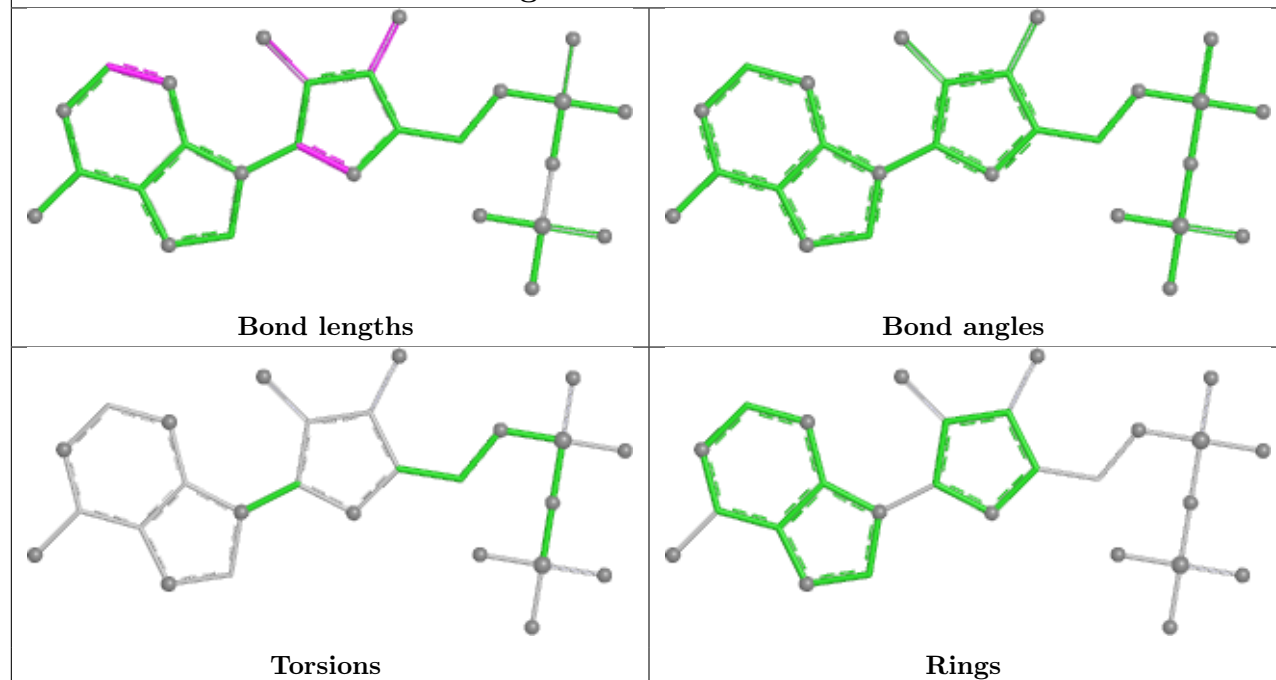
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	4032	NET	1	0
7	C	4027	ADP	1	0
9	A	4012	NET	3	0
8	G	4076	ORN	2	0
7	A	4007	ADP	2	0

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.

