



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:08 PM UTC

PDB ID : 1KEE / pdb_00001kee
Title : Inactivation of the Amidotransferase Activity of Carbamoyl Phosphate Synthetase by the Antibiotic Acivicin
Authors : Miles, B.W.; Thoden, J.B.; Holden, H.M.; Raushel, F.M.
Deposited on : 2001-11-15
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

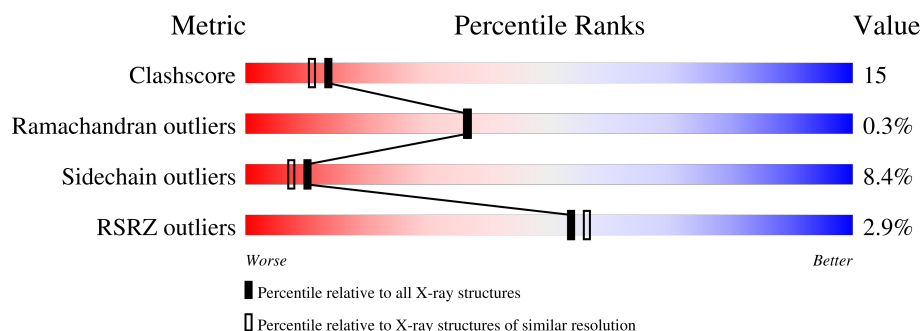
1 Overall quality at a glance ⓘ

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))
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	4% 69% 24% 5% .
1	C	1073	3% 69% 25% 5% .
1	E	1073	3% 71% 24% . .
1	G	1073	4% 66% 28% 5% . .
2	B	382	% 65% 30% . .
2	D	382	% 66% 27% 5% . .

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Mol	Chain	Length	Quality of chain
2	F	382	 % 64% 28% 7% •
2	H	382	 2% 59% 36% • •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	143	B	269	X	-	-	-
2	143	D	269	X	-	-	-
2	143	F	269	X	-	-	-
2	143	H	269	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48896 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	1058	Total	C	N	O	S	0	5	0
			8181	5136	1425	1575	45			
1	C	1058	Total	C	N	O	S	0	2	0
			8172	5130	1425	1572	45			
1	E	1058	Total	C	N	O	S	0	8	0
			8204	5150	1430	1579	45			
1	G	1058	Total	C	N	O	S	0	0	0
			8160	5123	1422	1570	45			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	1	0
			2912	1834	513	555	10			
2	D	379	Total	C	N	O	S	0	1	0
			2907	1831	510	556	10			
2	F	379	Total	C	N	O	S	0	0	0
			2905	1830	510	555	10			
2	H	379	Total	C	N	O	S	0	0	0
			2905	1830	510	555	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	143	CYS	modified residue	UNP P00907
D	269	143	CYS	modified residue	UNP P00907
F	269	143	CYS	modified residue	UNP P00907
H	269	143	CYS	modified residue	UNP P00907

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

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

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

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

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

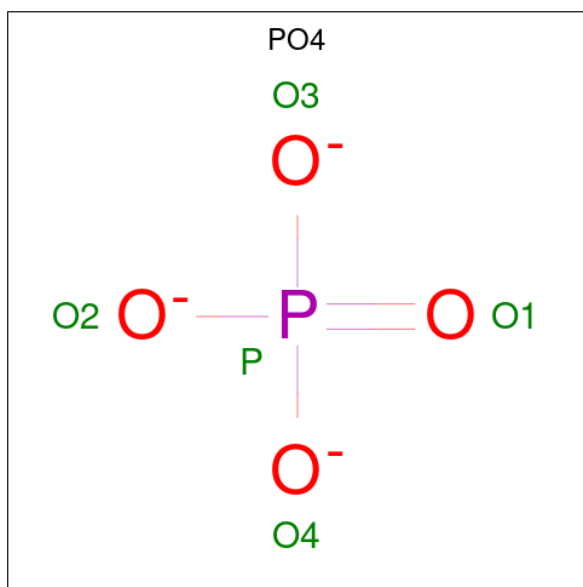
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Cl 5 5	0	0
5	B	1	Total Cl 1 1	0	0
5	C	5	Total Cl 5 5	0	0
5	D	1	Total Cl 1 1	0	0
5	E	4	Total Cl 4 4	0	0
5	F	1	Total Cl 1 1	0	0

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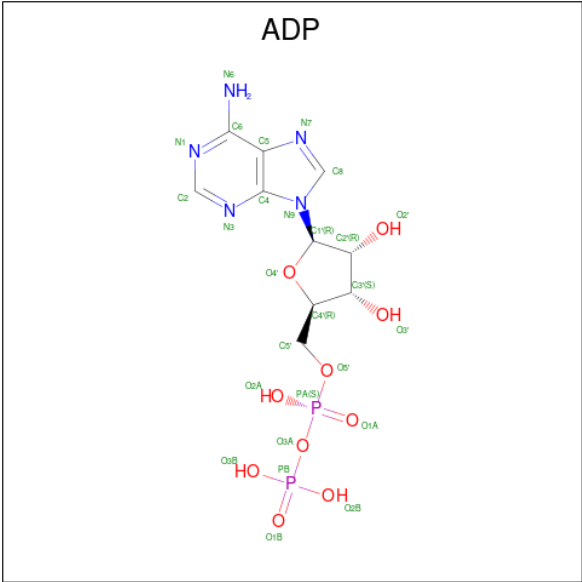
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	4	Total	Cl	0	0
			4	4		
5	H	1	Total	Cl	0	0
			1	1		

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



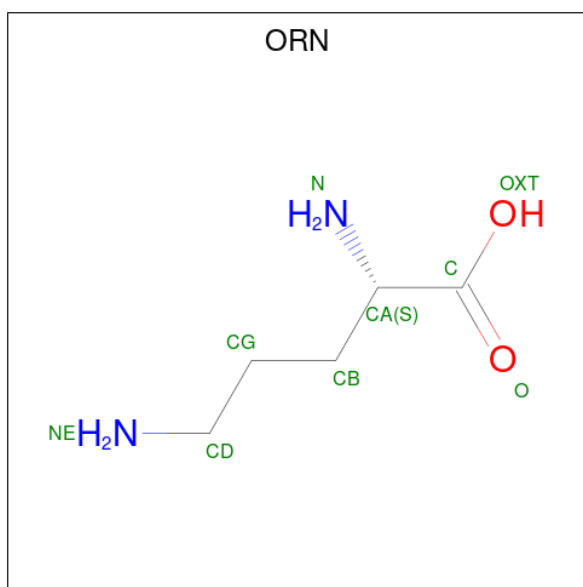
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

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



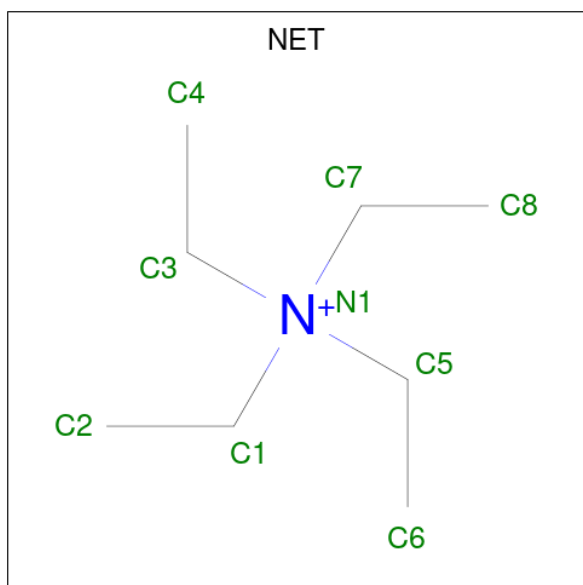
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

- Molecule 8 is L-ornithine (CCD ID: ORN) (formula: C₅H₁₂N₂O₂).



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

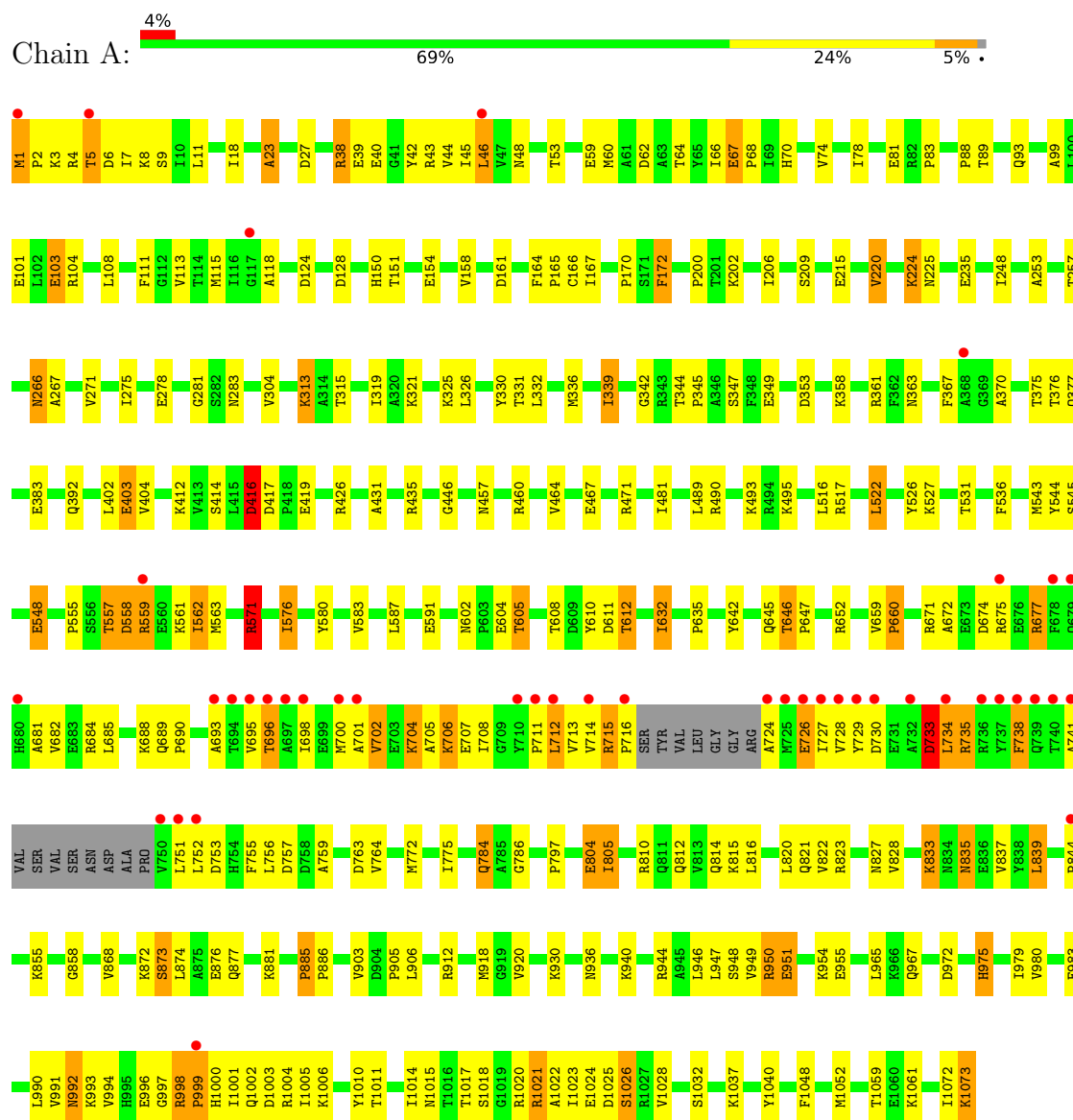
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	841	Total O 841 841	0	0
10	B	230	Total O 230 230	0	0
10	C	783	Total O 783 783	0	0
10	D	304	Total O 304 304	0	0
10	E	886	Total O 886 886	0	0
10	F	263	Total O 263 263	0	0
10	G	678	Total O 678 678	0	0
10	H	191	Total O 191 191	0	0

3 Residue-property plots

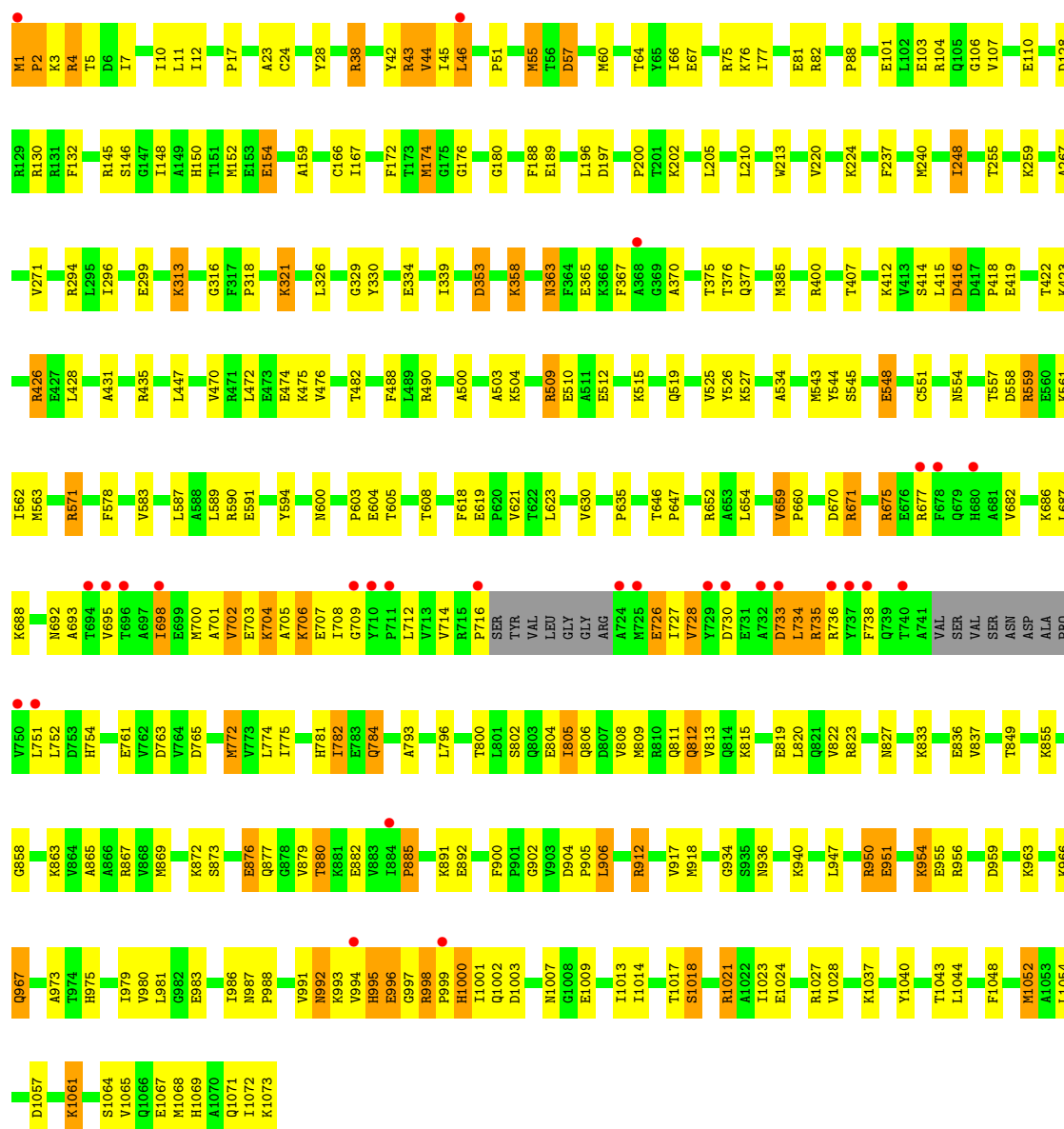
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

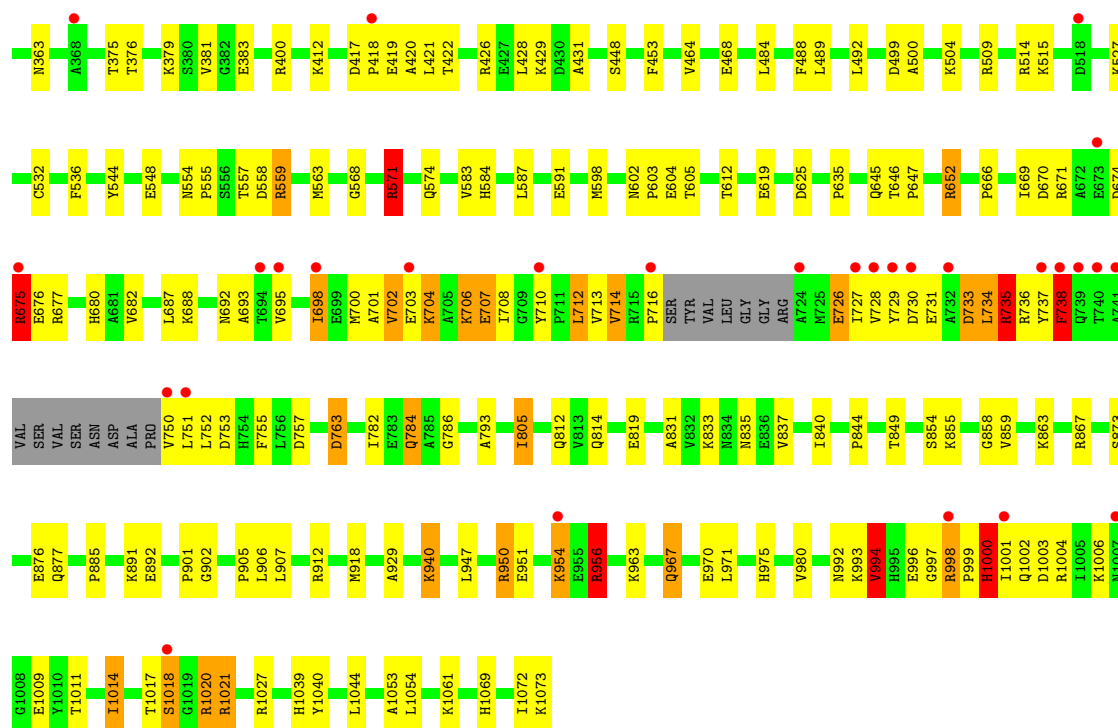
- Molecule 1: Carbamoyl-phosphate synthetase large chain



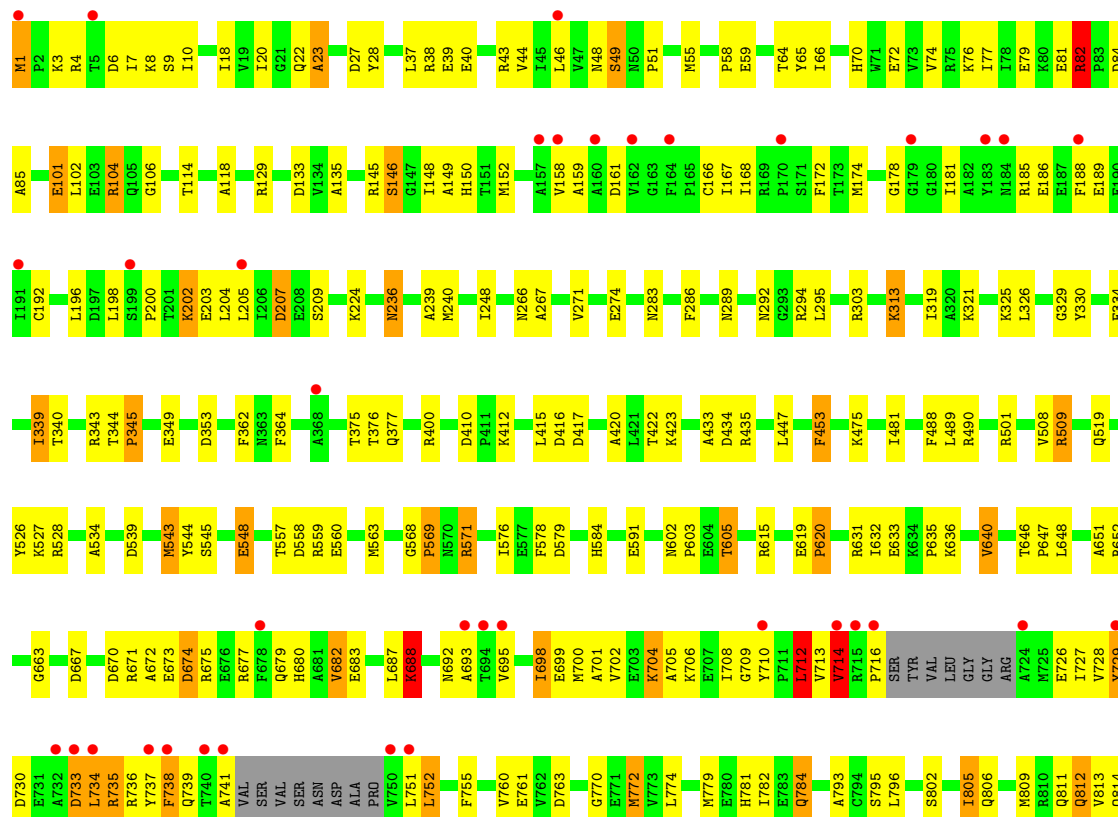
- Molecule 1: Carbamoyl-phosphate synthetase large chain

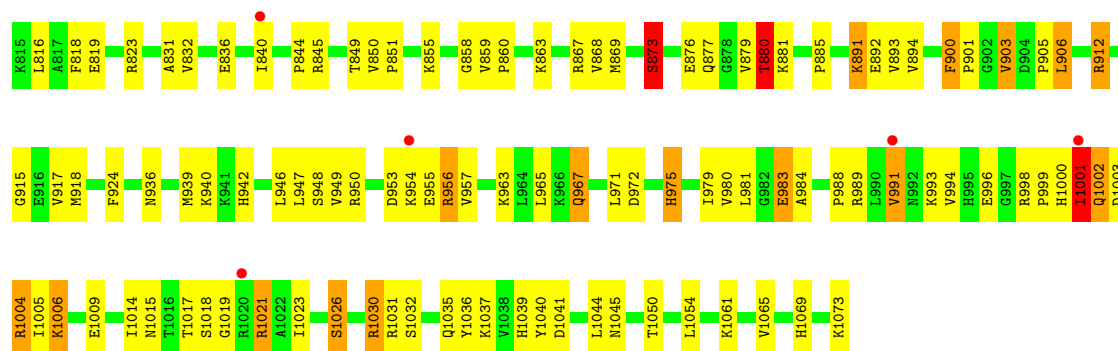




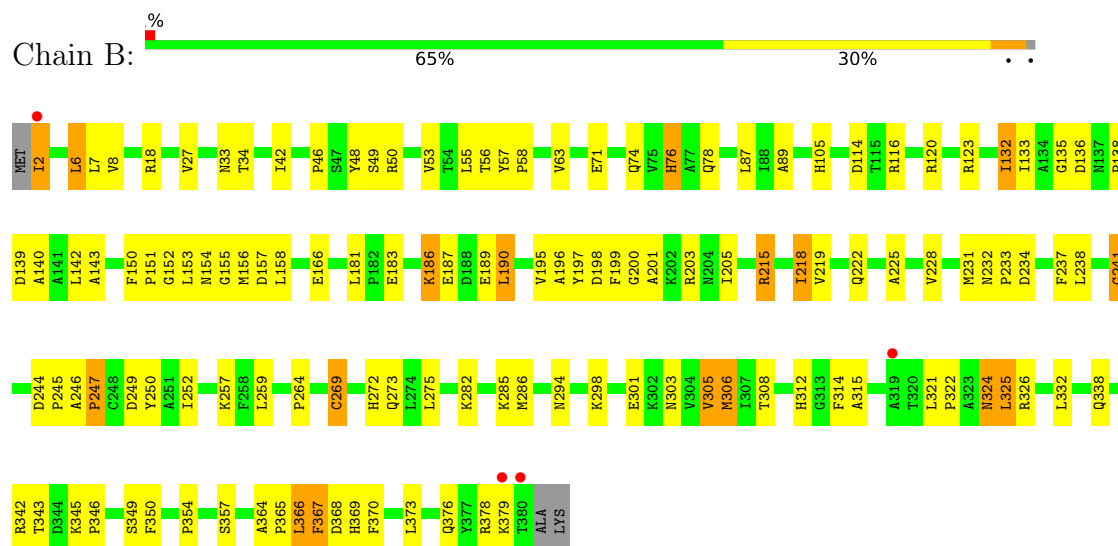


• Molecule 1: Carbamoyl-phosphate synthetase large chain

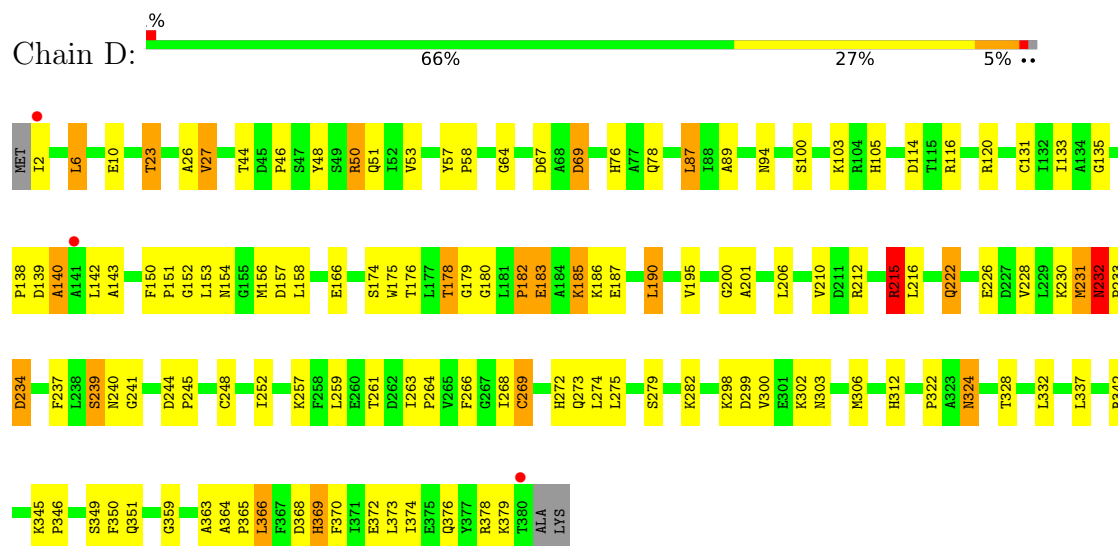




• Molecule 2: Carbamoyl-phosphate synthetase small chain

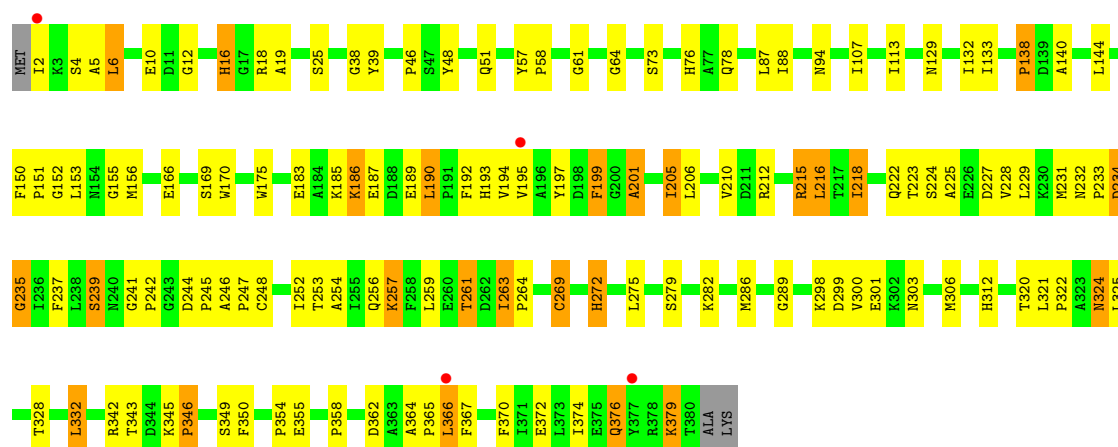


• Molecule 2: Carbamoyl-phosphate synthetase small chain

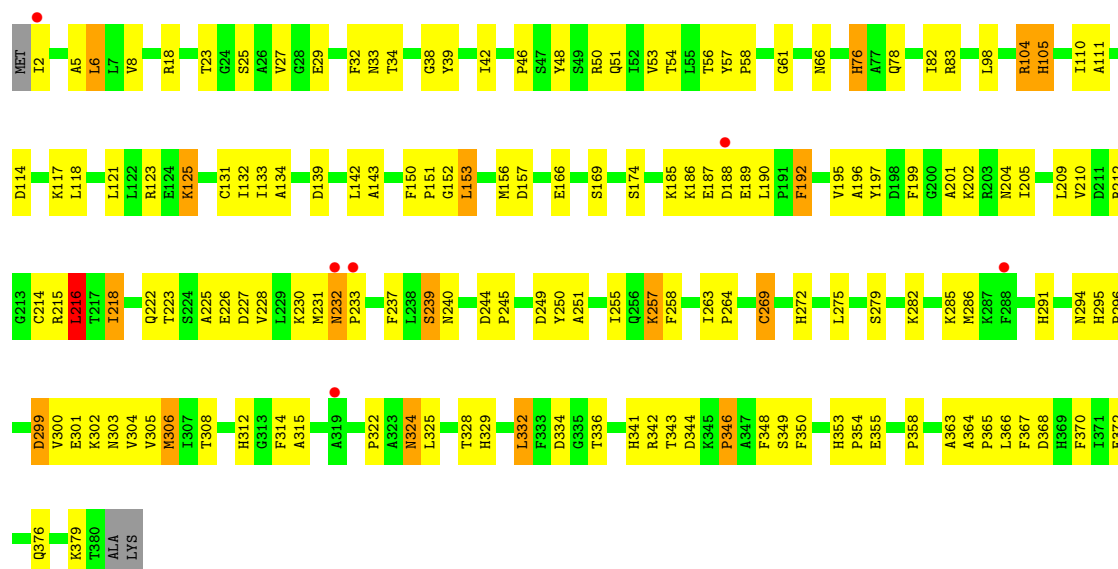


• Molecule 2: Carbamoyl-phosphate synthetase small chain





• 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	152.40Å 164.40Å 333.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.9 (30.00-2.10) 88.9 (30.00-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.186 , 0.211 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 116.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48896	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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, NET, ORN, ADP, K, PO4, 143, CL

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	1.06	0/8327	1.54	63/11257 (0.6%)
1	C	1.04	1/8306 (0.0%)	1.52	54/11228 (0.5%)
1	E	1.05	0/8362	1.51	59/11302 (0.5%)
1	G	1.03	0/8286	1.55	68/11202 (0.6%)
2	B	0.99	0/2961	1.50	25/4019 (0.6%)
2	D	1.01	0/2956	1.52	25/4013 (0.6%)
2	F	1.01	0/2950	1.51	19/4005 (0.5%)
2	H	0.98	0/2950	1.54	21/4005 (0.5%)
All	All	1.03	1/45098 (0.0%)	1.53	334/61031 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	1	0
2	D	1	0
2	F	1	0
2	H	1	0
All	All	4	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	GLU	CA-CB	5.24	1.61	1.53