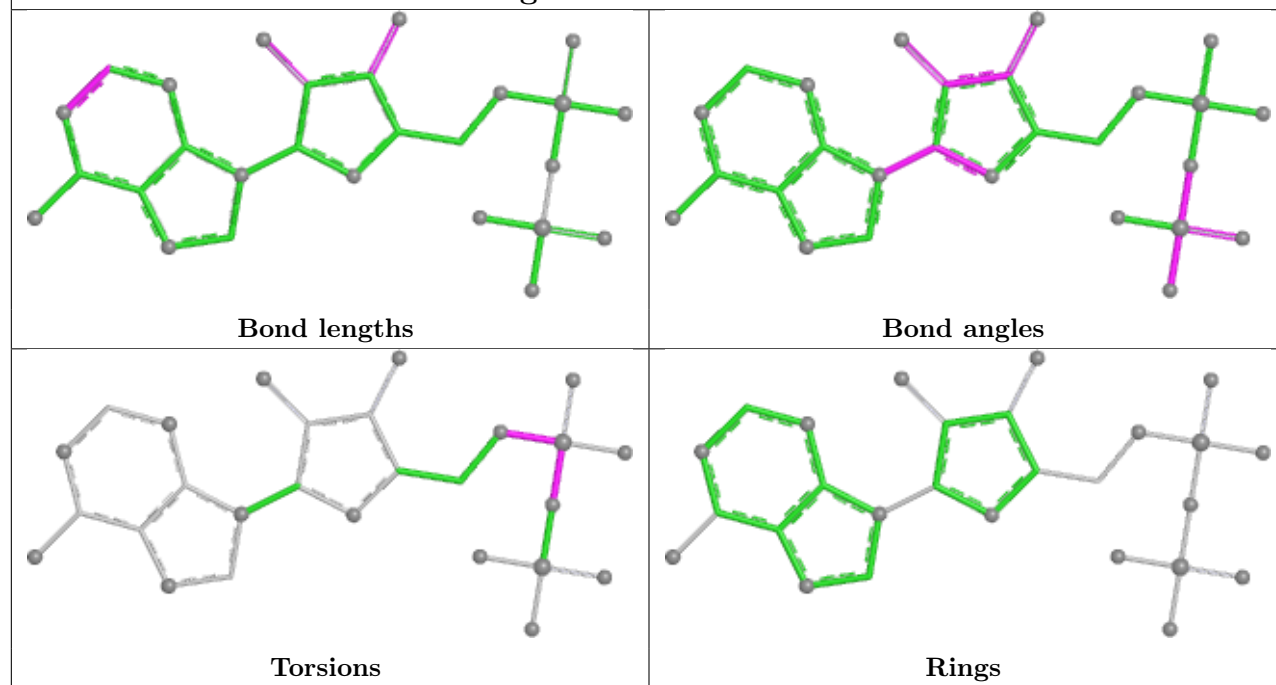




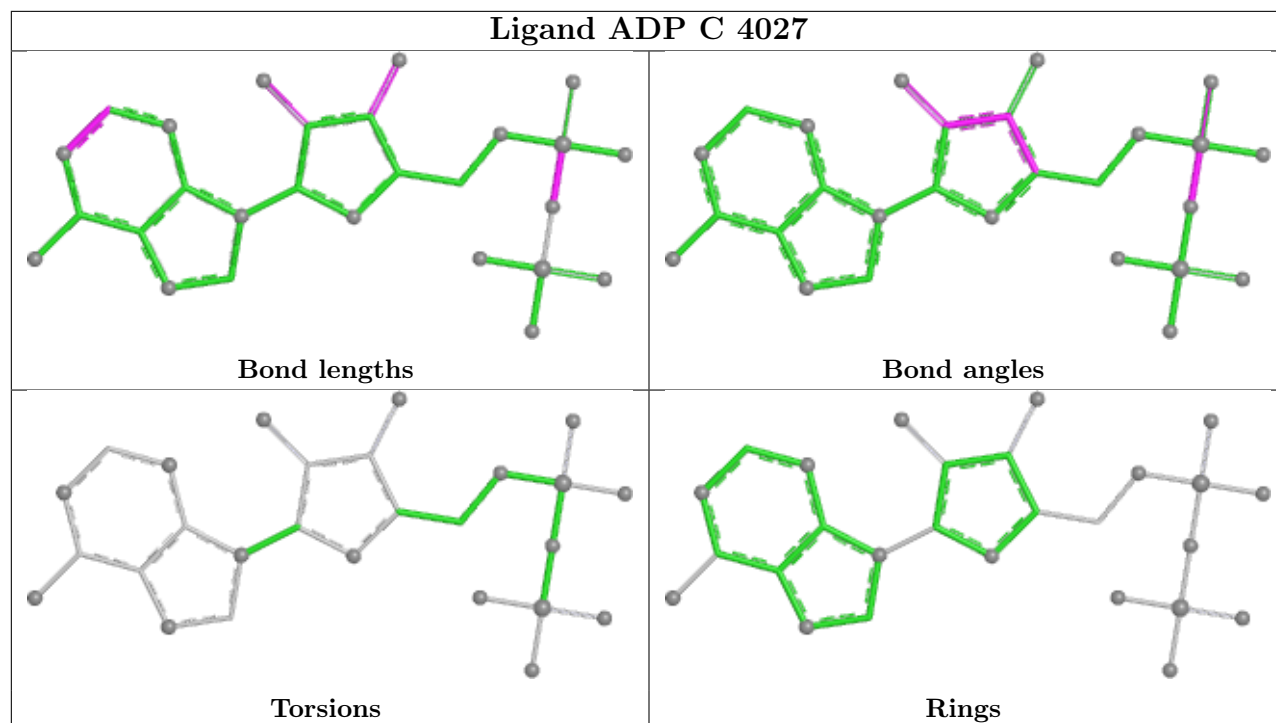
Ligand ADP G 4072



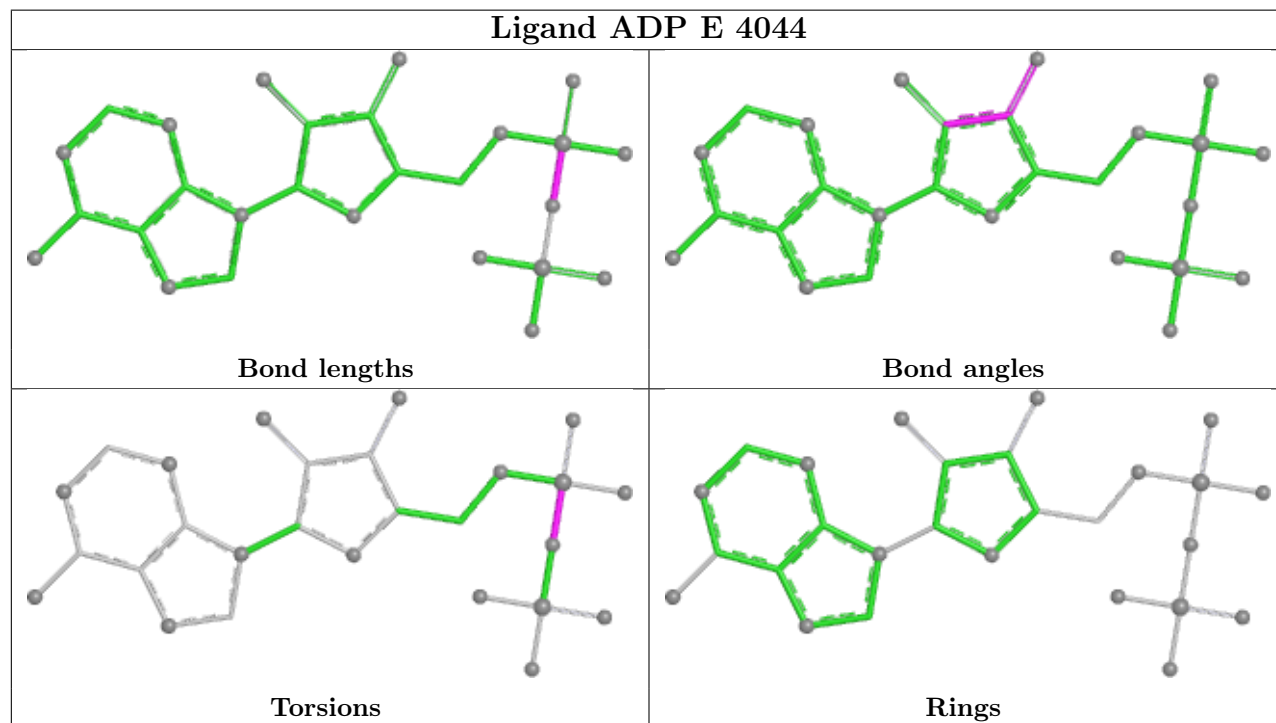
Ligand ADP G 4066

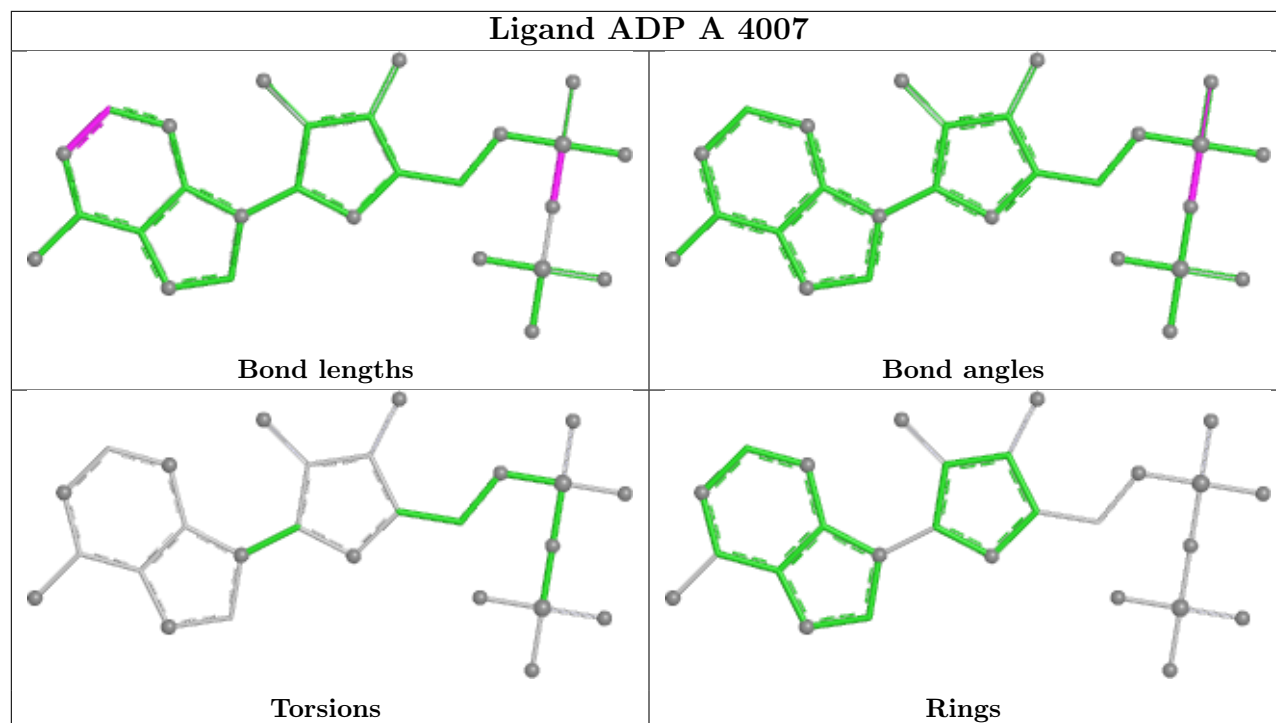


Ligand ADP C 4027



Ligand ADP E 4044





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1059/1073 (98%)	-0.58	21 (1%)	65	67	14, 29, 71, 100	6 (0%)
1	C	1059/1073 (98%)	-0.50	20 (1%)	66	69	14, 31, 76, 100	5 (0%)
1	E	1059/1073 (98%)	-0.62	14 (1%)	75	77	13, 27, 75, 100	6 (0%)
1	G	1059/1073 (98%)	-0.32	22 (2%)	63	66	17, 36, 81, 100	6 (0%)
2	B	375/382 (98%)	0.11	15 (4%)	42	44	21, 47, 84, 100	1 (0%)
2	D	375/382 (98%)	-0.36	4 (1%)	78	80	17, 33, 71, 100	2 (0%)
2	F	375/382 (98%)	-0.27	3 (0%)	82	84	15, 36, 76, 100	3 (0%)
2	H	375/382 (98%)	0.31	14 (3%)	45	47	26, 51, 90, 100	1 (0%)
All	All	5736/5820 (98%)	-0.39	113 (1%)	65	67	13, 33, 79, 100	30 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	363	ALA	7.5
1	E	368	ALA	7.4
1	G	368	ALA	5.9
1	A	750	VAL	5.2
2	H	363	ALA	5.1
1	A	716	PRO	5.0
1	G	751	LEU	4.9
2	B	363	ALA	4.8
2	F	364	ALA	4.8
2	B	358	PRO	4.3
1	E	1	MET	3.9
2	D	358	PRO	3.8
1	A	1	MET	3.8
1	C	1	MET	3.7
1	G	1	MET	3.7
1	A	751	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	994	VAL	3.6
1	A	741	ALA	3.5
1	E	341	GLY	3.5
1	A	717	SER	3.5
1	C	368	ALA	3.5
1	C	724	ALA	3.5
1	A	368	ALA	3.5
1	G	750	VAL	3.5
1	A	999	PRO	3.2
1	G	737	TYR	3.2
1	G	738	PHE	3.1
2	B	325	LEU	3.1
1	A	752	LEU	3.0
1	C	2	PRO	2.9
1	C	751	LEU	2.9
1	C	738	PHE	2.9
2	H	171	THR	2.8
1	C	703	GLU	2.8
1	A	729	TYR	2.8
2	B	225	ALA	2.8
2	H	364	ALA	2.8
1	C	678	PHE	2.8
2	B	2	ILE	2.8
2	H	188	ASP	2.7
1	G	729	TYR	2.7
1	C	999	PRO	2.7
1	A	739	GLN	2.7
2	F	358	PRO	2.7
1	A	700	MET	2.6