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	885	PRO	N-CA-CB	10.80	108.84	103.22
1	C	885	PRO	N-CA-CB	10.56	109.11	103.19
1	A	283	ASN	CA-CB-CG	10.35	122.95	112.60
1	C	557	THR	CA-C-N	9.89	133.71	120.65
1	C	557	THR	C-N-CA	9.89	133.71	120.65
1	A	605	THR	N-CA-C	9.66	123.60	110.55
1	A	757	ASP	CA-CB-CG	9.16	121.76	112.60
2	D	157	ASP	CA-CB-CG	8.66	121.27	112.60
1	C	605	THR	N-CA-C	8.65	123.14	110.59
1	C	659	VAL	N-CA-C	8.63	116.05	108.63
1	E	209	SER	N-CA-C	8.62	122.27	109.59
1	G	996	GLU	N-CA-C	8.53	121.72	111.82
1	C	998	ARG	N-CA-C	8.46	121.74	108.55
2	F	16	HIS	CA-CB-CG	-8.38	105.42	113.80
1	G	605	THR	N-CA-C	8.38	122.74	110.59
1	C	998	ARG	O-C-N	7.91	126.77	121.71
1	C	782	ILE	N-CA-C	-7.88	103.57	110.74
1	C	811	GLN	CB-CA-C	7.88	124.24	110.85
1	E	339	ILE	N-CA-C	7.73	122.86	112.04
2	B	105	HIS	CA-CB-CG	-7.72	106.08	113.80
1	A	682	VAL	N-CA-C	-7.67	103.32	110.53
1	E	782	ILE	N-CA-C	-7.66	103.77	110.74
1	E	557	THR	CA-C-N	7.59	130.67	120.65
1	E	557	THR	C-N-CA	7.59	130.67	120.65
1	G	1001	ILE	CA-C-N	7.52	130.36	120.28
1	G	1001	ILE	C-N-CA	7.52	130.36	120.28
1	E	605	THR	N-CA-C	7.47	122.00	110.42
2	H	232	ASN	CA-CB-CG	-7.47	105.13	112.60
1	A	999	PRO	N-CA-CB	7.46	110.81	102.60
1	E	499	ASP	CA-CB-CG	7.38	119.98	112.60
1	E	885	PRO	N-CA-CB	7.32	107.03	103.22
2	H	188	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	23	ALA	N-CA-C	7.24	119.49	109.29
1	C	716	PRO	N-CA-CB	7.17	110.89	103.00
1	G	953	ASP	CA-CB-CG	7.11	119.71	112.60
1	A	416	ASP	CA-CB-CG	-7.08	105.52	112.60
2	H	353	HIS	CA-CB-CG	-7.07	106.73	113.80
2	F	372	GLU	CB-CA-C	-7.07	99.79	110.88
1	C	210	LEU	N-CA-C	-7.04	103.26	112.41
1	C	558	ASP	N-CA-C	7.01	118.61	110.97
1	G	339	ILE	N-CA-C	6.99	122.08	113.00
1	G	578	PHE	CA-CB-CG	-6.97	106.83	113.80
1	C	558	ASP	N-CA-CB	-6.95	99.77	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	PRO	N-CA-CB	6.94	110.63	103.00
1	G	716	PRO	N-CA-CB	6.93	110.62	103.00
1	A	660	PRO	N-CA-CB	6.91	107.35	102.65
1	A	738	PHE	CA-CB-CG	-6.91	106.89	113.80
1	A	557	THR	CA-C-N	6.90	134.72	121.54
1	A	557	THR	C-N-CA	6.90	134.72	121.54
1	C	353	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	367	PHE	CA-CB-CG	-6.88	106.92	113.80
1	G	793	ALA	N-CA-C	-6.88	101.26	110.55
1	C	23	ALA	N-CA-C	6.87	118.97	109.29
1	C	128	ASP	CA-CB-CG	6.86	119.46	112.60
1	E	716	PRO	N-CA-CB	6.85	110.53	103.00
1	C	995	HIS	CA-CB-CG	6.76	120.56	113.80
1	C	1000	HIS	CA-CB-CG	-6.73	107.07	113.80
1	C	714	VAL	N-CA-C	6.69	117.38	107.15
1	A	248	ILE	N-CA-C	-6.68	100.07	108.89
1	E	283	ASN	CA-CB-CG	6.65	119.25	112.60
1	C	885	PRO	O-C-N	6.64	124.37	121.31
1	A	457	ASN	CA-CB-CG	-6.63	105.97	112.60
2	F	216	LEU	N-CA-C	6.61	120.81	110.17
2	B	53	VAL	N-CA-C	6.50	118.17	108.23
1	E	994	VAL	N-CA-C	6.47	117.22	110.62
2	F	234	ASP	N-CA-C	-6.46	104.88	112.89
1	E	793	ALA	N-CA-C	-6.44	100.09	110.32
1	C	590	ARG	N-CA-C	-6.43	104.19	111.14
1	C	154	GLU	N-CA-C	-6.42	103.41	111.11
1	E	707	GLU	CA-C-N	6.41	128.64	120.56
1	E	707	GLU	C-N-CA	6.41	128.64	120.56
1	A	319	ILE	N-CA-C	6.40	116.89	110.23
1	G	23	ALA	N-CA-C	6.38	118.29	109.29
1	E	558	ASP	N-CA-C	6.36	117.90	110.97
1	E	712	LEU	N-CA-C	6.35	119.88	109.72
2	F	346	PRO	N-CA-CB	6.34	106.69	102.25
1	G	682	VAL	O-C-N	6.34	128.12	121.91
1	C	255	THR	N-CA-C	6.33	120.31	112.59
1	E	885	PRO	O-C-N	6.32	124.12	121.15
1	E	532	CYS	N-CA-C	6.30	120.60	112.41
2	D	53	VAL	N-CA-C	6.29	117.86	108.54
2	H	157	ASP	CA-CB-CG	6.27	118.87	112.60
2	F	10	GLU	CB-CA-C	-6.26	100.03	110.68
1	G	44	VAL	N-CA-C	6.23	117.09	107.99
2	B	201	ALA	N-CA-C	6.22	119.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	970	GLU	N-CA-C	-6.20	100.09	109.95
1	G	893	VAL	N-CA-C	6.19	118.00	109.46
2	H	346	PRO	N-CA-CB	6.19	106.58	102.25
1	C	435	ARG	N-CA-C	6.18	118.53	111.11
2	D	359	GLY	CA-C-N	6.18	126.14	119.78
2	D	359	GLY	C-N-CA	6.18	126.14	119.78
1	A	998	ARG	N-CA-C	6.17	116.06	108.11
1	E	1000	HIS	CA-CB-CG	-6.16	107.64	113.80
2	F	4	SER	N-CA-C	6.15	119.18	110.50
1	A	733	ASP	CA-CB-CG	6.14	118.75	112.60
1	C	682	VAL	O-C-N	6.14	127.91	121.89
1	A	543	MET	N-CA-C	6.13	119.19	109.81
1	G	557	THR	CA-C-N	6.13	133.25	121.54
1	G	557	THR	C-N-CA	6.13	133.25	121.54
1	C	44	VAL	N-CA-C	6.12	116.92	107.99
2	F	374	ILE	CB-CA-C	-6.11	103.79	112.22
1	A	949	VAL	N-CA-C	6.07	118.60	109.20
2	B	241	GLY	CA-C-N	6.06	126.25	120.31
2	B	241	GLY	C-N-CA	6.06	126.25	120.31
1	G	186	GLU	CA-C-N	6.04	128.37	120.28
1	G	186	GLU	C-N-CA	6.04	128.37	120.28
1	E	558	ASP	CB-CA-C	-6.04	101.67	110.96
2	H	76	HIS	CA-CB-CG	-6.02	107.78	113.80
2	D	368	ASP	CA-CB-CG	-6.02	106.58	112.60
1	E	612	THR	N-CA-C	6.01	119.87	112.54
1	G	569	PRO	CB-CA-C	-6.01	103.11	110.98
1	A	1010	TYR	N-CA-C	6.00	119.61	109.76
1	G	319	ILE	N-CA-C	6.00	116.66	110.36
1	G	712	LEU	N-CA-C	6.00	119.31	109.72
1	A	417	ASP	CA-CB-CG	5.99	118.59	112.60
2	B	76	HIS	CA-CB-CG	-5.99	107.81	113.80
1	G	283	ASN	CA-CB-CG	5.99	118.59	112.60
2	H	53	VAL	N-CA-C	5.96	116.69	107.99
2	D	182	PRO	CB-CA-C	-5.96	103.43	111.12
1	E	786	GLY	N-CA-C	-5.94	107.22	113.58
1	G	885	PRO	O-C-N	5.94	123.94	121.15
1	G	1002	GLN	N-CA-C	-5.93	104.81	111.28
1	A	885	PRO	CA-C-N	5.92	126.44	120.04
1	A	885	PRO	C-N-CA	5.92	126.44	120.04
2	D	183	GLU	N-CA-C	-5.92	102.16	110.50
2	H	227	ASP	CA-C-N	5.91	128.09	120.88
2	H	227	ASP	C-N-CA	5.91	128.09	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	900	PHE	CA-C-N	5.90	126.05	119.32
1	G	900	PHE	C-N-CA	5.90	126.05	119.32
2	D	215	ARG	CB-CA-C	5.88	119.23	109.53
2	F	201	ALA	N-CA-C	5.86	118.96	110.28
1	C	543	MET	N-CA-C	5.86	118.60	109.52
1	A	858	GLY	CA-C-N	-5.86	116.99	123.43
1	A	858	GLY	C-N-CA	-5.86	116.99	123.43
1	C	431	ALA	N-CA-C	5.83	118.81	110.24
1	G	453	PHE	CA-CB-CG	-5.83	107.97	113.80
1	E	559	ARG	N-CA-C	5.82	118.69	110.14
1	E	338	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	57	ASP	N-CA-C	-5.80	102.47	109.83
1	G	248	ILE	N-CA-C	-5.79	101.34	109.21
2	B	136	ASP	CA-C-N	-5.78	116.61	122.74
2	B	136	ASP	C-N-CA	-5.78	116.61	122.74
2	F	235	GLY	O-C-N	5.78	129.14	123.76
1	C	793	ALA	N-CA-C	-5.78	102.75	110.55
1	A	994	VAL	N-CA-C	5.78	117.21	110.62
1	A	729	TYR	N-CA-C	5.77	120.44	113.41
1	E	996	GLU	CA-C-N	-5.76	112.47	121.97
1	E	996	GLU	C-N-CA	-5.76	112.47	121.97
1	C	367	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	67	GLU	O-C-N	5.75	125.39	121.71
1	G	674	ASP	CA-C-N	5.75	128.77	120.38
1	G	674	ASP	C-N-CA	5.75	128.77	120.38
1	C	339	ILE	N-CA-C	5.74	120.47	113.00
1	E	287	ALA	CA-C-N	-5.73	115.02	122.99
1	E	287	ALA	C-N-CA	-5.73	115.02	122.99
1	G	993	LYS	N-CA-C	-5.72	103.09	110.19
1	A	786	GLY	N-CA-C	-5.71	107.47	113.58
1	G	714	VAL	N-CA-C	5.71	115.47	107.37
1	A	78	ILE	CB-CA-C	-5.70	104.56	112.02
1	G	584	HIS	CA-CB-CG	-5.69	108.11	113.80
1	C	557	THR	CA-C-O	5.68	125.15	118.90
1	E	738	PHE	CA-CB-CG	-5.68	108.12	113.80
1	G	39	GLU	CB-CA-C	-5.67	99.47	110.46
1	E	619	GLU	O-C-N	5.66	125.33	121.71
1	C	67	GLU	O-C-N	5.66	125.96	121.55
1	A	44	VAL	N-CA-C	5.65	116.44	108.36
2	H	98	LEU	N-CA-C	5.65	117.44	111.28
1	E	62	ASP	CA-CB-CG	-5.64	106.96	112.60
1	C	515	LYS	CA-C-O	5.63	126.39	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	GLU	CB-CA-C	-5.63	103.97	111.63
2	B	346	PRO	N-CA-CB	5.63	106.58	102.81
1	E	88	PRO	CB-CA-C	-5.63	102.28	111.56
1	A	536	PHE	CA-CB-CG	-5.62	108.18	113.80
2	B	367	PHE	CA-CB-CG	-5.60	108.20	113.80
1	E	584	HIS	CA-CB-CG	-5.60	108.20	113.80
2	H	105	HIS	CA-CB-CG	-5.60	108.20	113.80
1	E	239	ALA	N-CA-C	5.60	117.13	110.19
1	E	571	ARG	N-CA-CB	5.59	120.39	111.56
1	E	726	GLU	CB-CG-CD	5.58	122.08	112.60
1	A	712	LEU	N-CA-C	5.57	118.48	109.40
1	C	619	GLU	O-C-N	5.56	125.88	121.55
2	B	308	THR	N-CA-C	5.55	117.85	109.41
1	E	1039	HIS	CA-CB-CG	-5.55	108.25	113.80
1	C	959	ASP	CA-CB-CG	-5.54	107.06	112.60
2	H	240	ASN	N-CA-C	-5.54	103.39	110.53
1	E	625	ASP	CA-CB-CG	-5.53	107.07	112.60
1	C	578	PHE	CA-CB-CG	-5.52	108.28	113.80
1	C	316	GLY	N-CA-C	-5.52	107.64	115.43
1	C	248	ILE	N-CA-C	-5.52	100.63	108.58
1	E	735	ARG	O-C-N	5.52	127.77	122.03
2	F	320	THR	CB-CA-C	-5.51	101.24	110.56
1	G	207	ASP	N-CA-C	5.51	118.56	109.85
1	G	209	SER	N-CA-C	5.51	118.22	109.96
2	F	199	PHE	N-CA-C	-5.48	106.48	112.72
1	A	111	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	557	THR	N-CA-C	-5.46	106.98	113.97
1	E	453	PHE	CA-CB-CG	-5.45	108.35	113.80
1	G	101	GLU	N-CA-C	-5.45	104.99	111.69
1	G	885	PRO	N-CA-C	5.44	116.40	110.58
2	D	239	SER	N-CA-C	5.44	117.10	110.41
1	C	407	THR	N-CA-C	-5.42	105.47	113.61
1	A	209	SER	N-CA-C	5.42	118.38	109.76
1	A	1025	ASP	CA-CB-CG	5.42	118.02	112.60
2	B	157	ASP	CA-CB-CG	5.42	118.02	112.60
2	H	216	LEU	N-CA-C	5.42	118.39	109.72
1	A	610	TYR	N-CA-CB	5.41	119.92	110.18
1	G	27	ASP	N-CA-C	-5.41	104.80	111.40
1	G	880	THR	N-CA-CB	-5.40	102.65	111.18
2	D	234	ASP	N-CA-C	-5.39	106.54	113.23
1	G	295	LEU	N-CA-C	5.39	117.74	109.07
1	G	984	ALA	CA-C-N	-5.39	113.86	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	984	ALA	C-N-CA	-5.39	113.86	122.10
1	G	364	PHE	N-CA-C	5.38	117.90	111.71
1	G	738	PHE	CA-CB-CG	-5.38	108.42	113.80
1	E	7	ILE	N-CA-C	5.37	115.59	107.80
1	E	714	VAL	N-CA-C	5.37	115.37	107.15
2	H	303	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	161	ASP	N-CA-C	5.37	118.30	111.69
2	H	308	THR	N-CA-C	5.36	117.83	109.52
1	C	726	GLU	CB-CG-CD	5.36	121.71	112.60
2	F	10	GLU	CB-CG-CD	-5.35	103.50	112.60
2	D	10	GLU	CB-CA-C	-5.35	102.25	110.81
1	A	39	GLU	CB-CA-C	-5.34	100.76	110.63
1	C	554	ASN	CB-CA-C	-5.33	107.42	111.20
1	G	266	ASN	CA-CB-CG	5.32	117.92	112.60
1	G	699	GLU	CA-C-N	5.32	127.41	120.28
1	G	699	GLU	C-N-CA	5.32	127.41	120.28
1	A	266	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	612	THR	N-CA-C	5.30	117.81	111.71
1	E	993	LYS	N-CA-C	-5.30	103.89	110.41
1	G	345	PRO	CB-CA-C	-5.30	102.91	110.75
2	D	23	THR	CA-C-N	-5.29	113.24	121.97
2	D	23	THR	C-N-CA	-5.29	113.24	121.97
2	F	239	SER	N-CA-C	5.29	116.75	110.19
1	A	726	GLU	N-CA-CB	5.29	120.19	111.62
1	A	339	ILE	N-CA-C	5.29	119.44	112.04
1	A	559	ARG	N-CA-C	5.29	118.25	110.59
1	G	353	ASP	CA-CB-CG	5.28	117.88	112.60
2	D	105	HIS	CA-CB-CG	-5.27	108.53	113.80
1	G	760	VAL	N-CA-CB	5.27	116.46	110.72
2	B	305	VAL	CA-C-N	-5.26	114.42	122.62
2	B	305	VAL	C-N-CA	-5.26	114.42	122.62
1	G	239	ALA	N-CA-C	5.26	116.71	110.19
1	C	370	ALA	N-CA-C	5.25	117.91	110.50
1	G	620	PRO	N-CA-CB	5.25	108.00	103.27
1	A	642	TYR	N-CA-C	5.25	120.55	113.72
1	E	247	SER	CB-CA-C	-5.25	101.14	109.80
1	G	729	TYR	N-CA-C	5.25	119.68	113.12
1	G	133	ASP	CA-C-O	5.24	126.02	120.10
1	A	993	LYS	N-CA-C	-5.24	103.96	110.41
2	F	237	PHE	CA-CB-CG	-5.24	108.56	113.80
1	A	645	GLN	O-C-N	5.24	127.67	122.12
1	A	715	ARG	CG-CD-NE	5.24	123.52	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	89	ALA	N-CA-C	-5.23	101.17	109.96
1	G	543	MET	N-CA-C	5.23	117.81	109.81
2	H	174	SER	N-CA-C	5.22	117.60	110.55
2	D	67	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	1057	ASP	CA-CB-CG	5.21	117.81	112.60
2	H	299	ASP	N-CA-C	-5.21	98.19	107.98
1	E	27	ASP	N-CA-C	-5.21	105.29	111.69
2	F	299	ASP	N-CA-C	-5.21	98.83	107.99
1	G	82	ARG	CG-CD-NE	-5.20	100.56	112.00
1	C	28	TYR	N-CA-C	-5.20	105.51	111.07
2	D	69	ASP	CA-CB-CG	5.20	117.80	112.60
2	H	379	LYS	N-CA-CB	5.20	119.15	110.32
1	G	23	ALA	CA-C-N	5.19	127.96	120.38
1	G	23	ALA	C-N-CA	5.19	127.96	120.38
1	G	1039	HIS	CA-CB-CG	-5.18	108.62	113.80
1	A	580	TYR	N-CA-CB	-5.18	102.50	110.16
1	G	688	LYS	N-CA-C	5.18	117.17	108.73
1	A	1011	THR	N-CA-CB	5.17	118.42	110.61
2	D	231	MET	N-CA-C	5.16	118.83	112.54
1	C	987	ASN	CB-CA-C	-5.15	105.30	110.65
1	G	993	LYS	CA-C-N	-5.14	113.98	120.56
1	G	993	LYS	C-N-CA	-5.14	113.98	120.56
2	H	204	ASN	N-CA-CB	5.14	117.77	110.06
1	G	924	PHE	N-CA-C	-5.13	105.68	111.28
1	A	873	SER	N-CA-C	5.13	117.15	110.43
2	H	239	SER	N-CA-C	5.12	116.94	110.33
2	B	325	LEU	N-CA-C	5.12	117.44	107.71
1	A	557	THR	O-C-N	5.12	128.67	122.48
2	D	369	HIS	CA-CB-CG	-5.11	108.69	113.80
2	B	155	GLY	CA-C-N	-5.10	115.98	122.77
2	B	155	GLY	C-N-CA	-5.10	115.98	122.77
1	C	900	PHE	CA-C-N	5.10	125.14	119.32
1	C	900	PHE	C-N-CA	5.10	125.14	119.32
2	F	362	ASP	CA-CB-CG	5.10	117.70	112.60
2	D	190	LEU	CA-C-N	5.10	124.60	119.19
2	D	190	LEU	C-N-CA	5.10	124.60	119.19
1	E	536	PHE	CA-CB-CG	-5.10	108.70	113.80
2	B	89	ALA	N-CA-C	-5.10	101.40	109.76
2	B	247	PRO	CA-C-N	-5.10	114.67	122.21
2	B	247	PRO	C-N-CA	-5.10	114.67	122.21
1	E	230	ILE	N-CA-CB	5.10	117.78	111.41
2	B	326	ARG	N-CA-C	5.09	117.68	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	255	THR	N-CA-C	5.09	118.98	112.26
1	E	431	ALA	N-CA-C	5.09	117.72	110.24
1	E	956	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	G	942	HIS	N-CA-C	5.08	115.87	108.14
1	E	23	ALA	N-CA-C	5.08	121.62	110.80
1	A	571	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	A	172	PHE	CA-CB-CG	-5.06	108.74	113.80
1	C	558	ASP	CA-CB-CG	5.06	117.66	112.60
1	G	435	ARG	N-CA-C	5.06	117.45	111.33
2	F	272	HIS	CA-CB-CG	5.05	118.86	113.80
1	E	737	TYR	O-C-N	5.05	127.49	122.03
1	A	522	LEU	CB-CA-C	5.05	120.11	111.68
2	B	200	GLY	CA-C-N	5.05	127.94	120.82
2	B	200	GLY	C-N-CA	5.05	127.94	120.82
2	H	295	HIS	N-CA-C	5.04	116.88	109.42
2	D	232	ASN	CA-C-N	5.04	124.97	119.78
2	D	232	ASN	C-N-CA	5.04	124.97	119.78
2	D	232	ASN	CA-CB-CG	-5.04	107.56	112.60
1	A	726	GLU	CB-CG-CD	5.04	121.16	112.60
2	B	132	ILE	CB-CA-C	-5.04	103.33	110.83
1	C	132	PHE	CA-CB-CG	-5.04	108.77	113.80
2	B	369	HIS	CA-C-O	5.03	125.79	120.10
1	A	170	PRO	N-CA-CB	5.03	107.72	103.35
1	E	998[A]	ARG	O-C-N	5.03	125.45	121.88
1	E	998[B]	ARG	O-C-N	5.03	125.45	121.88
1	C	955	GLU	N-CA-C	5.02	116.56	111.14
1	A	1014	ILE	CB-CA-C	5.02	117.52	110.99
1	C	154	GLU	CG-CD-OE1	5.02	129.95	118.40
1	C	900	PHE	O-C-N	5.02	125.30	121.23
1	E	763	ASP	CA-CB-CG	5.02	117.62	112.60
2	F	138	PRO	N-CA-CB	5.02	107.78	103.27
1	A	706	LYS	N-CA-C	-5.01	105.81	111.28
1	E	4	ARG	N-CA-C	5.01	117.31	110.24
1	E	189	GLU	CA-C-N	5.01	127.76	120.79
1	E	189	GLU	C-N-CA	5.01	127.76	120.79
1	G	364	PHE	CA-CB-CG	-5.01	108.79	113.80
1	G	286	PHE	N-CA-C	5.01	117.28	109.52
2	D	140	ALA	N-CA-C	5.00	116.73	111.28
1	A	604	GLU	N-CA-C	5.00	117.62	111.82

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	269	143	CD
2	D	269	143	CD
2	F	269	143	CD
2	H	269	143	CD

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	8181	0	8215	224	0
1	C	8172	0	8206	238	0
1	E	8204	0	8235	214	0
1	G	8160	0	8196	268	0
2	B	2912	0	2874	90	0
2	D	2907	0	2866	90	0
2	F	2905	0	2864	84	0
2	H	2905	0	2864	109	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	7	0	0	1	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	1	0
5	B	1	0	0	0	0
5	C	5	0	0	1	0
5	D	1	0	0	0	0
5	E	4	0	0	1	0
5	F	1	0	0	0	0
5	G	4	0	0	1	0
5	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	5	0	0	0	0
6	C	5	0	0	1	0
6	E	5	0	0	0	0
6	G	5	0	0	1	0
7	A	54	0	24	1	0
7	C	54	0	24	1	0
7	E	54	0	24	4	0
7	G	54	0	24	3	0
8	A	9	0	11	0	0
8	C	9	0	11	1	0
8	E	9	0	11	1	0
8	G	9	0	11	2	0
9	A	9	0	20	4	0
9	C	9	0	20	0	0
9	E	9	0	20	1	0
9	G	9	0	20	1	0
10	A	841	0	0	23	0
10	B	230	0	0	5	0
10	C	783	0	0	20	0
10	D	304	0	0	7	0
10	E	886	0	0	20	0
10	F	263	0	0	1	0
10	G	678	0	0	14	0
10	H	191	0	0	3	0
All	All	48896	0	44540	1305	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 15.

All (1305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LEU:HD22	1:E:46:LEU:O	1.37	1.20
1:A:46:LEU:O	1:A:46:LEU:HD22	1.42	1.18
2:D:228:VAL:HA	2:D:231:MET:HE2	1.22	1.16
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.27	1.14
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.32	1.09
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.27	1.07
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.36	1.07
1:G:46:LEU:HD11	1:G:64:THR:HG23	1.36	1.06
1:E:46:LEU:HD21	1:E:64:THR:HG23	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.45	0.98
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.29	0.97
2:B:286:MET:HE1	2:B:312:HIS:ND1	1.82	0.95
1:C:967:GLN:HG3	1:C:1054:LEU:HD13	1.48	0.95
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.49	0.94
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.49	0.94
1:C:38[A]:ARG:HG3	1:C:38[A]:ARG:HH11	1.29	0.94
1:A:784:GLN:HE21	1:A:784:GLN:H	1.16	0.94
1:A:46:LEU:O	1:A:46:LEU:CD2	2.17	0.93
2:D:50:ARG:HH11	2:D:158:LEU:HD22	1.35	0.92
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.16	0.91
1:E:46:LEU:O	1:E:46:LEU:CD2	2.18	0.90
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.54	0.90
1:E:1:MET:H2	1:E:224:LYS:NZ	1.68	0.90
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.54	0.89
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.07	0.89
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.53	0.89
1:G:901:PRO:HD2	5:G:5084:CL:CL	2.08	0.89
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.02	0.89
2:H:286:MET:HE2	2:H:315:ALA:HB2	1.54	0.89
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.51	0.89
1:A:46:LEU:CD2	1:A:46:LEU:C	2.44	0.88
1:E:1:MET:N	1:E:224:LYS:HZ1	1.72	0.87
1:E:728:VAL:CG1	1:E:733:ASP:HB3	2.04	0.87
1:E:46:LEU:HD22	1:E:46:LEU:C	2.00	0.87
1:E:1:MET:H2	1:E:224:LYS:HZ1	0.91	0.86
2:B:286:MET:HE2	2:B:315:ALA:HB2	1.56	0.86
1:C:1001:ILE:HD12	1:C:1002:GLN:N	1.89	0.86
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.10	0.86
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.06	0.86
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.56	0.85
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.05	0.85
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.58	0.85
1:E:146:SER:HB2	1:E:205:LEU:HD11	1.58	0.85
2:F:195:VAL:HG23	2:F:233:PRO:HB3	1.55	0.85
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.56	0.84
2:F:259:LEU:HD13	2:F:342:ARG:NH1	1.91	0.84
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.59	0.84
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.57	0.84
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.56	0.84
1:C:46:LEU:HD12	1:C:46:LEU:C	2.03	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LEU:CD2	1:E:46:LEU:C	2.50	0.83
1:G:698:ILE:HD12	1:G:698:ILE:H	1.43	0.83
1:A:46:LEU:HD21	1:A:64:THR:HG23	1.59	0.82
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.95	0.82
2:B:187:GLU:HG2	2:B:215[A]:ARG:HD2	1.61	0.82
2:H:286:MET:HE1	2:H:312:HIS:CE1	2.15	0.82
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.61	0.81
1:A:46:LEU:HD22	1:A:46:LEU:C	2.02	0.81
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.63	0.81
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.46	0.81
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.15	0.81
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.43	0.81
2:B:324:ASN:HD22	2:B:324:ASN:N	1.76	0.80
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.45	0.80
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.10	0.80
1:E:994:VAL:HG13	1:E:1000:HIS:ND1	1.97	0.80
2:F:228:VAL:HA	2:F:231:MET:CE	2.12	0.79
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.63	0.79
2:H:286:MET:HE1	2:H:312:HIS:ND1	1.96	0.79
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.12	0.78
2:B:71:GLU:O	2:B:203:ARG:HG3	1.83	0.78
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.66	0.78
1:E:1:MET:N	1:E:224:LYS:NZ	2.30	0.78
1:A:726:GLU:HG3	1:A:727:ILE:H	1.47	0.78
1:E:994:VAL:HG13	1:E:1000:HIS:CE1	2.19	0.78
1:G:784:GLN:H	1:G:784:GLN:HE21	1.29	0.77
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.66	0.77
1:G:873:SER:O	1:G:877:GLN:HG3	1.85	0.77
2:D:228:VAL:CA	2:D:231:MET:HE2	2.10	0.77
1:E:3:LYS:HB2	1:E:42:TYR:OH	1.84	0.77
4:E:5053:K:K	10:E:5816:HOH:O	1.94	0.77
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.20	0.77
2:F:228:VAL:HA	2:F:231:MET:HE3	1.67	0.77
1:E:1001:ILE:HD12	1:E:1002:GLN:N	1.99	0.76
1:C:951:GLU:O	1:C:954:LYS:HB3	1.86	0.76
1:A:873:SER:O	1:A:877:GLN:HG3	1.85	0.76
2:D:185:LYS:HD3	2:D:190:LEU:HD21	1.66	0.76
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.68	0.76
2:D:322:PRO:HB2	2:D:324:ASN:ND2	2.01	0.76
1:C:882:GLU:HB2	10:C:5495:HOH:O	1.84	0.76
1:E:967[A]:GLN:HG3	1:E:1054:LEU:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:GLN:H	1:A:784:GLN:NE2	1.83	0.75
1:G:936:ASN:HB2	10:G:3407:HOH:O	1.86	0.75
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.68	0.75
2:F:322:PRO:HB2	2:F:324:ASN:ND2	2.01	0.75
2:H:322:PRO:HB2	2:H:324:ASN:ND2	2.02	0.75
1:E:734:LEU:HD12	1:E:734:LEU:O	1.87	0.74
1:G:784:GLN:H	1:G:784:GLN:NE2	1.85	0.74
1:C:734:LEU:O	1:C:734:LEU:HD12	1.88	0.74
1:G:967:GLN:HG3	1:G:1054:LEU:HD13	1.67	0.73
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.04	0.73
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.18	0.73
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.24	0.72
2:H:187:GLU:HG2	2:H:215:ARG:CD	2.18	0.72
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.03	0.72
2:B:325:LEU:O	10:B:5179:HOH:O	2.06	0.72
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.71	0.72
1:G:702:VAL:HG11	1:G:735:ARG:NH2	2.04	0.72
1:A:646:THR:HB	1:A:647:PRO:HD3	1.71	0.72
1:E:784:GLN:H	1:E:784:GLN:HE21	1.35	0.72
1:E:736:ARG:NH2	10:E:5947:HOH:O	2.22	0.72
1:A:375:THR:HG23	1:A:377:GLN:H	1.54	0.72
1:C:772:MET:SD	1:C:880:THR:HG22	2.30	0.72
1:E:151:THR:OG1	1:E:153[B]:GLU:HG2	1.90	0.71
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.04	0.71
1:A:313:LYS:HE2	1:A:608:THR:O	1.88	0.71
1:G:1001:ILE:HD12	1:G:1002:GLN:N	2.06	0.71
1:G:965:LEU:HG	1:G:971:LEU:HD11	1.72	0.71
2:H:300:VAL:HG22	2:H:328:THR:O	1.90	0.71
2:D:345:LYS:HB3	2:D:346:PRO:HD2	1.73	0.70
1:C:784:GLN:H	1:C:784:GLN:HE21	1.37	0.70
1:A:734:LEU:HD12	1:A:734:LEU:O	1.92	0.69
1:A:751:LEU:HD23	10:A:5738:HOH:O	1.92	0.69
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.73	0.69
2:H:152:GLY:O	2:H:156:MET:HE3	1.92	0.69
2:H:269:143:HE	2:H:312:HIS:HB3	1.74	0.69
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.73	0.69
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.22	0.69
1:G:687:LEU:HD13	1:G:812:GLN:HG2	1.73	0.69
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.28	0.69
1:C:734:LEU:HD11	1:C:738:PHE:CE2	2.28	0.69
1:C:954:LYS:HB2	10:C:5808:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LEU:HD12	1:C:46:LEU:O	1.92	0.69
1:G:734:LEU:HD12	1:G:734:LEU:O	1.92	0.69
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.28	0.68
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.56	0.68
2:F:186:LYS:O	2:F:189:GLU:HB2	1.93	0.68
1:A:950:ARG:HD3	10:A:5560:HOH:O	1.94	0.68
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.08	0.68
2:F:187:GLU:CG	2:F:215:ARG:HD2	2.20	0.68
1:G:166:CYS:C	1:G:167:ILE:HD12	2.18	0.68
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.94	0.68
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.23	0.68
1:C:548:GLU:OE1	2:D:114:ASP:HA	1.92	0.68
1:C:1001:ILE:HD12	1:C:1002:GLN:H	1.58	0.68
2:F:150:PHE:CD2	2:F:151:PRO:HD2	2.29	0.67
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.77	0.67
1:A:1021:ARG:HG3	1:A:1021:ARG:HH11	1.60	0.67
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.29	0.67
2:D:152:GLY:O	2:D:156:MET:HE3	1.94	0.67
1:G:46:LEU:C	1:G:46:LEU:HD12	2.20	0.67
1:C:802:SER:O	1:C:806:GLN:HG3	1.95	0.67
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.10	0.67
1:G:726:GLU:HG3	1:G:727:ILE:N	2.09	0.67
1:E:784:GLN:H	1:E:784:GLN:NE2	1.92	0.67
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.95	0.67
1:C:416:ASP:O	1:C:418:PRO:HD3	1.94	0.67
2:B:324:ASN:ND2	2:B:324:ASN:N	2.44	0.67
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.76	0.66
1:A:681:ALA:O	1:A:685:LEU:HG	1.95	0.66
2:F:324:ASN:N	2:F:324:ASN:HD22	1.94	0.66
1:E:468:GLU:HG3	10:E:5429:HOH:O	1.95	0.66
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.78	0.66
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.77	0.66
1:A:715:ARG:HB3	10:A:5668:HOH:O	1.96	0.66
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.60	0.66
1:A:997:GLY:O	1:A:998:ARG:HG3	1.96	0.66
1:C:82:ARG:NH1	10:C:5109:HOH:O	2.26	0.66
1:E:703:GLU:O	1:E:706:LYS:HB2	1.96	0.66
1:G:64:THR:O	1:G:1065:VAL:HG23	1.96	0.65
2:B:324:ASN:HD22	2:B:324:ASN:H	1.44	0.65
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.31	0.65
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:ARG:NH2	1:E:81:GLU:OE2	2.28	0.65
1:E:645:GLN:HG3	10:E:5756:HOH:O	1.96	0.65
1:C:559:ARG:NH1	10:C:5704:HOH:O	2.29	0.65
2:H:186:LYS:O	2:H:189:GLU:HB2	1.96	0.65
2:B:259:LEU:HD13	2:B:342:ARG:NH1	2.11	0.65
1:E:997:GLY:C	1:E:998[B]:ARG:HG3	2.22	0.65
2:F:248:CYS:O	2:F:252:ILE:HD12	1.96	0.65
1:C:509:ARG:NH1	1:C:512:GLU:OE1	2.29	0.65
1:E:278:GLU:HG2	10:E:5679:HOH:O	1.96	0.65
1:C:698:ILE:HD12	1:C:698:ILE:H	1.60	0.65
1:C:865:ALA:O	1:C:869:MET:HG3	1.97	0.65
1:G:712:LEU:HD23	1:G:752:LEU:HG	1.79	0.65
1:G:539:ASP:HB2	10:G:3694:HOH:O	1.96	0.64
1:C:130:ARG:HB2	1:C:148:ILE:CD1	2.27	0.64
2:B:298:LYS:HE2	2:B:303:ASN:OD1	1.96	0.64
1:C:313:LYS:HE2	1:C:608:THR:O	1.96	0.64
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.78	0.64
1:G:698:ILE:HD12	1:G:698:ILE:N	2.12	0.64
1:C:902:GLY:O	1:C:1027:ARG:NH2	2.30	0.64
1:A:358:LYS:HD2	1:A:383:GLU:OE1	1.97	0.64
9:A:5012:NET:H22	9:A:5012:NET:H42	1.80	0.64
2:B:139:ASP:OD2	2:B:142:LEU:HB2	1.96	0.64
1:C:110:GLU:OE2	10:C:5132:HOH:O	2.14	0.64
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.78	0.64
1:G:667:ASP:OD2	1:G:677:ARG:NH2	2.30	0.64
1:A:954:LYS:O	1:A:980:VAL:HG11	1.98	0.64
1:C:675:ARG:H	1:C:675:ARG:CD	2.08	0.64
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.79	0.64
1:G:701:ALA:O	1:G:705:ALA:N	2.30	0.64
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.78	0.64
1:C:809:MET:O	1:C:813:VAL:HG23	1.98	0.64
1:C:998:ARG:CB	1:C:999:PRO:HA	2.27	0.64
1:A:804:GLU:HB3	10:A:5750:HOH:O	1.98	0.63
1:C:873:SER:O	1:C:877:GLN:HG3	1.98	0.63
1:A:471:ARG:HB2	10:A:5388:HOH:O	1.98	0.63
2:F:324:ASN:HD22	2:F:324:ASN:H	1.45	0.63
2:B:272:HIS:ND1	2:B:349:SER:OG	2.30	0.63
2:B:286:MET:HE1	2:B:312:HIS:CE1	2.34	0.63
2:B:338:GLN:NE2	10:B:5234:HOH:O	2.24	0.63
1:C:973:ALA:O	1:C:991:VAL:HG12	1.98	0.63
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:VAL:HA	2:B:231:MET:HE3	1.81	0.63
2:H:299:ASP:OD1	2:H:302:LYS:HD2	1.98	0.63
2:D:78:GLN:NE2	10:D:1782:HOH:O	2.29	0.63
1:G:710:TYR:HB3	1:G:729:TYR:O	1.99	0.63
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.81	0.63
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.81	0.63
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.98	0.63
1:C:1017:THR:HG21	1:C:1023:ILE:HA	1.81	0.63
2:F:223:THR:CG2	2:F:228:VAL:HG23	2.29	0.62
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.33	0.62
1:G:1004:ARG:O	1:G:1009:GLU:HG3	1.99	0.62
2:H:275:LEU:HD23	2:H:349:SER:OG	1.98	0.62
2:F:324:ASN:O	2:F:342:ARG:HD2	2.00	0.62
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.34	0.62
1:E:58:PRO:HD2	1:E:59:GLU:OE2	2.00	0.62
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.27	0.62
2:H:324:ASN:HD22	2:H:324:ASN:H	1.48	0.62
2:F:46:PRO:O	2:F:242:PRO:HG3	2.00	0.62
1:C:726:GLU:HG3	1:C:727:ILE:H	1.65	0.62
2:D:228:VAL:O	2:D:231:MET:N	2.29	0.62
1:G:646:THR:HB	1:G:647:PRO:HD3	1.82	0.62
1:G:1030:ARG:HH11	1:G:1030:ARG:HG3	1.64	0.62
1:A:816:LEU:HD11	1:A:839:LEU:HD21	1.82	0.62
1:E:954:LYS:O	1:E:980:VAL:HG11	2.00	0.62
2:H:34:THR:HA	2:H:56:THR:OG1	1.99	0.62
1:E:734:LEU:HD11	1:E:738:PHE:CE2	2.34	0.62
2:H:344:ASP:OD2	2:H:344:ASP:N	2.30	0.62
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.80	0.61
1:E:736:ARG:HH21	1:E:1020:ARG:HG2	1.65	0.61
1:C:267:ALA:O	1:C:271:VAL:HG23	2.00	0.61
1:E:4:ARG:HA	10:E:5629:HOH:O	2.00	0.61
1:A:89:THR:O	1:A:304:VAL:HG22	2.00	0.61
2:B:135:GLY:O	2:B:138:PRO:HD3	2.00	0.61
2:B:324:ASN:ND2	2:B:324:ASN:H	1.95	0.61
1:C:562:ILE:HG21	1:C:589:LEU:HD13	1.81	0.61
2:D:212:ARG:HG3	2:D:212:ARG:HH11	1.65	0.61
1:G:267:ALA:O	1:G:271:VAL:HG23	1.99	0.61
1:A:481:ILE:HG22	10:A:5397:HOH:O	2.00	0.61
2:B:190:LEU:HB2	2:B:215[B]:ARG:HB3	1.81	0.61
1:C:703:GLU:O	1:C:706:LYS:HB2	2.00	0.61
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:SER:O	1:A:1015:ASN:HA	2.00	0.61
2:B:186:LYS:O	2:B:189:GLU:HB2	2.01	0.61
2:B:286:MET:HE2	2:B:315:ALA:CB	2.27	0.61
1:E:950:ARG:HD3	10:E:5603:HOH:O	2.00	0.61
1:G:202:LYS:HG3	10:G:3585:HOH:O	2.00	0.61
1:A:726:GLU:HG3	1:A:727:ILE:N	2.13	0.61
1:A:738:PHE:O	1:A:741:ALA:HB3	2.01	0.61
2:B:275:LEU:HD23	2:B:349:SER:HB3	1.81	0.61
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.30	0.61
1:C:1017:THR:HG22	1:C:1023:ILE:HG13	1.83	0.61
1:G:101:GLU:OE2	1:G:104:ARG:NH2	2.29	0.61
1:G:698:ILE:H	1:G:698:ILE:CD1	2.11	0.61
1:G:1030:ARG:HG3	1:G:1030:ARG:NH1	2.14	0.61
2:H:249:ASP:OD2	2:H:250:TYR:N	2.31	0.61
1:A:1:MET:H1	1:A:224:LYS:HE3	1.66	0.61
1:A:695:VAL:HG11	1:A:701:ALA:CA	2.31	0.61
1:G:809:MET:O	1:G:813:VAL:HG23	1.99	0.61
1:A:471:ARG:HD2	10:A:5687:HOH:O	2.00	0.61
1:A:1000:HIS:CD2	1:A:1002[B]:GLN:HB3	2.36	0.61
1:E:1000:HIS:O	1:E:1004[B]:ARG:HG3	2.01	0.61
1:G:168:ILE:CG2	1:G:204:LEU:HD22	2.31	0.61
1:A:991:VAL:HG23	1:A:1004:ARG:NH1	2.16	0.60
1:A:1073:LYS:NZ	10:A:5860:HOH:O	2.33	0.60
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.48	0.60
1:E:103:GLU:HG3	1:E:104:ARG:N	2.15	0.60
1:E:1021:ARG:HH11	1:E:1021:ARG:CG	2.14	0.60
2:H:78:GLN:NE2	10:H:4012:HOH:O	2.34	0.60
1:A:1021:ARG:HH11	1:A:1021:ARG:CG	2.14	0.60
2:H:324:ASN:HD22	2:H:324:ASN:N	1.99	0.60
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.82	0.60
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.49	0.60
1:G:1:MET:HA	1:G:224:LYS:HE3	1.83	0.60
1:A:822:VAL:O	1:A:823:ARG:HD3	2.02	0.60
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.09	0.60
2:H:269:143:HE	2:H:312:HIS:CB	2.30	0.60
2:F:350:PHE:HB2	2:F:366:LEU:HD22	1.82	0.60
1:G:1036:TYR:C	1:G:1037:LYS:HG2	2.25	0.60
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.84	0.60
1:G:998:ARG:HA	1:G:999:PRO:C	2.26	0.60
1:A:944:ARG:HD3	1:A:972:ASP:OD1	2.02	0.60
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.83	0.60
1:C:64:THR:O	1:C:1065:VAL:HG23	2.01	0.59
1:C:447:LEU:HD23	1:G:447:LEU:HD23	1.84	0.59
1:A:115:MET:HG2	1:A:118:ALA:O	2.03	0.59
1:C:426:ARG:HD3	1:C:426:ARG:C	2.27	0.59
1:A:728:VAL:HG11	1:A:734:LEU:HA	1.84	0.59
2:B:249:ASP:OD2	2:B:250:TYR:N	2.33	0.59
1:E:698:ILE:O	1:E:702:VAL:HG23	2.03	0.59
1:G:734:LEU:HD12	1:G:734:LEU:C	2.27	0.59
2:B:225:ALA:O	2:B:228:VAL:HB	2.02	0.59
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.84	0.59
1:E:65:TYR:OH	1:E:80:LYS:HE2	2.03	0.59
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.02	0.59
1:C:695:VAL:CG1	1:C:701:ALA:HB2	2.17	0.59
1:E:710:TYR:HB3	1:E:729:TYR:O	2.03	0.59
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.17	0.59
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.85	0.59
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.84	0.59
2:D:226:GLU:O	2:D:230:LYS:HG3	2.02	0.59
1:A:419:GLU:HB2	10:A:5681:HOH:O	2.02	0.59
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.33	0.59
1:C:563:MET:CE	1:C:635:PRO:HG3	2.32	0.59
2:F:195:VAL:CG2	2:F:233:PRO:HB3	2.29	0.59
1:G:1019:GLY:O	1:G:1023:ILE:HG13	2.03	0.59
1:G:1021:ARG:HG3	1:G:1021:ARG:HH11	1.67	0.59
2:F:228:VAL:HA	2:F:231:MET:HE2	1.84	0.58
2:F:376:GLN:HA	2:F:379:LYS:HZ2	1.68	0.58
1:G:343:ARG:HB3	10:G:4159:HOH:O	2.02	0.58
1:C:38[A]:ARG:HG3	1:C:38[A]:ARG:NH1	2.03	0.58
1:A:150:HIS:N	1:A:154:GLU:OE2	2.37	0.58
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.68	0.58
1:G:1021:ARG:HH11	1:G:1021:ARG:CG	2.16	0.58
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.85	0.58
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.33	0.58
1:A:46:LEU:C	1:A:46:LEU:HD23	2.26	0.58
2:D:233:PRO:HG2	2:D:263:ILE:HD13	1.85	0.58
1:E:130:ARG:HG3	1:E:148:ILE:HG13	1.85	0.58
2:F:218:ILE:HD13	2:F:218:ILE:N	2.18	0.58
1:G:687:LEU:CD1	1:G:812:GLN:HG2	2.34	0.58
1:A:1000:HIS:CD2	1:A:1002[A]:GLN:HB3	2.39	0.58
2:D:222:GLN:NE2	10:D:2212:HOH:O	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:967[B]:GLN:HG2	1:E:1054:LEU:HD13	1.84	0.58
1:C:950:ARG:HD3	10:C:5578:HOH:O	2.02	0.58
1:G:1:MET:H1	1:G:224:LYS:HZ2	1.52	0.57
1:A:730:ASP:H	1:A:733:ASP:HB2	1.67	0.57
2:B:259:LEU:HD13	2:B:342:ARG:HH12	1.69	0.57
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.33	0.57
1:C:702:VAL:O	1:C:705:ALA:HB3	2.04	0.57
1:C:1061:LYS:HG2	10:C:5552:HOH:O	2.04	0.57
2:D:27:VAL:O	2:D:78:GLN:HG2	2.05	0.57
1:C:46:LEU:C	1:C:46:LEU:CD1	2.75	0.57
1:G:738:PHE:O	1:G:741:ALA:HB3	2.04	0.57
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.39	0.57
1:E:1:MET:HB3	1:E:2:PRO:HD3	1.87	0.57
2:F:286:MET:HE3	2:F:289:GLY:HA2	1.85	0.57
1:A:695:VAL:CG2	1:A:752:LEU:HD22	2.34	0.57
1:C:671:ARG:HG2	1:C:677:ARG:NH1	2.20	0.57
1:A:734:LEU:HD12	1:A:734:LEU:C	2.28	0.57
1:C:43:ARG:NH2	1:C:81:GLU:OE2	2.36	0.57
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.40	0.57
1:A:43:ARG:NH2	1:A:81:GLU:OE2	2.29	0.57
1:A:489:LEU:HD22	1:A:516:LEU:HD23	1.87	0.57
1:C:130:ARG:HB2	1:C:148:ILE:HD12	1.86	0.57
2:F:232:ASN:N	2:F:233:PRO:HD3	2.18	0.57
1:G:954:LYS:O	1:G:957:VAL:HG12	2.05	0.57
2:H:228:VAL:HA	2:H:231:MET:HE3	1.87	0.57
2:H:334:ASP:OD2	2:H:336:THR:HG23	2.05	0.57
1:C:75:ARG:HG3	1:C:107:VAL:CG1	2.35	0.57
1:C:998:ARG:CG	1:C:999:PRO:HA	2.35	0.57
1:C:1068:MET:O	1:C:1071:GLN:HB2	2.05	0.57
1:G:663:GLY:CA	1:G:869:MET:HG2	2.35	0.57
1:C:1:MET:HA	1:C:224:LYS:HE3	1.86	0.56
1:E:757:ASP:O	1:E:833:LYS:NZ	2.29	0.56
1:G:814:GLN:HG3	1:G:818:PHE:CE2	2.40	0.56
2:D:206:LEU:O	2:D:210:VAL:HG23	2.05	0.56
1:A:70:HIS:O	1:A:74:VAL:HG23	2.05	0.56
1:A:426:ARG:HD3	1:A:426:ARG:C	2.31	0.56
1:E:559:ARG:HB3	10:E:5812:HOH:O	2.04	0.56
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.86	0.56
1:G:46:LEU:CD1	1:G:64:THR:HG23	2.25	0.56
1:G:152:MET:HE1	1:G:189:GLU:HA	1.87	0.56
1:G:560:GLU:OE1	1:G:636:LYS:HE3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:302:LYS:HB2	2:H:304:VAL:HG22	1.86	0.56
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.20	0.56
2:D:259:LEU:HD13	2:D:342:ARG:NH1	2.20	0.56
1:C:353:ASP:OD1	2:D:116:ARG:HD2	2.06	0.56
1:C:358:LYS:HE3	10:C:5075:HOH:O	2.05	0.56
2:H:46:PRO:HA	2:H:76:HIS:CG	2.41	0.56
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.87	0.56
1:G:735:ARG:O	1:G:738:PHE:N	2.38	0.56
2:D:324:ASN:N	2:D:324:ASN:HD22	2.01	0.56
1:E:1017:THR:HG22	1:E:1018:SER:N	2.21	0.56
1:E:956:ARG:HB3	1:E:1044:LEU:CD2	2.36	0.56
1:A:646:THR:CB	1:A:647:PRO:HD3	2.36	0.56
2:D:200:GLY:HA2	10:D:2059:HOH:O	2.06	0.56
1:E:646:THR:HB	1:E:647:PRO:HD3	1.88	0.56
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.88	0.56
2:H:244:ASP:OD2	2:H:245:PRO:HD2	2.05	0.56
2:B:78:GLN:NE2	2:B:78:GLN:HA	2.19	0.55
2:H:251:ALA:O	2:H:255:ILE:HG13	2.06	0.55
1:A:353:ASP:OD1	2:B:116:ARG:HD2	2.06	0.55
1:A:918:MET:HE2	1:A:920:VAL:HG22	1.89	0.55
1:E:702:VAL:CG1	1:E:731:GLU:HG3	2.35	0.55
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.70	0.55
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.87	0.55
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.42	0.55
1:C:734:LEU:HD12	1:C:734:LEU:C	2.29	0.55
1:E:735:ARG:O	1:E:738:PHE:N	2.39	0.55
1:C:784:GLN:H	1:C:784:GLN:NE2	2.04	0.55
1:E:671:ARG:NH2	1:E:819:GLU:O	2.40	0.55
1:G:956:ARG:HB3	1:G:1044:LEU:HD21	1.87	0.55
2:D:300:VAL:HG22	2:D:328:THR:O	2.07	0.55
1:E:196:LEU:HG	1:E:204:LEU:HD11	1.86	0.55
2:H:368:ASP:HB2	10:H:4261:HOH:O	2.06	0.55
1:C:975:HIS:HE2	1:E:992:ASN:ND2	2.05	0.55
1:E:805:ILE:HD13	1:E:837:VAL:CG2	2.37	0.55
1:C:12:ILE:N	1:C:45:ILE:O	2.33	0.55
2:D:46:PRO:HA	2:D:76:HIS:CG	2.41	0.55
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.07	0.55
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.06	0.55
1:E:677:ARG:O	1:E:680:HIS:HB2	2.05	0.55
1:C:698:ILE:HD12	1:C:698:ILE:N	2.22	0.55
2:D:279:SER:O	2:D:322:PRO:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:814:GLN:NE2	10:E:5516:HOH:O	2.40	0.55