1	A	738	PHE	2.6
2	B	169	SER	2.6
1	G	695	VAL	2.6
2	H	275	LEU	2.6
1	E	698	ILE	2.6
2	H	377	TYR	2.6
2	D	363	ALA	2.6
1	G	2	PRO	2.6
1	E	740	THR	2.5
2	D	380	THR	2.5
1	G	717	SER	2.5
1	E	1008	GLY	2.5
1	G	672	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	323	ALA	2.5
1	G	683	GLU	2.4
1	C	1073	LYS	2.4
2	B	229	LEU	2.4
1	C	741	ALA	2.4
2	H	373	LEU	2.4
2	B	377	TYR	2.4
2	B	165	ALA	2.4
2	H	321	LEU	2.4
1	A	341	GLY	2.4
1	A	342	GLY	2.4
1	E	1020	ARG	2.4
1	C	732	ALA	2.3
2	D	364	ALA	2.3
2	H	356	ALA	2.3
1	C	700	MET	2.3
1	G	708	ILE	2.3
1	C	696	THR	2.3
2	B	260	GLU	2.3
1	C	716	PRO	2.3
2	B	380	THR	2.3
2	H	184	ALA	2.3
1	G	954	LYS	2.3
1	A	714	VAL	2.3
1	G	724	ALA	2.3
1	C	698	ILE	2.2
1	C	682	VAL	2.2
1	A	693	ALA	2.2
1	A	701	ALA	2.2
1	A	696	THR	2.2
1	E	729	TYR	2.2
1	C	740	THR	2.2
1	G	991	VAL	2.2
2	H	228	VAL	2.2
1	C	695	VAL	2.1
1	C	750	VAL	2.1
1	G	714	VAL	2.1
2	H	229	LEU	2.1
1	E	997	GLY	2.1
1	E	737	TYR	2.1
2	B	379	LYS	2.1
2	B	355	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	376	GLN	2.1
1	A	675	ARG	2.1
1	G	341	GLY	2.1
1	E	702	VAL	2.1
1	E	717	SER	2.1
1	G	693	ALA	2.1
2	H	233	PRO	2.0
1	G	678	PHE	2.0
1	E	732	ALA	2.0
2	H	225	ALA	2.0
1	A	559	ARG	2.0
1	G	715	ARG	2.0
1	E	342	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	C	4037	1/1	0.83	0.14	81,81,81,81	0
4	K	G	4074	1/1	0.90	0.11	86,86,86,86	0
5	CL	G	4081	1/1	0.91	0.13	75,75,75,75	0
5	CL	E	4060	1/1	0.93	0.08	56,56,56,56	0
5	CL	D	4043	1/1	0.93	0.11	80,80,80,80	0
5	CL	E	4063	1/1	0.94	0.07	59,59,59,59	0
8	ORN	A	4011	9/9	0.94	0.07	15,23,32,38	0
8	ORN	C	4031	9/9	0.94	0.09	19,26,46,57	0
4	K	G	4078	1/1	0.95	0.07	53,53,53,53	0
5	CL	G	4084	1/1	0.95	0.07	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ORN	E	4054	9/9	0.95	0.07	17,28,35,38	0