1:G:40:GLU:CG	1:G:325:LYS:HE2	2.37	0.54
2:H:218:ILE:N	2:H:218:ILE:HD13	2.22	0.54
1:A:695:VAL:CG1	1:A:701:ALA:HB2	2.19	0.54
1:A:814:GLN:NE2	10:A:5474:HOH:O	2.40	0.54
1:E:358:LYS:HG2	1:E:359:ILE:N	2.21	0.54
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.88	0.54
1:G:814:GLN:HG3	1:G:818:PHE:HE2	1.73	0.54
1:A:704:LYS:O	1:A:707:GLU:HB2	2.06	0.54
1:A:602:ASN:CG	1:A:605:THR:HG23	2.32	0.54
1:C:101:GLU:OE2	1:C:104:ARG:NH2	2.33	0.54
2:D:156:MET:SD	2:D:158:LEU:HD21	2.48	0.54
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.07	0.54
1:E:196:LEU:HG	1:E:204:LEU:CD1	2.37	0.54
1:G:340:THR:O	1:G:343:ARG:HB2	2.08	0.54
1:A:675:ARG:NH2	10:A:5504:HOH:O	2.29	0.54
1:C:224:LYS:HE2	1:C:329:GLY:O	2.07	0.54
2:D:178:THR:HG22	2:D:179:GLY:N	2.22	0.54
1:E:734:LEU:HD12	1:E:734:LEU:C	2.29	0.54
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.22	0.54
1:C:1021:ARG:HH11	1:C:1021:ARG:HG3	1.71	0.54
1:G:28:TYR:CE1	1:G:313:LYS:HE3	2.43	0.54
1:A:267:ALA:O	1:A:271:VAL:HG23	2.08	0.54
2:D:150:PHE:CD2	2:D:151:PRO:HD2	2.43	0.54
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.42	0.54
1:G:1:MET:N	1:G:224:LYS:NZ	2.55	0.54
1:A:224:LYS:NZ	10:A:5023:HOH:O	2.40	0.54
1:A:315:THR:O	1:A:531:THR:HG22	2.08	0.54
2:B:27:VAL:O	2:B:78:GLN:HG2	2.08	0.54
2:B:232:ASN:N	2:B:233:PRO:HD3	2.22	0.54
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.43	0.54
2:D:231:MET:HA	10:D:2215:HOH:O	2.08	0.54
1:E:28:TYR:CE1	1:E:313:LYS:HE3	2.42	0.54
1:G:796:LEU:C	1:G:796:LEU:HD23	2.33	0.54
1:G:991:VAL:HG21	1:G:1001:ILE:HG22	1.90	0.54
2:F:298:LYS:HE2	2:F:303:ASN:OD1	2.08	0.54
1:G:167:ILE:HD12	1:G:167:ILE:N	2.22	0.54
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.39	0.53
1:A:698:ILE:O	1:A:702:VAL:HG23	2.07	0.53
1:C:1:MET:HB3	1:C:334:GLU:OE2	2.08	0.53
1:C:992:ASN:O	1:C:1000:HIS:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:998:ARG:HG2	1:C:999:PRO:HA	1.90	0.53
2:D:275:LEU:HD23	2:D:349:SER:HB3	1.89	0.53
1:E:99:ALA:HB1	1:E:115:MET:HE2	1.90	0.53
2:F:376:GLN:HA	2:F:379:LYS:NZ	2.23	0.53
1:G:733:ASP:HA	1:G:736:ARG:HH11	1.72	0.53
2:B:152:GLY:O	2:B:156:MET:HE3	2.07	0.53
1:E:736:ARG:NH2	1:E:1020:ARG:HG2	2.23	0.53
1:A:1000:HIS:HD2	1:A:1003:ASP:N	1.97	0.53
1:C:994:VAL:HA	1:C:1000:HIS:CB	2.38	0.53
9:E:5056:NET:H42	9:E:5056:NET:H22	1.90	0.53
1:G:181:ILE:HD11	1:G:376:THR:HG23	1.91	0.53
2:H:232:ASN:N	2:H:233:PRO:HD3	2.23	0.53
2:B:46:PRO:HA	2:B:76:HIS:CG	2.43	0.53
1:E:417:ASP:OD2	1:E:418:PRO:HD2	2.08	0.53
1:A:1000:HIS:O	1:A:1003:ASP:HB2	2.08	0.53
2:D:350:PHE:HB2	2:D:366:LEU:HD22	1.91	0.53
2:F:279:SER:O	2:F:322:PRO:HG3	2.08	0.53
1:A:659:VAL:HG13	1:A:660:PRO:HD2	1.91	0.53
2:D:100:SER:O	10:D:1835:HOH:O	2.18	0.53
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.39	0.53
1:G:74:VAL:HG11	1:G:102:LEU:HD11	1.89	0.53
2:H:54:THR:HG21	2:H:118:LEU:HD23	1.89	0.53
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.38	0.53
1:G:663:GLY:HA3	1:G:869:MET:HG2	1.91	0.53
2:F:185:LYS:HD2	2:F:190:LEU:HD21	1.90	0.53
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.90	0.53
1:C:75:ARG:HG3	1:C:107:VAL:HG11	1.91	0.53
1:C:772:MET:CE	1:C:880:THR:HG22	2.39	0.53
2:D:26:ALA:O	2:D:131:CYS:HA	2.09	0.53
1:G:106:GLY:HA2	10:G:3478:HOH:O	2.09	0.53
1:A:225:ASN:ND2	1:A:331:THR:HG21	2.24	0.52
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.24	0.52
1:C:872:LYS:HG3	1:C:876:GLU:HB3	1.91	0.52
1:C:885:PRO:HG2	10:C:5510:HOH:O	2.07	0.52
1:E:997:GLY:O	1:E:998[B]:ARG:HG3	2.09	0.52
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.90	0.52
1:G:236:ASN:HD22	1:G:236:ASN:N	2.07	0.52
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.39	0.52
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.40	0.52
2:F:201:ALA:HB2	2:F:239:SER:CB	2.40	0.52
1:C:772:MET:HE1	1:C:880:THR:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:ARG:NH1	2:D:158:LEU:HD22	2.13	0.52
1:E:735:ARG:O	1:E:738:PHE:HB2	2.10	0.52
2:F:194:VAL:HG13	2:F:235:GLY:O	2.09	0.52
1:G:150:HIS:CD2	1:G:203:GLU:HB2	2.44	0.52
1:A:5:THR:C	1:A:7:ILE:H	2.17	0.52
1:A:344:THR:HB	1:A:345:PRO:HD2	1.92	0.52
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.39	0.52
1:C:46:LEU:HD11	1:C:64:THR:HG23	1.92	0.52
1:C:166:CYS:C	1:C:167:ILE:HD12	2.34	0.52
2:D:363:ALA:C	2:D:365:PRO:HD2	2.34	0.52
1:G:375:THR:HG23	1:G:377:GLN:H	1.74	0.52
1:A:548:GLU:OE1	2:B:114:ASP:HA	2.09	0.52
1:C:623:LEU:HD12	1:C:654:LEU:HD23	1.92	0.52
2:D:298:LYS:HE2	2:D:303:ASN:OD1	2.09	0.52
1:E:78:ILE:HG23	1:E:83:PRO:HD2	1.92	0.52
1:E:146:SER:HB3	1:E:207:ASP:OD1	2.09	0.52
1:G:680:HIS:O	1:G:683:GLU:HB2	2.09	0.52
2:H:187:GLU:CG	2:H:215:ARG:HD2	2.22	0.52
1:A:9:SER:OG	1:A:83:PRO:HA	2.10	0.52
2:D:324:ASN:HD22	2:D:324:ASN:H	1.57	0.52
1:G:1:MET:H1	1:G:224:LYS:NZ	2.08	0.52
1:G:146:SER:HB2	1:G:205:LEU:HD11	1.92	0.52
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.30	0.52
1:A:220:VAL:O	1:A:281:GLY:HA2	2.09	0.52
2:B:354:PRO:HB2	2:B:367:PHE:CE2	2.43	0.52
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.45	0.52
1:A:1:MET:HE3	2:B:303:ASN:HD22	1.75	0.51
1:A:103:GLU:HG2	10:A:5598:HOH:O	2.08	0.51
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.10	0.51
1:C:363:ASN:ND2	1:C:365:GLU:OE1	2.39	0.51
1:E:166:CYS:C	1:E:167:ILE:HD12	2.34	0.51
1:E:652:ARG:HD2	1:E:666:PRO:HB2	1.92	0.51
1:A:999:PRO:HD2	1:G:983:GLU:OE1	2.10	0.51
1:C:562:ILE:HG21	1:C:589:LEU:CD1	2.39	0.51
1:G:713:VAL:HG12	1:G:713:VAL:O	2.08	0.51
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.92	0.51
1:A:339:ILE:HD11	1:A:531:THR:HG23	1.93	0.51
1:C:998:ARG:HA	1:C:999:PRO:C	2.34	0.51
1:A:1000:HIS:CD2	1:A:1003:ASP:N	2.76	0.51
1:C:709:GLY:O	1:C:754:HIS:ND1	2.43	0.51
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.71	0.51
1:E:750:VAL:O	1:E:750:VAL:HG12	2.10	0.51
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.29	0.51
2:H:32:PHE:O	2:H:291:HIS:HB2	2.09	0.51
2:H:142:LEU:HD12	2:H:142:LEU:O	2.10	0.51
1:A:124:ASP:O	1:A:128:ASP:HB3	2.11	0.51
1:A:724:ALA:N	10:A:5721:HOH:O	2.44	0.51
1:C:630:VAL:HG11	1:C:659:VAL:HG22	1.93	0.51
1:C:772:MET:HE1	1:C:880:THR:CA	2.40	0.51
1:E:1061:LYS:NZ	10:E:5578:HOH:O	2.42	0.51
2:F:194:VAL:HG13	2:F:235:GLY:C	2.35	0.51
1:G:3:LYS:HB3	1:G:330:TYR:CE1	2.45	0.51
1:G:129:ARG:HB3	1:G:205:LEU:HD22	1.93	0.51
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.92	0.51
2:D:201:ALA:HB2	2:D:239:SER:CB	2.41	0.51
1:E:375:THR:OG1	1:E:376:THR:N	2.43	0.51
1:A:1001:ILE:HD12	1:A:1002[B]:GLN:HB2	1.91	0.51
1:C:994:VAL:HA	1:C:1000:HIS:CG	2.46	0.51
1:E:1:MET:O	1:E:329:GLY:O	2.29	0.51
1:C:728:VAL:CG1	1:C:733:ASP:HB3	2.36	0.51
2:D:174:SER:O	2:D:182:PRO:HD3	2.10	0.51
1:G:509:ARG:HH11	1:G:509:ARG:HB2	1.76	0.51
2:B:199:PHE:O	2:B:241:GLY:HA3	2.10	0.51
1:C:38[B]:ARG:NH2	10:C:5086:HOH:O	2.27	0.51
2:B:120:ARG:HD2	10:B:5054:HOH:O	2.11	0.51
2:D:369:HIS:O	2:D:372:GLU:HB2	2.11	0.51
1:G:954:LYS:O	1:G:980:VAL:HG11	2.11	0.51
1:A:979:ILE:O	1:A:983:GLU:HG3	2.11	0.50
2:B:50:ARG:HD2	2:B:158:LEU:HD21	1.94	0.50
2:B:324:ASN:HA	2:B:343:THR:OG1	2.11	0.50
1:C:782:ILE:N	1:C:782:ILE:HD12	2.26	0.50
2:F:241:GLY:O	2:F:269:143:OF	2.28	0.50
1:C:197:ASP:OD2	1:C:1037:LYS:NZ	2.34	0.50
1:C:704:LYS:O	1:C:707:GLU:HB2	2.11	0.50
1:G:415:LEU:HB2	10:G:3828:HOH:O	2.11	0.50
1:G:1017:THR:CG2	1:G:1023:ILE:HG12	2.42	0.50
1:C:1052:MET:HG2	10:C:5817:HOH:O	2.11	0.50
1:E:126:ALA:HB3	1:E:302:PRO:HG3	1.93	0.50
1:G:814:GLN:CG	1:G:818:PHE:HE2	2.23	0.50
1:C:804:GLU:O	1:C:808:VAL:HG23	2.11	0.50
1:E:713:VAL:HB	1:E:753:ASP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:THR:HA	10:A:5644:HOH:O	2.11	0.50
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.12	0.50
1:A:1001:ILE:O	1:A:1005:ILE:HG13	2.11	0.50
2:B:245:PRO:HG3	2:B:273:GLN:OE1	2.11	0.50
1:C:774:LEU:HD22	1:C:879:VAL:HG12	1.93	0.50
1:E:907:LEU:HD11	8:E:5055:ORN:HD3	1.93	0.50
1:G:181:ILE:HG13	1:G:376:THR:HG23	1.94	0.50
2:H:139:ASP:OD2	2:H:142:LEU:HB2	2.10	0.50
1:A:166:CYS:C	1:A:167:ILE:HD12	2.37	0.50
1:A:690:PRO:HG3	1:A:756:LEU:HD11	1.94	0.50
1:E:267:ALA:O	1:E:271:VAL:HG23	2.11	0.50
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.94	0.50
1:G:135:ALA:HB1	1:G:274:GLU:CG	2.42	0.50
2:H:324:ASN:O	2:H:342:ARG:HD2	2.12	0.50
2:D:248:CYS:O	2:D:252:ILE:HG13	2.11	0.50
1:G:51:PRO:HG3	1:G:918:MET:HB2	1.94	0.50
1:A:695:VAL:HG21	1:A:752:LEU:HD22	1.93	0.50
1:C:46:LEU:HD21	1:C:55:MET:O	2.11	0.50
1:C:986:ILE:O	1:C:988:PRO:HD3	2.12	0.50
1:E:138:LYS:HD3	1:E:274:GLU:OE1	2.12	0.50
1:E:225:ASN:ND2	1:E:331:THR:HG21	2.26	0.50
1:G:700:MET:O	1:G:704:LYS:HB2	2.10	0.50
2:H:367:PHE:O	2:H:370:PHE:HB3	2.11	0.50
2:B:234:ASP:OD1	2:B:378:ARG:NH1	2.44	0.49
1:C:698:ILE:H	1:C:698:ILE:CD1	2.22	0.49
1:E:39:GLU:HG3	10:E:5114:HOH:O	2.12	0.49
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.93	0.49
1:C:152:MET:SD	1:C:189:GLU:HG2	2.52	0.49
2:F:354:PRO:HB2	2:F:367:PHE:CE2	2.47	0.49
1:G:224:LYS:HE2	1:G:329:GLY:O	2.12	0.49
1:G:400:ARG:HB3	10:G:3730:HOH:O	2.12	0.49
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.94	0.49
1:C:11:LEU:HA	1:C:45:ILE:O	2.12	0.49
1:C:167:ILE:HD12	1:C:167:ILE:N	2.27	0.49
1:G:755:PHE:CD1	7:G:2072:ADP:C2	3.00	0.49
2:B:286:MET:CE	2:B:315:ALA:HB2	2.35	0.49
1:C:519:GLN:NE2	10:C:5775:HOH:O	2.45	0.49
1:C:993:LYS:O	1:C:1000:HIS:HB3	2.13	0.49
1:C:997:GLY:O	1:C:998:ARG:HG3	2.13	0.49
1:G:1017:THR:HG22	1:G:1023:ILE:HG12	1.94	0.49
1:C:482:THR:HB	10:C:5689:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:LYS:HB3	2:D:346:PRO:CD	2.40	0.49
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.47	0.49
1:G:948:SER:O	1:G:1015:ASN:HA	2.13	0.49
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.60	0.49
1:C:701:ALA:O	1:C:705:ALA:N	2.37	0.49
1:C:980:VAL:HG13	10:C:5728:HOH:O	2.13	0.49
1:E:500:ALA:O	1:E:504:LYS:HG3	2.12	0.49
1:E:854:SER:HA	1:E:859:VAL:O	2.12	0.49
1:A:375:THR:OG1	1:A:376:THR:N	2.35	0.49
2:B:259:LEU:O	2:B:345:LYS:HE3	2.13	0.49
1:E:568:GLY:O	1:E:602:ASN:HB2	2.12	0.49
1:E:831:ALA:HB2	1:E:840:ILE:HD11	1.95	0.49
1:E:929:ALA:HB2	1:E:1053:ALA:HB1	1.93	0.49
1:G:1030:ARG:HH11	1:G:1030:ARG:CG	2.25	0.49
2:D:269:143:HE	2:D:312:HIS:CB	2.43	0.49
1:E:693:ALA:HB3	1:E:708:ILE:HD11	1.93	0.49
2:F:223:THR:HG21	2:F:228:VAL:HG23	1.93	0.49
2:F:225:ALA:O	2:F:229:LEU:HG	2.12	0.49
1:G:129:ARG:NH2	7:G:2066:ADP:O3B	2.39	0.49
2:H:38:GLY:HA3	2:H:358:PRO:HB3	1.95	0.49
1:A:998:ARG:CB	1:A:999:PRO:HA	2.43	0.49
1:C:1017:THR:CG2	1:C:1023:ILE:HG13	2.42	0.49
2:D:237:PHE:CE1	2:D:268:ILE:HD12	2.47	0.49
2:D:241:GLY:O	2:D:269:143:OF	2.30	0.49
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.48	0.49
1:G:772:MET:HE1	1:G:880:THR:HA	1.95	0.49
2:H:324:ASN:ND2	2:H:324:ASN:H	2.10	0.49
2:H:350:PHE:HD2	2:H:354:PRO:HD3	1.78	0.49
1:A:402:LEU:O	1:A:403:GLU:HB2	2.13	0.48
1:A:775:ILE:HG13	1:A:810:ARG:HG2	1.94	0.48
1:A:951:GLU:OE1	1:A:951:GLU:HA	2.10	0.48
2:B:364:ALA:N	2:B:365:PRO:HD2	2.28	0.48
1:C:772:MET:HE1	1:C:880:THR:HG22	1.95	0.48
1:E:224:LYS:HE2	1:E:329:GLY:O	2.13	0.48
2:H:322:PRO:HG2	2:H:324:ASN:HD21	1.78	0.48
1:A:392:GLN:OE1	1:A:495:LYS:HD3	2.13	0.48
2:B:367:PHE:O	2:B:370:PHE:HB3	2.13	0.48
1:C:490:ARG:HD3	10:C:5655:HOH:O	2.13	0.48
1:C:500:ALA:O	1:C:504:LYS:HG3	2.13	0.48
2:B:34:THR:HA	2:B:56:THR:OG1	2.13	0.48
2:B:133:ILE:HD12	2:B:143:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:VAL:HG11	1:C:701:ALA:CA	2.43	0.48
1:E:998[A]:ARG:HB3	1:E:999:PRO:HA	1.95	0.48
1:G:362:PHE:CD2	1:G:433:ALA:HB1	2.48	0.48
1:G:410:ASP:OD1	1:G:501:ARG:NH1	2.47	0.48
1:A:772:MET:HG3	1:A:874:LEU:HD12	1.95	0.48
1:C:509:ARG:HD3	10:C:5680:HOH:O	2.14	0.48
1:C:956:ARG:HB3	1:C:1044:LEU:HD21	1.96	0.48
1:C:1064:SER:OG	1:C:1067:GLU:HG3	2.12	0.48
2:F:169:SER:HA	2:F:216:LEU:O	2.13	0.48
1:C:561:LYS:HE2	10:C:5448:HOH:O	2.12	0.48
1:E:213:TRP:O	1:E:239:ALA:HB1	2.12	0.48
1:G:774:LEU:HD22	1:G:879:VAL:HG12	1.96	0.48
1:C:1:MET:CB	1:C:2:PRO:HD3	2.43	0.48
2:D:135:GLY:O	2:D:138:PRO:HD3	2.13	0.48
1:E:172:PHE:CB	1:E:200:PRO:HG2	2.31	0.48
1:E:676:GLU:O	1:E:680:HIS:ND1	2.46	0.48
1:G:65:TYR:CE2	1:G:77:ILE:HG23	2.49	0.48
1:A:164:PHE:HA	1:A:165:PRO:C	2.39	0.48
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.78	0.48
1:E:426:ARG:C	1:E:426:ARG:HD3	2.37	0.48
1:E:464:VAL:HG11	2:F:88:ILE:HD13	1.96	0.48
1:E:571:ARG:HD3	1:E:574:GLN:HB2	1.95	0.48
1:G:181:ILE:CG1	1:G:376:THR:HG23	2.42	0.48
1:G:702:VAL:HG11	1:G:735:ARG:HH22	1.76	0.48
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.95	0.48
1:A:460:ARG:O	1:A:464:VAL:HG13	2.12	0.48
1:A:954:LYS:HB3	1:A:980:VAL:HG21	1.96	0.48
1:C:24:CYS:HB2	1:C:604:GLU:HB3	1.94	0.48
1:C:600:ASN:O	1:C:618:PHE:HA	2.13	0.48
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.95	0.48
1:G:733:ASP:O	1:G:736:ARG:NH1	2.46	0.48
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.77	0.48
1:A:88:PRO:HB3	1:A:99:ALA:HB2	1.95	0.48
1:C:375:THR:HG23	1:C:377:GLN:H	1.79	0.48
2:D:142:LEU:HD12	2:D:142:LEU:O	2.14	0.48
2:F:245:PRO:C	2:F:247:PRO:HD2	2.39	0.48
1:G:947:LEU:HD12	1:G:947:LEU:N	2.29	0.48
2:H:341:HIS:CD2	2:H:348:PHE:HB3	2.48	0.48
1:A:759:ALA:HB2	1:A:833:LYS:HG3	1.95	0.48
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.49	0.48
2:D:228:VAL:O	2:D:231:MET:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:805:ILE:HD13	1:E:837:VAL:HG23	1.96	0.48
2:F:350:PHE:HB2	2:F:366:LEU:CD2	2.43	0.48
1:G:965:LEU:HA	1:G:965:LEU:HD23	1.75	0.48
1:G:972:ASP:HA	1:G:989:ARG:O	2.14	0.48
1:G:18:ILE:HG23	1:G:23:ALA:HA	1.96	0.47
1:G:150:HIS:HD2	1:G:203:GLU:HB2	1.77	0.47
1:G:344:THR:HB	1:G:345:PRO:HD2	1.95	0.47
1:G:730:ASP:H	1:G:733:ASP:HB2	1.79	0.47
1:G:735:ARG:O	1:G:738:PHE:HB2	2.14	0.47
1:A:1020:ARG:NH2	1:A:1023:ILE:HG21	2.29	0.47
2:F:332:LEU:HD12	2:F:332:LEU:HA	1.62	0.47
2:B:6:LEU:HD12	2:B:7:LEU:N	2.29	0.47
1:G:174:MET:HB2	6:G:2071:PO4:O1	2.14	0.47
2:H:264:PRO:HA	2:H:346:PRO:HB2	1.97	0.47
1:C:872:LYS:HG2	1:C:877:GLN:HG2	1.97	0.47
2:F:12:GLY:HA2	2:F:144:LEU:HD13	1.96	0.47
1:G:38:ARG:HG3	1:G:38:ARG:HH11	1.79	0.47
1:A:713:VAL:HG12	1:A:713:VAL:O	2.15	0.47
1:C:822:VAL:O	1:C:823:ARG:HD3	2.14	0.47
1:E:167:ILE:HD12	1:E:167:ILE:N	2.29	0.47
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.27	0.47
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.44	0.47
1:C:213:TRP:CZ3	1:C:296:ILE:HD12	2.49	0.47
2:D:103:LYS:NZ	10:D:1769:HOH:O	2.48	0.47
2:F:275:LEU:HD23	2:F:349:SER:OG	2.14	0.47
1:G:135:ALA:HB1	1:G:274:GLU:HG3	1.96	0.47
1:G:196:LEU:HG	1:G:204:LEU:HD11	1.96	0.47
1:G:671:ARG:HG2	1:G:677:ARG:CZ	2.45	0.47
1:G:688:LYS:HE3	1:G:836:GLU:CD	2.39	0.47
1:A:27:ASP:OD2	1:A:53:THR:HB	2.15	0.47
1:A:266:ASN:ND2	10:A:5275:HOH:O	2.45	0.47
1:A:583:VAL:HG13	1:A:612:THR:CG2	2.45	0.47
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.49	0.47
1:C:17:PRO:HG3	1:C:917:VAL:CG1	2.44	0.47
1:E:902:GLY:O	1:E:1027:ARG:NH2	2.48	0.47
1:E:1000:HIS:CD2	1:E:1000:HIS:H	2.28	0.47
1:E:1021:ARG:HH11	1:E:1021:ARG:HG2	1.80	0.47
2:F:269:143:O	2:F:272:HIS:HB3	2.15	0.47
1:G:569:PRO:O	1:G:571:ARG:HD2	2.14	0.47
1:G:1005:ILE:HG21	1:G:1032:SER:HB3	1.96	0.47
2:H:202:LYS:NZ	2:H:355:GLU:OE1	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	1.96	0.47
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.50	0.47
1:G:70:HIS:HE1	1:G:72:GLU:HG3	1.79	0.47
1:C:671:ARG:NH2	1:C:819:GLU:O	2.48	0.47
1:G:48:ASN:O	1:G:66:ILE:HA	2.14	0.47
1:G:181:ILE:CD1	1:G:376:THR:HG23	2.45	0.47
2:H:38:GLY:HA3	2:H:358:PRO:CB	2.45	0.47
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.33	0.47
1:E:692:ASN:HA	1:E:752:LEU:O	2.15	0.47
1:G:9:SER:O	1:G:84:ASP:HB2	2.15	0.47
1:G:632:ILE:HG13	1:G:633:GLU:N	2.30	0.47
1:G:1001:ILE:CD1	1:G:1002:GLN:N	2.75	0.47
1:A:675:ARG:NH2	10:A:5768:HOH:O	2.49	0.46
1:C:735:ARG:O	1:C:738:PHE:N	2.47	0.46
2:D:264:PRO:HB3	2:D:373:LEU:HB3	1.98	0.46
1:E:46:LEU:HD13	1:E:46:LEU:N	2.30	0.46
1:E:891:LYS:HG2	1:E:892:GLU:N	2.29	0.46
1:G:1:MET:O	1:G:334:GLU:OE1	2.33	0.46
1:A:735:ARG:O	1:A:738:PHE:N	2.47	0.46
1:C:57:ASP:HB2	1:C:60:MET:HG2	1.98	0.46
1:C:726:GLU:CG	1:C:727:ILE:N	2.78	0.46
1:C:995:HIS:O	1:C:997:GLY:N	2.48	0.46
2:D:139:ASP:OD2	2:D:142:LEU:HB2	2.15	0.46
1:E:169:ARG:NH1	7:E:2045:ADP:O2A	2.47	0.46
1:E:863:LYS:O	1:E:867:ARG:HG3	2.15	0.46
1:G:434:ASP:HB2	10:G:3716:HOH:O	2.15	0.46
1:G:734:LEU:O	1:G:737:TYR:HB3	2.15	0.46
2:H:29:GLU:HB2	2:H:153:LEU:HD22	1.97	0.46
2:H:210:VAL:HG22	2:H:214:CYS:O	2.15	0.46
1:A:930:LYS:HE3	10:A:5080:HOH:O	2.15	0.46
1:E:702:VAL:O	1:E:706:LYS:HD3	2.15	0.46
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.50	0.46
2:D:116:ARG:O	2:D:120:ARG:HG3	2.15	0.46
2:D:222:GLN:H	2:D:222:GLN:HE21	1.63	0.46
1:G:679:GLN:HG2	1:G:683:GLU:OE2	2.15	0.46
1:A:990:LEU:HG	1:G:979:ILE:CD1	2.46	0.46
2:B:196:ALA:O	2:B:219:VAL:HG22	2.14	0.46
1:C:695:VAL:HG21	1:C:701:ALA:CA	2.36	0.46
1:E:151:THR:CB	1:E:153[B]:GLU:HG2	2.45	0.46
1:E:317:PHE:CE1	1:E:322:VAL:HG21	2.51	0.46
1:E:726:GLU:CG	1:E:727:ILE:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:272:HIS:HA	2:F:349:SER:HB2	1.97	0.46
1:G:568:GLY:O	1:G:602:ASN:HB2	2.15	0.46
1:G:906:LEU:O	1:G:912:ARG:NH2	2.39	0.46
1:A:414:SER:OG	1:A:416:ASP:OD2	2.30	0.46
2:B:365:PRO:O	2:B:368:ASP:HB2	2.16	0.46
1:C:991:VAL:O	10:C:5809:HOH:O	2.21	0.46
1:C:1023:ILE:HG22	1:C:1024:GLU:N	2.31	0.46
2:F:248:CYS:C	2:F:252:ILE:HD12	2.41	0.46
1:G:1004:ARG:HA	1:G:1009:GLU:HG3	1.98	0.46
2:H:350:PHE:HB2	2:H:366:LEU:HD23	1.98	0.46
1:A:370:ALA:HB2	1:A:903:VAL:CG2	2.45	0.46
1:A:726:GLU:CG	1:A:727:ILE:N	2.78	0.46
1:C:802:SER:OG	1:C:805:ILE:HB	2.16	0.46
2:F:367:PHE:O	2:F:370:PHE:HB3	2.16	0.46
1:G:40:GLU:HG2	1:G:325:LYS:HE2	1.98	0.46
1:G:289:ASN:HB3	1:G:292:ASN:OD1	2.14	0.46
1:A:446:GLY:O	1:E:448:SER:N	2.45	0.46
1:E:51:PRO:HG3	1:E:918:MET:HB2	1.97	0.46
1:E:998[B]:ARG:HB3	1:E:999:PRO:HA	1.96	0.46
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.46	0.46
1:G:712:LEU:CD2	1:G:752:LEU:HG	2.44	0.46
1:A:835:ASN:HD22	1:A:835:ASN:HA	1.64	0.46
1:C:589:LEU:O	1:C:594:TYR:HB2	2.15	0.46
2:D:269:143:HE	2:D:312:HIS:HB2	1.98	0.46
1:E:313:LYS:NZ	1:E:603:PRO:O	2.49	0.46
1:G:563:MET:CE	1:G:635:PRO:HG3	2.45	0.46
1:G:695:VAL:CG1	1:G:700:MET:HB3	2.40	0.46
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.81	0.46
1:A:805:ILE:HD13	1:A:837:VAL:CG2	2.46	0.46
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.84	0.46
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.81	0.46
1:E:57:ASP:HB3	1:E:59:GLU:OE2	2.16	0.46
1:E:152:MET:SD	1:E:189:GLU:HG2	2.56	0.46
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.98	0.46
1:G:118:ALA:HA	10:G:3483:HOH:O	2.16	0.46
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.46	0.46
1:A:820:LEU:O	1:A:821:GLN:HB2	2.16	0.45
1:C:979:ILE:O	1:C:983:GLU:HG3	2.15	0.45
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.32	0.45
1:E:5:THR:O	1:E:8:LYS:NZ	2.49	0.45
1:E:147:GLY:HA3	1:E:158:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:VAL:O	1:G:161:ASP:HB3	2.15	0.45
1:G:548:GLU:OE1	2:H:114:ASP:HA	2.16	0.45
1:G:859:VAL:HA	1:G:860:PRO:HD2	1.82	0.45
2:H:212:ARG:HG3	2:H:212:ARG:HH11	1.80	0.45
1:A:6:ASP:OD2	1:A:6:ASP:N	2.45	0.45
1:A:701:ALA:O	1:A:705:ALA:N	2.40	0.45
2:B:2:ILE:HD12	10:B:5202:HOH:O	2.15	0.45
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.17	0.45
1:C:892:GLU:OE1	8:C:5033:ORN:NE	2.50	0.45
2:D:142:LEU:HD12	2:D:142:LEU:C	2.41	0.45
1:E:46:LEU:HD21	1:E:64:THR:CG2	2.26	0.45
1:E:258:ASP:O	1:E:262:GLN:HG2	2.16	0.45
1:E:675:ARG:CD	1:E:675:ARG:H	2.29	0.45
1:E:873:SER:O	1:E:877:GLN:HG3	2.17	0.45
1:E:998[B]:ARG:HG3	1:E:998[B]:ARG:HH11	1.81	0.45
2:F:324:ASN:HA	2:F:343:THR:OG1	2.16	0.45
1:G:1031:ARG:HE	1:G:1031:ARG:HB3	1.59	0.45
2:H:218:ILE:N	2:H:218:ILE:CD1	2.79	0.45
2:H:355:GLU:OE2	2:H:355:GLU:N	2.40	0.45
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.50	0.45
1:C:1:MET:N	1:C:2:PRO:CD	2.79	0.45
2:F:129:ASN:CG	2:F:150:PHE:HD1	2.25	0.45
1:G:784:GLN:HE21	1:G:784:GLN:N	2.04	0.45
2:H:192:PHE:O	2:H:215:ARG:HB3	2.16	0.45
1:A:583:VAL:O	1:A:587:LEU:HG	2.15	0.45
1:A:946:LEU:C	1:A:947:LEU:HD12	2.42	0.45
1:C:571:ARG:HD3	1:C:571:ARG:N	2.30	0.45
2:D:44:THR:O	2:D:46:PRO:HD3	2.17	0.45
1:A:583:VAL:HG13	1:A:612:THR:HG21	1.99	0.45
2:B:6:LEU:HD11	2:B:8:VAL:CG2	2.46	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
1:C:106:GLY:HA2	10:C:5129:HOH:O	2.17	0.45
1:C:237:PHE:HB3	1:C:248:ILE:O	2.16	0.45
1:C:385:MET:HB2	1:C:603:PRO:HG3	1.98	0.45
1:C:583:VAL:O	1:C:587:LEU:HG	2.15	0.45
2:F:78:GLN:NE2	10:F:2863:HOH:O	2.35	0.45
2:F:272:HIS:HA	2:F:349:SER:CB	2.47	0.45
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.98	0.45