8	ORN	G	4076	9/9	0.95	0.08	22,30,47,60	0
5	CL	A	4018	1/1	0.96	0.09	58,58,58,58	0
4	K	A	4013	1/1	0.96	0.07	55,55,55,55	0
5	CL	C	4040	1/1	0.96	0.07	59,59,59,59	0
9	NET	G	4077	9/9	0.96	0.06	23,28,36,42	0
7	ADP	G	4072	27/27	0.97	0.06	30,43,80,95	0
4	K	B	4014	1/1	0.97	0.06	42,42,42,42	0
4	K	C	4029	1/1	0.97	0.07	76,76,76,76	0
4	K	C	4034	1/1	0.97	0.06	51,51,51,51	0
4	K	E	4056	1/1	0.97	0.06	42,42,42,42	0
9	NET	A	4012	9/9	0.97	0.06	12,19,26,28	0
9	NET	C	4032	9/9	0.97	0.06	15,21,28,30	0
4	K	E	4057	1/1	0.97	0.06	55,55,55,55	0
5	CL	C	4039	1/1	0.98	0.06	45,45,45,45	0
5	CL	H	4085	1/1	0.98	0.06	52,52,52,52	0
7	ADP	A	4007	27/27	0.98	0.05	14,28,48,77	0
7	ADP	C	4027	27/27	0.98	0.05	16,33,62,83	0
7	ADP	E	4050	27/27	0.98	0.05	19,33,50,58	0
4	K	F	4058	1/1	0.98	0.04	39,39,39,39	0
5	CL	C	4041	1/1	0.98	0.03	27,27,27,27	0
4	K	D	4035	1/1	0.98	0.04	34,34,34,34	0
4	K	E	4052	1/1	0.98	0.05	61,61,61,61	0
5	CL	E	4061	1/1	0.98	0.04	41,41,41,41	0
4	K	C	4033	1/1	0.98	0.06	55,55,55,55	0
4	K	A	4009	1/1	0.98	0.10	80,80,80,80	0
9	NET	E	4055	9/9	0.98	0.06	12,19,31,35	0
5	CL	G	4083	1/1	0.98	0.07	58,58,58,58	0
5	CL	E	4062	1/1	0.99	0.04	48,48,48,48	0
4	K	G	4079	1/1	0.99	0.03	49,49,49,49	0
5	CL	E	4065	1/1	0.99	0.07	46,46,46,46	0
5	CL	G	4080	1/1	0.99	0.02	23,23,23,23	0
5	CL	A	4016	1/1	0.99	0.03	39,39,39,39	0
5	CL	G	4082	1/1	0.99	0.04	39,39,39,39	0
5	CL	A	4017	1/1	0.99	0.04	39,39,39,39	0
4	K	E	4053	1/1	0.99	0.03	23,23,23,23	0
5	CL	G	4086	1/1	0.99	0.04	47,47,47,47	0
5	CL	A	4020	1/1	0.99	0.07	45,45,45,45	0
6	PO4	A	4006	5/5	0.99	0.04	16,22,28,30	0
6	PO4	C	4026	5/5	0.99	0.03	14,15,19,24	0
6	PO4	E	4049	5/5	0.99	0.03	17,17,21,25	0
6	PO4	G	4071	5/5	0.99	0.03	15,16,17,32	0

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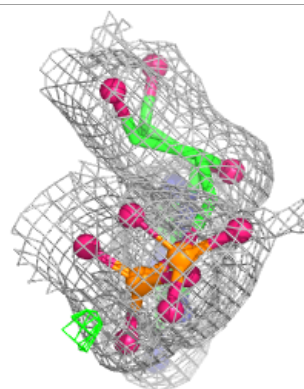
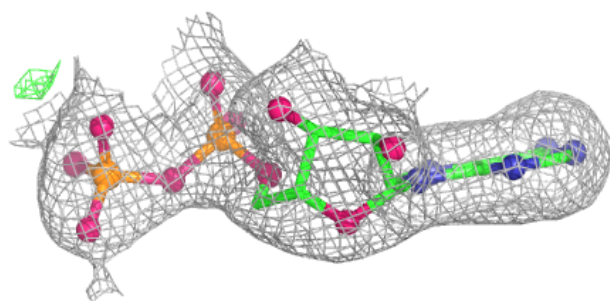
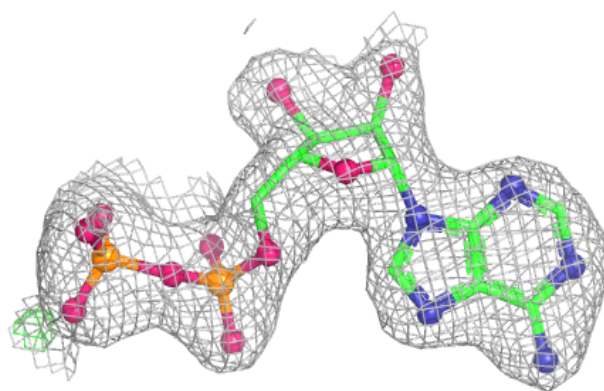
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ADP	A	4001	27/27	0.99	0.04	12,22,32,38	0
5	CL	B	4019	1/1	0.99	0.02	33,33,33,33	0
7	ADP	C	4021	27/27	0.99	0.04	12,19,24,45	0
5	CL	C	4036	1/1	0.99	0.03	26,26,26,26	0
7	ADP	E	4044	27/27	0.99	0.03	8,20,25,28	0
4	K	A	4010	1/1	0.99	0.02	21,21,21,21	0
7	ADP	G	4066	27/27	0.99	0.04	9,22,31,38	0
5	CL	C	4038	1/1	0.99	0.02	33,33,33,33	0
4	K	C	4025	1/1	0.99	0.02	25,25,25,25	0
4	K	A	4005	1/1	0.99	0.02	25,25,25,25	0
4	K	G	4070	1/1	0.99	0.02	30,30,30,30	0
5	CL	C	4042	1/1	0.99	0.03	45,45,45,45	0
4	K	E	4048	1/1	0.99	0.02	23,23,23,23	0
5	CL	E	4059	1/1	0.99	0.02	24,24,24,24	0
4	K	G	4075	1/1	0.99	0.03	37,37,37,37	0
4	K	C	4030	1/1	0.99	0.02	26,26,26,26	0
3	MN	C	4023	1/1	1.00	0.02	24,24,24,24	0
4	K	C	4024	1/1	1.00	0.01	19,19,19,19	0
3	MN	C	4028	1/1	1.00	0.02	39,39,39,39	0
3	MN	E	4045	1/1	1.00	0.03	24,24,24,24	0
3	MN	E	4046	1/1	1.00	0.02	21,21,21,21	0
5	CL	A	4015	1/1	1.00	0.02	23,23,23,23	0
3	MN	E	4051	1/1	1.00	0.02	36,36,36,36	0
3	MN	G	4067	1/1	1.00	0.02	25,25,25,25	0
5	CL	F	4064	1/1	1.00	0.02	33,33,33,33	0
3	MN	G	4068	1/1	1.00	0.01	22,22,22,22	0
4	K	E	4047	1/1	1.00	0.02	19,19,19,19	0
3	MN	G	4073	1/1	1.00	0.02	49,49,49,49	0
4	K	A	4004	1/1	1.00	0.01	20,20,20,20	0
3	MN	A	4002	1/1	1.00	0.01	21,21,21,21	0
3	MN	A	4003	1/1	1.00	0.03	21,21,21,21	0
3	MN	A	4008	1/1	1.00	0.01	28,28,28,28	0
3	MN	C	4022	1/1	1.00	0.02	21,21,21,21	0
4	K	G	4069	1/1	1.00	0.02	24,24,24,24	0