1:A:734:LEU:CD1	1:A:738:PHE:CE2	3.00	0.45
2:B:232:ASN:N	2:B:233:PRO:CD	2.80	0.45
2:D:364:ALA:N	2:D:365:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:GLY:N	7:E:2045:ADP:O2B	2.42	0.45
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.51	0.45
1:A:944:ARG:HD3	1:A:972:ASP:CG	2.42	0.45
2:D:175:TRP:HA	2:D:180:GLY:O	2.17	0.45
2:D:370:PHE:O	2:D:374:ILE:HG13	2.17	0.45
1:E:282:SER:OG	1:E:302:PRO:HA	2.17	0.45
1:E:698:ILE:CD1	1:E:698:ILE:N	2.79	0.45
1:G:292:ASN:OD1	1:G:294:ARG:HB2	2.16	0.45
1:G:475:LYS:HD3	1:G:488:PHE:CZ	2.52	0.45
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.52	0.45
1:G:1017:THR:CG2	1:G:1018:SER:N	2.79	0.45
2:H:363:ALA:C	2:H:365:PRO:HD2	2.42	0.45
1:A:1:MET:N	1:A:224:LYS:HE3	2.29	0.45
1:A:321:LYS:NZ	1:A:611:ASP:OD1	2.49	0.45
1:A:998:ARG:HA	1:A:999:PRO:C	2.39	0.45
1:A:1023:ILE:HG22	1:A:1024:GLU:N	2.32	0.45
1:C:534:ALA:HB1	2:D:120:ARG:HG2	1.98	0.45
1:C:761:GLU:CG	1:C:781:HIS:CE1	3.00	0.45
1:E:598:MET:HE2	1:E:598:MET:HB2	1.79	0.45
1:G:10:ILE:HD13	1:G:37:LEU:HD13	1.98	0.45
1:G:640:VAL:HG21	1:G:651:ALA:HB2	1.99	0.45
1:G:671:ARG:NH2	1:G:819:GLU:O	2.50	0.45
1:A:555:PRO:HG3	1:A:632:ILE:HD12	1.99	0.45
1:A:1061:LYS:HD3	10:A:5534:HOH:O	2.16	0.45
1:C:525:VAL:HB	1:C:551:CYS:HA	1.98	0.45
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.46	0.45
1:E:75:ARG:HG3	1:E:107:VAL:HG13	1.98	0.45
1:E:147:GLY:HA3	1:E:158:VAL:CG1	2.47	0.45
1:G:772:MET:HE1	1:G:880:THR:CA	2.47	0.45
2:B:33:ASN:HB3	2:B:55:LEU:HD23	1.98	0.45
2:B:74:GLN:HG3	2:B:76:HIS:NE2	2.32	0.45
1:C:1:MET:H3	1:C:2:PRO:HD2	1.81	0.45
1:C:735:ARG:O	1:C:738:PHE:HB2	2.17	0.45
1:E:144:ALA:HB1	1:E:208:GLU:HG2	1.99	0.45
1:G:167:ILE:N	1:G:167:ILE:CD1	2.80	0.45
1:A:1001:ILE:HD12	1:A:1002[A]:GLN:HB2	1.97	0.44
1:A:1022:ALA:O	1:A:1026:SER:OG	2.30	0.44
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.52	0.44
1:G:527:LYS:O	1:G:543:MET:HB3	2.17	0.44
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.99	0.44
2:H:6:LEU:CD1	2:H:8:VAL:HG23	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ALA:HB3	1:A:844:PRO:CG	2.46	0.44
1:C:159:ALA:HB2	1:C:188:PHE:CZ	2.52	0.44
1:C:176:GLY:HA3	1:C:377:GLN:HA	1.97	0.44
1:C:400:ARG:HD3	10:C:5346:HOH:O	2.18	0.44
1:C:726:GLU:HG3	1:C:727:ILE:N	2.30	0.44
2:F:46:PRO:HA	2:F:76:HIS:CG	2.51	0.44
1:G:782:ILE:O	1:G:1045:ASN:HB3	2.16	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.44
1:A:167:ILE:HD12	1:A:167:ILE:N	2.32	0.44
1:A:257:THR:HG22	2:B:63:VAL:HG21	2.00	0.44
1:C:736:ARG:CZ	1:C:736:ARG:HB3	2.48	0.44
1:E:168:ILE:HD13	1:E:191:ILE:CG2	2.47	0.44
1:E:687:LEU:HD22	1:E:812:GLN:HG2	2.00	0.44
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.99	0.44
1:G:148:ILE:HG22	1:G:149:ALA:N	2.33	0.44
1:G:894:VAL:HG22	1:G:915:GLY:C	2.42	0.44
2:H:150:PHE:CD2	2:H:151:PRO:HD2	2.52	0.44
2:H:324:ASN:HA	2:H:343:THR:OG1	2.17	0.44
2:H:325:LEU:HD23	2:H:325:LEU:HA	1.59	0.44
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.49	0.44
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.99	0.44
1:A:698:ILE:HD12	1:A:698:ILE:H	1.82	0.44
2:B:197:TYR:HB3	2:B:199:PHE:CZ	2.52	0.44
1:C:259:LYS:HD2	2:D:69:ASP:OD2	2.18	0.44
2:D:324:ASN:ND2	2:D:324:ASN:H	2.16	0.44
1:E:755:PHE:CD1	7:E:2051:ADP:C2	3.06	0.44
1:E:1004[B]:ARG:NH2	10:E:5070:HOH:O	2.50	0.44
1:A:1073:LYS:HD2	1:A:1073:LYS:N	2.32	0.44
2:D:212:ARG:HH11	2:D:212:ARG:CG	2.30	0.44
1:E:901:PRO:HD2	5:E:5063:CL:CL	2.54	0.44
2:F:193:HIS:N	2:F:234:ASP:OD2	2.42	0.44
2:F:212:ARG:HG3	2:F:212:ARG:HH11	1.82	0.44
2:F:246:ALA:N	2:F:247:PRO:HD2	2.31	0.44
2:F:254:ALA:O	2:F:257:LYS:HB2	2.17	0.44
1:G:726:GLU:CG	1:G:727:ILE:N	2.79	0.44
1:G:812:GLN:O	1:G:816:LEU:HD12	2.17	0.44
2:H:38:GLY:O	2:H:358:PRO:HG3	2.17	0.44
1:A:11:LEU:HA	1:A:45:ILE:O	2.18	0.44
1:C:687:LEU:HD11	1:C:812:GLN:HG2	1.95	0.44
2:D:195:VAL:HG21	2:D:231:MET:HE3	1.99	0.44
2:D:232:ASN:N	2:D:233:PRO:HD3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:N	1:E:224:LYS:CE	2.80	0.44
2:F:246:ALA:N	2:F:247:PRO:CD	2.80	0.44
1:G:349:GLU:O	2:H:294:ASN:HB2	2.17	0.44
1:G:734:LEU:CD1	1:G:738:PHE:CE2	2.99	0.44
1:A:1:MET:CB	1:A:2:PRO:HD3	2.48	0.44
1:A:571:ARG:HD3	1:A:571:ARG:N	2.32	0.44
2:D:274:LEU:HD23	2:D:274:LEU:HA	1.75	0.44
1:E:59:GLU:HG2	1:E:60:MET:HE2	1.99	0.44
1:E:583:VAL:O	1:E:587:LEU:HG	2.17	0.44
1:E:687:LEU:HD22	1:E:812:GLN:CG	2.48	0.44
1:G:159:ALA:HB2	1:G:188:PHE:CZ	2.52	0.44
1:G:534:ALA:O	2:H:123:ARG:HD3	2.17	0.44
1:G:802:SER:O	1:G:806:GLN:HG3	2.18	0.44
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.53	0.44
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.48	0.44
2:B:181:LEU:HD23	2:B:181:LEU:HA	1.80	0.44
2:B:285:LYS:HG3	2:B:314:PHE:CZ	2.52	0.44
1:A:659:VAL:CG1	1:A:660:PRO:HD2	2.47	0.44
1:A:991:VAL:CG2	1:A:1004:ARG:NH1	2.80	0.44
1:C:51:PRO:HG3	1:C:918:MET:HB2	2.00	0.44
1:E:554:ASN:N	1:E:555:PRO:HD3	2.33	0.44
1:E:704:LYS:O	1:E:707:GLU:HB2	2.17	0.44
1:E:994:VAL:HG13	1:E:1000:HIS:CG	2.51	0.44
2:H:350:PHE:CG	2:H:366:LEU:CD2	3.00	0.44
1:A:700:MET:O	1:A:704:LYS:HB2	2.18	0.43
2:D:6:LEU:HD21	2:D:140:ALA:HA	2.00	0.43
1:G:148:ILE:CG2	1:G:149:ALA:N	2.81	0.43
1:G:489:LEU:HD12	1:G:489:LEU:HA	1.83	0.43
2:H:305:VAL:HG12	2:H:306:MET:N	2.32	0.43
1:C:240:MET:HE3	7:C:2023:ADP:C4	2.53	0.43
1:C:734:LEU:CD1	1:C:738:PHE:CE2	3.00	0.43
2:D:299:ASP:OD1	2:D:302:LYS:HD2	2.19	0.43
1:G:240:MET:HE3	1:G:240:MET:HB3	1.86	0.43
1:G:602:ASN:HA	1:G:603:PRO:HD2	1.93	0.43
2:H:364:ALA:N	2:H:365:PRO:HD2	2.33	0.43
1:A:93:GLN:HG2	5:A:5017:CL:CL	2.56	0.43
1:A:344:THR:HB	1:A:345:PRO:CD	2.48	0.43
1:A:735:ARG:O	1:A:738:PHE:HB2	2.17	0.43
1:E:488:PHE:O	1:E:492:LEU:HG	2.18	0.43
1:E:753:ASP:HB2	10:E:5830:HOH:O	2.17	0.43
2:F:324:ASN:ND2	2:F:324:ASN:H	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:481:ILE:HD13	1:G:508:VAL:HG11	1.99	0.43
1:G:879:VAL:HA	10:G:3925:HOH:O	2.17	0.43
1:G:946:LEU:C	1:G:947:LEU:HD12	2.43	0.43
2:H:212:ARG:HG3	2:H:212:ARG:NH1	2.33	0.43
1:A:99:ALA:HB1	1:A:115:MET:CE	2.48	0.43
1:A:696:THR:OG1	1:A:700:MET:HE1	2.18	0.43
1:C:695:VAL:CG2	1:C:752:LEU:HD22	2.48	0.43
1:E:726:GLU:OE1	1:E:1020:ARG:HD3	2.18	0.43
2:F:6:LEU:HD13	2:F:16:HIS:CE1	2.53	0.43
2:F:155:GLY:N	2:F:244:ASP:OD1	2.46	0.43
2:F:364:ALA:N	2:F:365:PRO:HD2	2.33	0.43
1:G:805:ILE:HD12	1:G:832:VAL:HG11	2.00	0.43
1:G:891:LYS:HG2	1:G:892:GLU:N	2.31	0.43
1:G:955:GLU:HB3	10:G:3973:HOH:O	2.17	0.43
1:G:1002:GLN:O	1:G:1006:LYS:HB3	2.18	0.43
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.61	0.43
1:A:602:ASN:ND2	1:A:605:THR:HG23	2.33	0.43
1:A:918:MET:HE2	1:A:920:VAL:CG2	2.48	0.43
1:C:174:MET:HB2	6:C:2028:PO4:O1	2.18	0.43
1:C:796:LEU:HD23	1:C:796:LEU:C	2.43	0.43
1:C:975:HIS:O	1:C:979:ILE:HG12	2.18	0.43
2:D:195:VAL:HG11	2:D:231:MET:HE1	2.00	0.43
1:E:106:GLY:HA2	10:E:5155:HOH:O	2.17	0.43
1:E:159:ALA:HB2	1:E:188:PHE:CZ	2.53	0.43
1:E:363:ASN:OD1	1:E:381:VAL:HG21	2.18	0.43
1:E:484:LEU:HD23	1:E:484:LEU:HA	1.76	0.43
1:G:188:PHE:O	1:G:192:CYS:HB2	2.18	0.43
1:G:646:THR:HB	1:G:647:PRO:CD	2.49	0.43
2:H:25:SER:HA	2:H:132:ILE:O	2.19	0.43
2:H:169:SER:HA	2:H:216:LEU:O	2.18	0.43
2:B:259:LEU:O	2:B:345:LYS:HD2	2.19	0.43
1:C:775:ILE:HD13	1:C:775:ILE:HA	1.89	0.43
1:C:967:GLN:HG3	1:C:1054:LEU:CD1	2.35	0.43
1:E:239:ALA:HB2	10:E:5283:HOH:O	2.17	0.43
1:G:674:ASP:HB3	1:G:677:ARG:HG3	2.00	0.43
1:G:1017:THR:HG22	1:G:1018:SER:N	2.32	0.43
1:C:621:VAL:O	1:C:621:VAL:HG12	2.18	0.43
1:C:646:THR:HB	1:C:647:PRO:HD3	2.00	0.43
1:C:947:LEU:N	1:C:947:LEU:HD12	2.33	0.43
2:D:364:ALA:N	2:D:365:PRO:HD2	2.34	0.43
1:E:139:ILE:HG13	1:E:141:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:LEU:HD11	2:H:8:VAL:HG22	1.98	0.43
1:E:141:LEU:HD23	1:E:141:LEU:HA	1.79	0.43
1:G:18:ILE:HD12	1:G:23:ALA:HA	2.01	0.43
1:G:196:LEU:HG	1:G:204:LEU:CD1	2.49	0.43
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.48	0.43
1:G:770:GLY:CA	1:G:823:ARG:NH1	2.82	0.43
1:G:1021:ARG:CG	1:G:1021:ARG:NH1	2.80	0.43
2:H:225:ALA:HA	2:H:258:PHE:CZ	2.54	0.43
1:A:885:PRO:HA	1:A:886:PRO:HD3	1.87	0.43
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.49	0.43
1:C:906:LEU:O	1:C:912:ARG:NH2	2.47	0.43
1:G:49:SER:O	1:G:51:PRO:HD3	2.18	0.43
1:G:713:VAL:HG23	1:G:755:PHE:HB2	2.01	0.43
1:G:755:PHE:CE1	7:G:2072:ADP:C2	3.07	0.43
1:G:900:PHE:O	1:G:903:VAL:HG23	2.19	0.43
1:G:1035:GLN:NE2	10:G:3567:HOH:O	2.51	0.43
9:G:5077:NET:H63	9:G:5077:NET:H31	1.84	0.43
2:H:5:ALA:HB3	2:H:110:ILE:HG13	2.01	0.43
1:A:576:ILE:HD13	1:A:576:ILE:HG21	1.71	0.43
1:A:764:VAL:O	1:A:827:ASN:HA	2.19	0.43
1:C:503:ALA:HB2	1:C:510:GLU:HA	2.00	0.43
2:F:25:SER:HA	2:F:132:ILE:O	2.19	0.43
1:G:46:LEU:HD12	1:G:46:LEU:O	2.17	0.43
1:A:151:THR:HB	10:A:5633:HOH:O	2.19	0.42
1:A:868:VAL:HA	1:A:872:LYS:O	2.19	0.42
9:A:5012:NET:H23	9:A:5012:NET:H71	1.72	0.42
1:C:698:ILE:O	1:C:702:VAL:HG23	2.19	0.42
1:E:101:GLU:OE2	1:E:104:ARG:NH2	2.37	0.42
1:G:178:GLY:HA3	1:G:198:LEU:HD23	2.00	0.42
2:H:114:ASP:O	2:H:117:LYS:HB3	2.19	0.42
1:C:934:GLY:C	1:C:936:ASN:H	2.27	0.42
1:E:146:SER:HB2	1:E:205:LEU:CD1	2.39	0.42
1:G:1000:HIS:O	1:G:1004:ARG:HG3	2.19	0.42
2:H:249:ASP:OD2	2:H:250:TYR:HD2	2.01	0.42
1:A:361:ARG:CZ	1:A:404:VAL:HG12	2.50	0.42
1:C:294:ARG:HD2	5:C:5040:CL:CL	2.57	0.42
2:D:324:ASN:O	2:D:342:ARG:HA	2.19	0.42
1:E:46:LEU:C	1:E:46:LEU:HD23	2.41	0.42
1:E:1021:ARG:CG	1:E:1021:ARG:NH1	2.80	0.42
2:F:325:LEU:HD23	2:F:325:LEU:HA	1.75	0.42
1:G:850:VAL:HB	1:G:851:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:ASN:HB2	10:A:5036:HOH:O	2.19	0.42
2:B:6:LEU:O	2:B:132:ILE:HA	2.20	0.42
1:C:1:MET:H3	1:C:2:PRO:CD	2.33	0.42
1:C:470:VAL:O	1:C:474:GLU:HG3	2.20	0.42
1:C:472:LEU:O	1:C:476:VAL:HG23	2.19	0.42
1:C:475:LYS:HD3	1:C:488:PHE:CZ	2.54	0.42
1:C:730:ASP:H	1:C:733:ASP:HB2	1.85	0.42
1:C:863:LYS:O	1:C:867:ARG:HG3	2.18	0.42
2:F:5:ALA:HB2	2:F:19:ALA:HB2	2.00	0.42
2:F:152:GLY:O	2:F:156:MET:HE3	2.20	0.42
1:A:40:GLU:OE1	1:A:325:LYS:NZ	2.30	0.42
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.85	0.42
1:A:558:ASP:HB3	1:A:559:ARG:H	1.59	0.42
1:C:10:ILE:HD12	1:C:42:TYR:HB3	2.02	0.42
2:D:234:ASP:CG	2:D:378:ARG:HH11	2.28	0.42
1:E:670:ASP:CB	1:E:677:ARG:HH21	2.22	0.42
1:E:734:LEU:CD1	1:E:738:PHE:CE2	3.02	0.42
1:G:22:GLN:HG3	1:G:174:MET:HE1	2.01	0.42
1:G:831:ALA:HB2	1:G:840:ILE:HD11	2.01	0.42
2:H:121:LEU:CD1	2:H:125:LYS:HD3	2.49	0.42
1:A:349:GLU:O	2:B:294:ASN:HB2	2.18	0.42
2:B:305:VAL:HG12	2:B:306:MET:N	2.35	0.42
2:B:378:ARG:NH1	2:B:378:ARG:HG2	2.33	0.42
1:C:904:ASP:HA	1:C:905:PRO:HD3	1.81	0.42
1:G:49:SER:HB2	1:G:917:VAL:HG12	2.02	0.42
1:G:168:ILE:HG23	1:G:204:LEU:HD22	2.00	0.42
1:G:663:GLY:HA2	1:G:869:MET:HG2	2.01	0.42
1:G:863:LYS:O	1:G:867:ARG:HG3	2.20	0.42
2:H:226:GLU:OE1	2:H:257:LYS:HE3	2.20	0.42
9:A:5012:NET:H31	9:A:5012:NET:H63	1.67	0.42
2:B:49:SER:HA	2:B:76:HIS:O	2.19	0.42
2:B:264:PRO:HB3	2:B:373:LEU:HB3	2.01	0.42
2:D:275:LEU:HD12	2:D:275:LEU:O	2.18	0.42
1:E:237:PHE:HB3	1:E:248:ILE:O	2.20	0.42
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.20	0.42
2:F:205:ILE:HG12	2:F:355:GLU:CD	2.45	0.42
2:F:261:THR:OG1	2:F:263:ILE:HG13	2.20	0.42
1:G:152:MET:HE1	1:G:189:GLU:O	2.19	0.42
1:G:152:MET:HE3	10:G:4139:HOH:O	2.19	0.42
1:A:1017:THR:CG2	1:A:1018:SER:N	2.82	0.42
1:E:327:ALA:HB2	10:E:5322:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:300:VAL:HG22	2:F:328:THR:O	2.19	0.42
1:G:619:GLU:HB3	1:G:620:PRO:HD2	2.02	0.42
1:G:939:MET:HE2	1:G:1050:THR:CG2	2.49	0.42
1:E:379:LYS:HE2	10:E:5358:HOH:O	2.19	0.42
1:E:733:ASP:HA	1:E:736:ARG:HH11	1.84	0.42
2:F:286:MET:HE1	2:F:312:HIS:CE1	2.55	0.42
1:G:159:ALA:HB2	1:G:188:PHE:CE2	2.55	0.42
2:H:209:LEU:HD23	2:H:209:LEU:HA	1.95	0.42
1:A:325:LYS:O	1:A:330:TYR:HB2	2.20	0.42
2:B:244:ASP:O	2:B:247:PRO:HD2	2.19	0.42
2:B:246:ALA:N	2:B:247:PRO:CD	2.82	0.42
1:C:180:GLY:HA2	1:C:376:THR:OG1	2.20	0.42
1:C:196:LEU:HD23	1:C:196:LEU:HA	1.95	0.42
1:C:695:VAL:HG11	1:C:701:ALA:N	2.35	0.42
1:E:252:PRO:HD3	1:E:352:ILE:HD11	2.01	0.42
1:E:728:VAL:HG12	1:E:733:ASP:HB3	1.95	0.42
1:G:375:THR:OG1	1:G:376:THR:N	2.52	0.42
2:H:296:PRO:HB2	2:H:332:LEU:HB2	2.01	0.42
2:H:324:ASN:O	2:H:342:ARG:HA	2.20	0.42
1:A:46:LEU:CD2	1:A:64:THR:HA	2.50	0.41
1:A:48:ASN:O	1:A:66:ILE:HA	2.20	0.41
1:A:602:ASN:ND2	1:A:605:THR:CG2	2.83	0.41
1:C:1:MET:O	1:C:329:GLY:O	2.38	0.41
1:C:820:LEU:HD23	1:C:820:LEU:HA	1.91	0.41
1:E:421:LEU:HD23	1:E:421:LEU:HA	1.90	0.41
2:H:42:ILE:HG23	2:H:48:TYR:CE2	2.55	0.41
2:H:324:ASN:ND2	2:H:324:ASN:N	2.67	0.41
1:A:704:LYS:HD2	1:A:704:LYS:HA	1.69	0.41
1:A:728:VAL:H	1:A:728:VAL:HG23	1.64	0.41
9:A:5012:NET:H42	9:A:5012:NET:C2	2.44	0.41
2:B:232:ASN:O	10:B:5245:HOH:O	2.22	0.41
1:C:11:LEU:HA	1:C:45:ILE:HB	2.02	0.41
1:C:670:ASP:HB3	1:C:677:ARG:NH2	2.34	0.41
1:C:1013:ILE:O	1:C:1040:TYR:HA	2.20	0.41
1:C:1048:PHE:O	1:C:1052:MET:HG3	2.19	0.41
1:C:1071:GLN:HE21	1:C:1071:GLN:HB3	1.70	0.41
1:G:46:LEU:C	1:G:46:LEU:CD1	2.89	0.41
1:A:702:VAL:HG11	1:A:735:ARG:NH2	2.35	0.41
2:B:46:PRO:HA	2:B:76:HIS:CB	2.50	0.41
2:B:190:LEU:HB2	2:B:215[A]:ARG:HB3	2.03	0.41
1:C:415:LEU:HA	1:C:415:LEU:HD23	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:ARG:CG	2:D:212:ARG:NH1	2.81	0.41
1:E:400:ARG:HD3	10:E:5372:HOH:O	2.19	0.41
1:E:1021:ARG:HH11	1:E:1021:ARG:HG3	1.84	0.41
2:F:6:LEU:HD21	2:F:140:ALA:HA	2.02	0.41
1:G:79:GLU:O	1:G:82:ARG:HD2	2.19	0.41
1:G:868:VAL:HG23	1:G:877:GLN:HE22	1.85	0.41
1:G:1041:ASP:HA	8:G:5076:ORN:O	2.20	0.41
2:H:33:ASN:HA	2:H:291:HIS:O	2.20	0.41
1:A:431:ALA:HB2	1:A:435:ARG:CZ	2.51	0.41
1:C:765:ASP:OD2	1:C:827:ASN:HB2	2.20	0.41
1:E:336:MET:HB3	1:E:342:GLY:HA2	2.02	0.41
1:E:855:LYS:HA	1:E:855:LYS:HD2	1.82	0.41
1:G:423:LYS:H	1:G:423:LYS:HG3	1.62	0.41
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.36	0.41
1:A:108:LEU:HD22	1:A:113:VAL:HB	2.02	0.41
1:A:332:LEU:HB3	1:A:347:SER:HB3	2.02	0.41
1:A:419:GLU:HG3	10:E:5067:HOH:O	2.19	0.41
1:A:517:ARG:HD2	1:A:522:LEU:O	2.21	0.41
2:B:71:GLU:C	2:B:203:ARG:HG3	2.45	0.41
2:B:269:143:HE	2:B:312:HIS:CB	2.51	0.41
2:B:269:143:HE	2:B:312:HIS:HB3	2.02	0.41
1:C:66:ILE:CG2	1:C:918:MET:HB3	2.50	0.41
2:D:372:GLU:HG3	10:D:2246:HOH:O	2.20	0.41
1:E:940:LYS:HG3	1:E:1011:THR:HB	2.01	0.41
2:H:82:ILE:O	2:H:111:ALA:HA	2.20	0.41
2:H:350:PHE:CD1	2:H:366:LEU:HD21	2.56	0.41
1:A:18:ILE:HG23	1:A:23:ALA:HA	2.02	0.41
1:A:828:VAL:CG1	1:A:839:LEU:HD11	2.51	0.41
2:B:6:LEU:HD21	2:B:140:ALA:HA	2.02	0.41
1:C:891:LYS:HG2	1:C:892:GLU:N	2.36	0.41
1:C:994:VAL:HA	1:C:1000:HIS:ND1	2.35	0.41
1:C:1017:THR:CG2	1:C:1018:SER:N	2.83	0.41
2:D:176:THR:O	2:D:180:GLY:N	2.52	0.41
1:E:237:PHE:HB3	1:E:248:ILE:HB	2.03	0.41
1:E:419:GLU:O	1:E:422:THR:HB	2.21	0.41
1:E:514:ARG:HD3	10:E:5436:HOH:O	2.20	0.41
1:E:669:ILE:HA	1:E:844:PRO:HG2	2.03	0.41
2:F:223:THR:HG22	2:F:228:VAL:HG23	2.03	0.41
1:G:688:LYS:HD3	10:G:4241:HOH:O	2.19	0.41
2:H:66:ASN:ND2	10:H:3649:HOH:O	2.35	0.41
2:B:259:LEU:HA	2:B:259:LEU:HD23	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LYS:HB2	2:B:332:LEU:HD11	2.02	0.41
1:C:1021:ARG:HH11	1:C:1021:ARG:CG	2.34	0.41
2:D:228:VAL:HG22	2:D:231:MET:CE	2.50	0.41
1:E:1:MET:CB	1:E:2:PRO:HD3	2.50	0.41
1:E:489:LEU:HD12	1:E:489:LEU:HA	1.88	0.41
1:E:755:PHE:CE1	7:E:2051:ADP:C2	3.08	0.41
1:G:994:VAL:HG13	1:G:1000:HIS:ND1	2.36	0.41
1:A:46:LEU:HD21	1:A:64:THR:CG2	2.42	0.41
1:A:467:GLU:O	1:A:471:ARG:HG2	2.21	0.41
1:A:695:VAL:HG23	1:A:752:LEU:HD22	2.01	0.41
1:C:318:PRO:HB2	1:C:321:LYS:HB2	2.03	0.41
1:C:992:ASN:ND2	1:E:975:HIS:NE2	2.68	0.41
2:D:272:HIS:HA	2:D:349:SER:HB2	2.02	0.41
1:G:892:GLU:OE1	8:G:5076:ORN:NE	2.51	0.41
2:H:23:THR:HG23	2:H:134:ALA:O	2.21	0.41
2:H:201:ALA:HB2	2:H:239:SER:CB	2.50	0.41
2:H:205:ILE:HG13	2:H:355:GLU:HG3	2.03	0.41
1:A:728:VAL:HG12	1:A:733:ASP:HB3	2.02	0.41
1:A:797:PRO:HB3	10:A:5497:HOH:O	2.20	0.41
2:B:378:ARG:HG2	2:B:378:ARG:HH11	1.85	0.41
1:C:150:HIS:N	1:C:154:GLU:OE2	2.54	0.41
1:C:385:MET:HB3	1:C:618:PHE:CE1	2.56	0.41
1:C:419:GLU:O	1:C:423:LYS:HG3	2.21	0.41
1:C:526:TYR:CE1	1:C:545:SER:HB3	2.56	0.41
1:C:805:ILE:HD13	1:C:837:VAL:CG2	2.51	0.41
1:C:833:LYS:O	1:C:836:GLU:HB2	2.21	0.41
1:E:170:PRO:HB3	1:E:199:SER:HB2	2.03	0.41
1:E:1001:ILE:CD1	1:E:1002:GLN:N	2.78	0.41
1:G:58:PRO:HD2	1:G:59:GLU:OE2	2.21	0.41
1:G:453:PHE:CD1	1:G:453:PHE:C	2.98	0.41
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.56	0.41
1:G:752:LEU:HD12	1:G:752:LEU:HA	1.73	0.41
1:A:215:GLU:OE1	7:A:2001:ADP:O3'	2.36	0.41
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.56	0.41
1:A:672:ALA:HB2	1:A:844:PRO:HG3	2.01	0.41
1:C:1:MET:N	1:C:2:PRO:HD2	2.36	0.41
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.56	0.41
1:E:224:LYS:C	1:E:226:ASP:H	2.29	0.41
2:F:272:HIS:HB2	2:F:349:SER:HB2	2.03	0.41
1:G:85:ALA:HB1	1:G:114:THR:O	2.21	0.41
1:G:726:GLU:HG3	1:G:727:ILE:H	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1026:SER:CB	1:G:1030:ARG:HH12	2.33	0.41
2:H:279:SER:O	2:H:322:PRO:HG3	2.21	0.41
1:A:59[B]:GLU:CG	1:A:60:MET:HE2	2.50	0.40
1:A:711:PRO:HG2	1:A:755:PHE:HD2	1.85	0.40
2:B:187:GLU:CG	2:B:215[A]:ARG:HD2	2.42	0.40
1:C:3:LYS:HB3	1:C:330:TYR:CZ	2.56	0.40
1:C:46:LEU:CD2	1:C:55:MET:O	2.69	0.40
1:C:423:LYS:HG3	1:C:423:LYS:H	1.46	0.40
1:C:805:ILE:CD1	1:C:837:VAL:CG2	2.99	0.40
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.71	0.40
1:E:1017:THR:CG2	1:E:1018:SER:N	2.84	0.40
1:G:763:ASP:HB3	1:G:779:MET:HE3	2.03	0.40
1:A:4:ARG:HD3	1:A:7:ILE:HD12	2.03	0.40
1:A:167:ILE:N	1:A:167:ILE:CD1	2.84	0.40
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.56	0.40
2:D:324:ASN:ND2	2:D:324:ASN:N	2.68	0.40
2:D:337:LEU:HD12	2:D:337:LEU:HA	1.83	0.40
1:G:6:ASP:OD2	1:G:6:ASP:N	2.49	0.40
1:G:579:ASP:OD1	1:G:605:THR:HB	2.21	0.40
1:G:738:PHE:HA	1:G:741:ALA:HB3	2.03	0.40
1:G:770:GLY:CA	1:G:823:ARG:CZ	3.00	0.40
1:G:770:GLY:HA3	1:G:823:ARG:CZ	2.52	0.40
2:D:201:ALA:HA	2:D:240:ASN:OD1	2.22	0.40
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.69	0.40
1:E:148:ILE:CG2	1:E:149:ALA:N	2.85	0.40
1:E:1001:ILE:HD12	1:E:1002:GLN:CA	2.52	0.40
2:F:38:GLY:HA3	2:F:358:PRO:HB3	2.02	0.40
1:G:1065:VAL:HG23	1:G:1065:VAL:H	1.59	0.40
2:H:196:ALA:HA	2:H:237:PHE:O	2.22	0.40
2:H:228:VAL:C	2:H:230:LYS:N	2.80	0.40
1:C:77:ILE:O	1:C:81:GLU:N	2.51	0.40
1:C:772:MET:HE1	1:C:880:THR:HA	2.04	0.40
1:C:992:ASN:ND2	1:C:996:GLU:HB3	2.36	0.40
1:E:728:VAL:HG11	1:E:734:LEU:HA	2.03	0.40
1:E:730:ASP:H	1:E:733:ASP:HB2	1.86	0.40
1:E:730:ASP:O	1:E:733:ASP:HB2	2.21	0.40
1:G:7:ILE:HG21	1:G:7:ILE:HD13	1.80	0.40
1:G:671:ARG:CG	1:G:677:ARG:NH1	2.82	0.40
2:H:121:LEU:HD11	2:H:125:LYS:HD3	2.03	0.40
1:A:561:LYS:C	1:A:562:ILE:HG12	2.45	0.40
1:A:681:ALA:HA	1:A:684:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:GLN:NE2	10:A:5766:HOH:O	2.29	0.40
1:A:975:HIS:CD2	1:A:975:HIS:C	2.99	0.40
1:A:1048:PHE:O	1:A:1052:MET:HG3	2.21	0.40
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.84	0.40
1:C:693:ALA:HB2	1:C:708:ILE:HD11	2.02	0.40
1:C:947:LEU:HG	1:C:1014:ILE:HG21	2.03	0.40
1:E:146:SER:HA	1:E:206:ILE:O	2.22	0.40
1:E:693:ALA:CB	1:E:708:ILE:HD11	2.52	0.40
2:F:206:LEU:HD22	2:F:216:LEU:HD13	2.04	0.40
1:G:1:MET:N	1:G:224:LYS:HZ1	2.19	0.40
1:G:709:GLY:O	1:G:712:LEU:HD12	2.20	0.40
1:G:975:HIS:CD2	1:G:975:HIS:C	3.00	0.40
1:G:981:LEU:HA	1:G:981:LEU:HD23	1.91	0.40
2:H:185:LYS:HD2	2:H:190:LEU:HD21	2.04	0.40
2:H:190:LEU:HD23	2:H:190:LEU:HA	1.78	0.40
2:H:197:TYR:HB3	2:H:199:PHE:CZ	2.57	0.40
2:H:350:PHE:CG	2:H:366:LEU:HD21	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1057/1073 (98%)	998 (94%)	56 (5%)	3 (0%)	36	36
1	C	1054/1073 (98%)	1002 (95%)	48 (5%)	4 (0%)	30	28
1	E	1060/1073 (99%)	1012 (96%)	45 (4%)	3 (0%)	36	36
1	G	1052/1073 (98%)	998 (95%)	49 (5%)	5 (0%)	24	22
2	B	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	376/382 (98%)	364 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	376/382 (98%)	362 (96%)	14 (4%)	0	100	100
All	All	5729/5820 (98%)	5462 (95%)	252 (4%)	15 (0%)	36	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	996	GLU
1	G	873	SER
1	A	558	ASP
1	A	975	HIS
1	E	675	ARG
1	E	954	LYS
1	G	975	HIS
1	G	558	ASP
1	G	739	GLN
1	A	646	THR
1	C	88	PRO
1	E	738	PHE
1	G	698	ILE
1	C	2	PRO
1	C	698	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	870/878 (99%)	802 (92%)	68 (8%)	11	9
1	C	867/878 (99%)	789 (91%)	78 (9%)	9	6
1	E	873/878 (99%)	811 (93%)	62 (7%)	13	11
1	G	865/878 (98%)	783 (90%)	82 (10%)	8	5
2	B	308/309 (100%)	281 (91%)	27 (9%)	9	7
2	D	308/309 (100%)	283 (92%)	25 (8%)	11	8
2	F	307/309 (99%)	272 (89%)	35 (11%)	5	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	307/309 (99%)	285 (93%)	22 (7%)	13	11
All	All	4705/4748 (99%)	4306 (92%)	399 (8%)	10	7