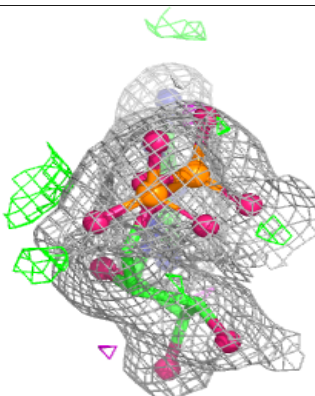
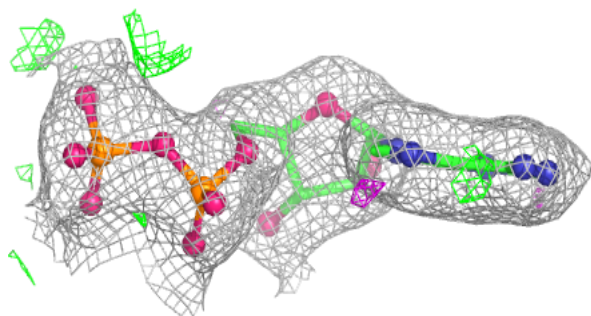
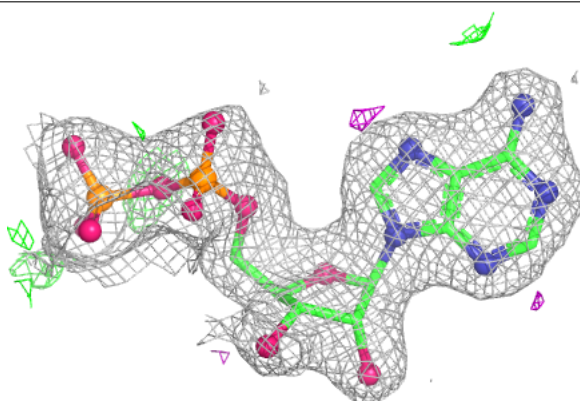
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP G 4072:

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

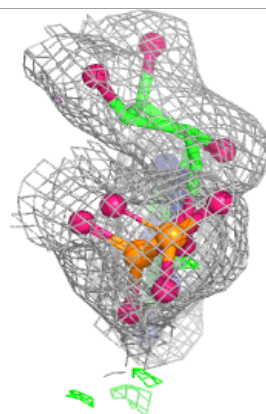
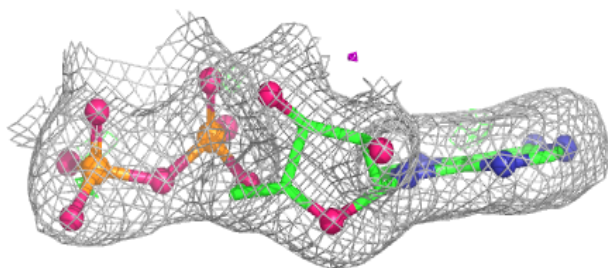
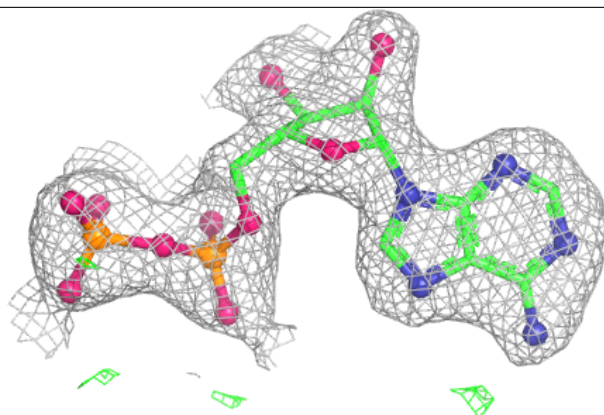
**Electron density around ADP A 4007:**

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

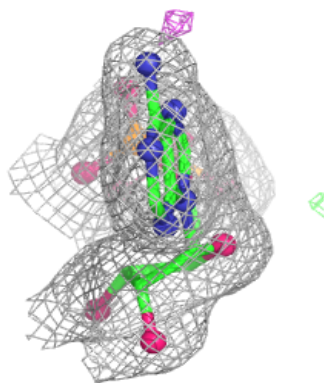
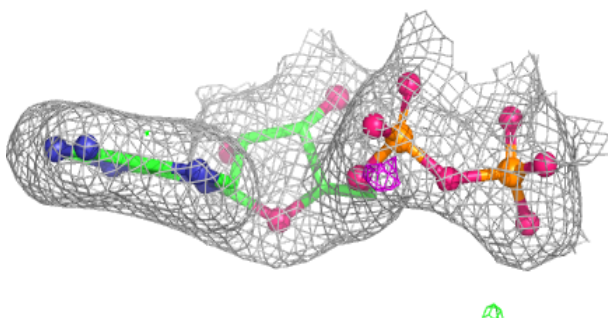
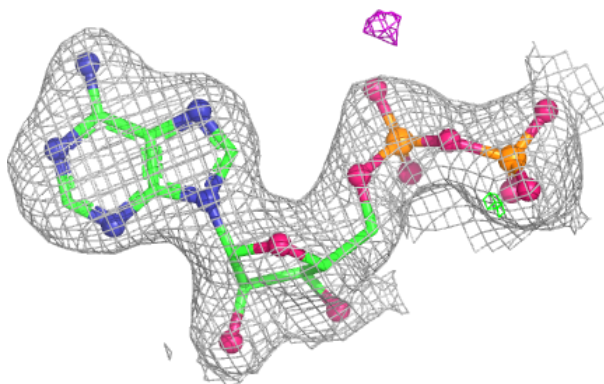


Electron density around ADP C 4027:

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

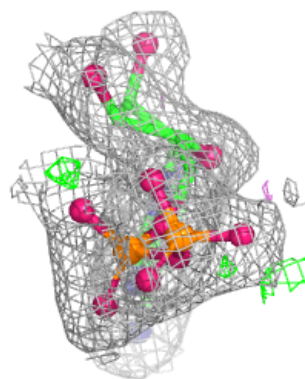
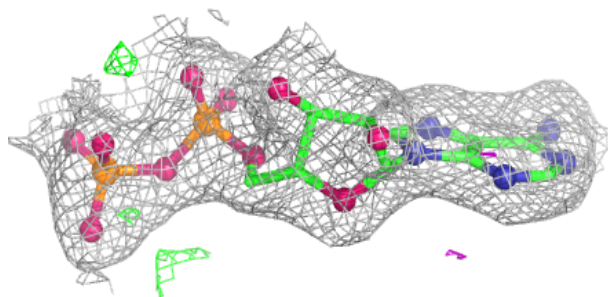
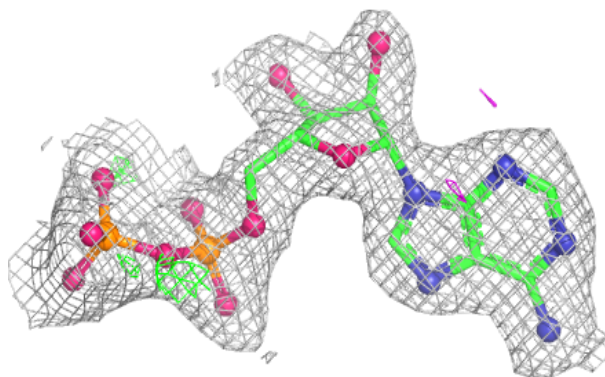
**Electron density around ADP E 4050:**