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	THR
1	A	8	LYS
1	A	38	ARG
1	A	46	LEU
1	A	62	ASP
1	A	103	GLU
1	A	202	LYS
1	A	220	VAL
1	A	224	LYS
1	A	275	ILE
1	A	278	GLU
1	A	313	LYS
1	A	326	LEU
1	A	363	ASN
1	A	412	LYS
1	A	416	ASP
1	A	490	ARG
1	A	548	GLU
1	A	557	THR
1	A	562	ILE
1	A	571	ARG
1	A	576	ILE
1	A	591	GLU
1	A	632	ILE
1	A	652	ARG
1	A	671	ARG
1	A	677	ARG
1	A	688	LYS
1	A	689	GLN
1	A	696	THR
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS
1	A	712	LEU
1	A	714	VAL

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Mol	Chain	Res	Type
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	753	ASP
1	A	763	ASP
1	A	784	GLN
1	A	804	GLU
1	A	805	ILE
1	A	815	LYS
1	A	833	LYS
1	A	835	ASN
1	A	839	LEU
1	A	855	LYS
1	A	876	GLU
1	A	881	LYS
1	A	906	LEU
1	A	912	ARG
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	955	GLU
1	A	967	GLN
1	A	992	ASN
1	A	1006	LYS
1	A	1021	ARG
1	A	1026	SER
1	A	1028	VAL
1	A	1032	SER
1	A	1037	LYS
1	A	1059	THR
1	A	1072	ILE
1	A	1073	LYS
2	B	2	ILE
2	B	6	LEU
2	B	18	ARG
2	B	87	LEU
2	B	123	ARG
2	B	153	LEU
2	B	154	ASN
2	B	166	GLU
2	B	183	GLU
2	B	186	LYS