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

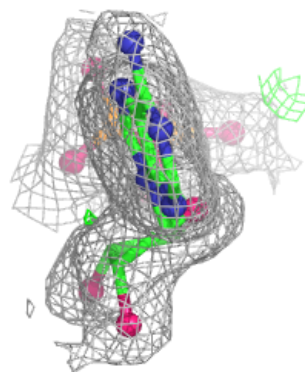
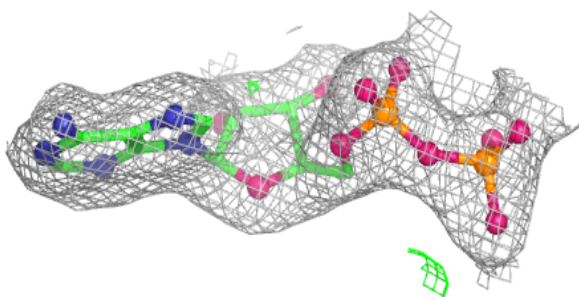
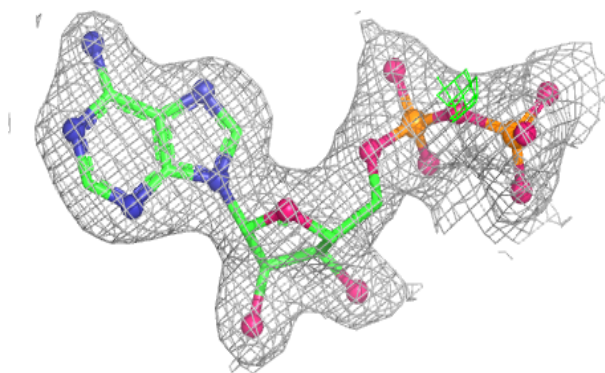


Electron density around ADP A 4001:

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

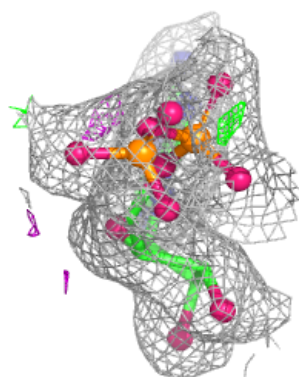
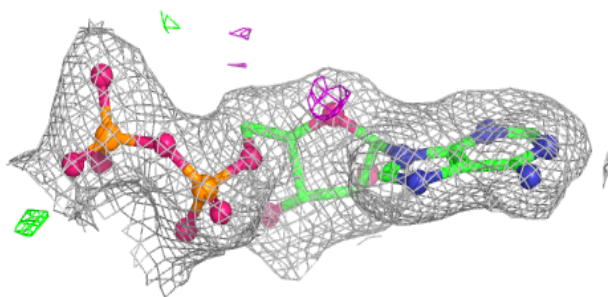
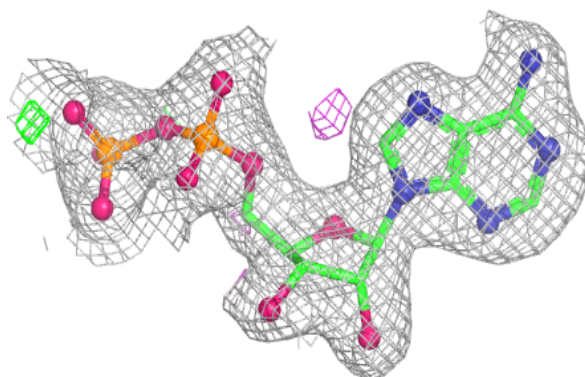
**Electron density around ADP C 4021:**

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

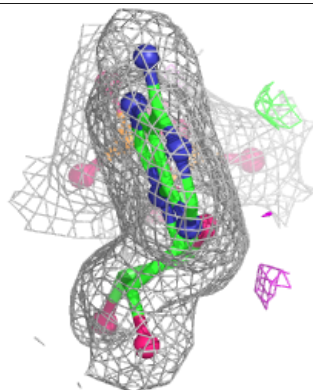
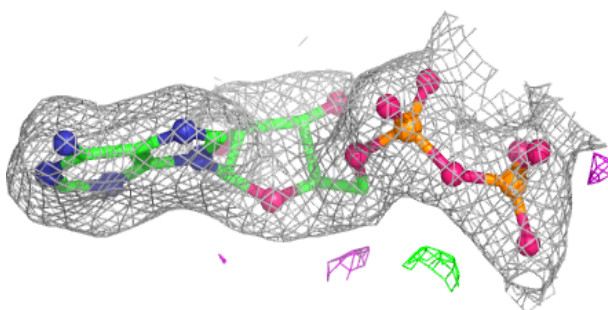
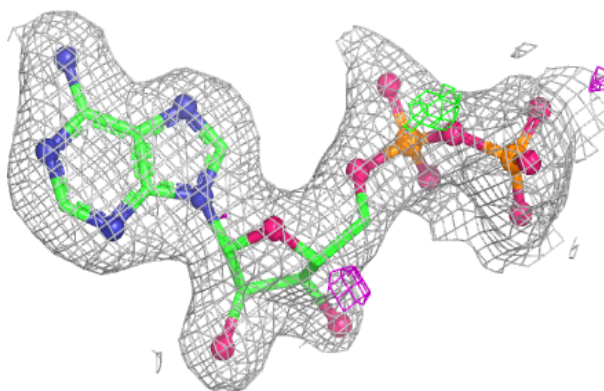


Electron density around ADP E 4044:

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

**Electron density around ADP G 4066:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.