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Mol	Chain	Res	Type
2	B	190	LEU
2	B	215[A]	ARG
2	B	215[B]	ARG
2	B	218	ILE
2	B	222	GLN
2	B	238	LEU
2	B	252	ILE
2	B	257	LYS
2	B	282	LYS
2	B	301	GLU
2	B	306	MET
2	B	321	LEU
2	B	324	ASN
2	B	357	SER
2	B	366	LEU
2	B	376	GLN
2	B	379	LYS
1	C	1	MET
1	C	4	ARG
1	C	5	THR
1	C	38[A]	ARG
1	C	38[B]	ARG
1	C	43	ARG
1	C	44	VAL
1	C	46	LEU
1	C	55	MET
1	C	76	LYS
1	C	103	GLU
1	C	145	ARG
1	C	174	MET
1	C	202	LYS
1	C	220	VAL
1	C	299	GLU
1	C	313	LYS
1	C	321	LYS
1	C	326	LEU
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	414	SER
1	C	416	ASP
1	C	422	THR

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Mol	Chain	Res	Type
1	C	426	ARG
1	C	428	LEU
1	C	509	ARG
1	C	548	GLU
1	C	559	ARG
1	C	571	ARG
1	C	591	GLU
1	C	652	ARG
1	C	671	ARG
1	C	675	ARG
1	C	686	LYS
1	C	688	LYS
1	C	692	ASN
1	C	702	VAL
1	C	704	LYS
1	C	706	LYS
1	C	712	LEU
1	C	728	VAL
1	C	733	ASP
1	C	734	LEU
1	C	735	ARG
1	C	751	LEU
1	C	763	ASP
1	C	772	MET
1	C	784	GLN
1	C	800	THR
1	C	805	ILE
1	C	812	GLN
1	C	815	LYS
1	C	849	THR
1	C	855	LYS
1	C	876	GLU
1	C	880	THR
1	C	906	LEU
1	C	912	ARG
1	C	940	LYS
1	C	950	ARG
1	C	951	GLU
1	C	954	LYS
1	C	963	LYS
1	C	966	LYS
1	C	967	GLN

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Mol	Chain	Res	Type
1	C	992	ASN
1	C	1007	ASN
1	C	1009[A]	GLU
1	C	1009[B]	GLU
1	C	1018	SER
1	C	1021	ARG
1	C	1028	VAL
1	C	1052	MET
1	C	1061	LYS
1	C	1072	ILE
1	C	1073	LYS
2	D	2	ILE
2	D	6	LEU
2	D	23	THR
2	D	27	VAL
2	D	50	ARG
2	D	87	LEU
2	D	153	LEU
2	D	154	ASN
2	D	166	GLU
2	D	178	THR
2	D	183	GLU
2	D	185	LYS
2	D	186	LYS
2	D	215	ARG
2	D	222	GLN
2	D	232	ASN
2	D	257	LYS
2	D	261	THR
2	D	282	LYS
2	D	306	MET
2	D	324	ASN
2	D	332	LEU
2	D	366	LEU
2	D	376	GLN
2	D	379	LYS
1	E	4	ARG
1	E	5	THR
1	E	8	LYS
1	E	46	LEU
1	E	103	GLU
1	E	115	MET

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Mol	Chain	Res	Type
1	E	119	THR
1	E	153[A]	GLU
1	E	153[B]	GLU
1	E	174	MET
1	E	220	VAL
1	E	275	ILE
1	E	313	LYS
1	E	321	LYS
1	E	339	ILE
1	E	358	LYS
1	E	412	LYS
1	E	428	LEU
1	E	429	LYS
1	E	509	ARG
1	E	515	LYS
1	E	548	GLU
1	E	571	ARG
1	E	591	GLU
1	E	652	ARG
1	E	675	ARG
1	E	688	LYS
1	E	698	ILE
1	E	702	VAL
1	E	704	LYS
1	E	706	LYS
1	E	712	LEU
1	E	714	VAL
1	E	733	ASP
1	E	734	LEU
1	E	735	ARG
1	E	751	LEU
1	E	763	ASP
1	E	784	GLN
1	E	805	ILE
1	E	835	ASN
1	E	849	THR
1	E	876	GLU
1	E	906	LEU
1	E	912	ARG
1	E	940	LYS
1	E	950	ARG
1	E	951	GLU

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Mol	Chain	Res	Type
1	E	956	ARG
1	E	963	LYS
1	E	967[A]	GLN
1	E	967[B]	GLN
1	E	971	LEU
1	E	994	VAL
1	E	1000	HIS
1	E	1006	LYS
1	E	1014	ILE
1	E	1018	SER
1	E	1020	ARG
1	E	1021	ARG
1	E	1072	ILE
1	E	1073	LYS
2	F	2	ILE
2	F	6	LEU
2	F	18	ARG
2	F	73	SER
2	F	87	LEU
2	F	107	ILE
2	F	113	ILE
2	F	153	LEU
2	F	166	GLU
2	F	175	TRP
2	F	183	GLU
2	F	186	LYS
2	F	190	LEU
2	F	192	PHE
2	F	205	ILE
2	F	210	VAL
2	F	215	ARG
2	F	218	ILE
2	F	222	GLN
2	F	224	SER
2	F	227	ASP
2	F	253	THR
2	F	256	GLN
2	F	257	LYS
2	F	261	THR
2	F	263	ILE
2	F	282	LYS
2	F	301	GLU

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Mol	Chain	Res	Type
2	F	306	MET
2	F	321	LEU
2	F	324	ASN
2	F	332	LEU
2	F	366	LEU
2	F	376	GLN
2	F	379	LYS
1	G	1	MET
1	G	4	ARG
1	G	8	LYS
1	G	20	ILE
1	G	49	SER
1	G	55	MET
1	G	76	LYS
1	G	82	ARG
1	G	104	ARG
1	G	145	ARG
1	G	146	SER
1	G	185	ARG
1	G	202	LYS
1	G	207	ASP
1	G	236	ASN
1	G	303	ARG
1	G	313	LYS
1	G	321	LYS
1	G	326	LEU
1	G	339	ILE
1	G	412	LYS
1	G	416	ASP
1	G	422	THR
1	G	490	ARG
1	G	509	ARG
1	G	519	GLN
1	G	548	GLU
1	G	559	ARG
1	G	571	ARG
1	G	576	ILE
1	G	591	GLU
1	G	631	ARG
1	G	640	VAL
1	G	648	LEU
1	G	652	ARG

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Mol	Chain	Res	Type
1	G	673	GLU
1	G	675	ARG
1	G	682	VAL
1	G	688	LYS
1	G	692	ASN
1	G	704	LYS
1	G	706	LYS
1	G	712	LEU
1	G	714	VAL
1	G	733	ASP
1	G	734	LEU
1	G	735	ARG
1	G	751	LEU
1	G	752	LEU
1	G	772	MET
1	G	784	GLN
1	G	795	SER
1	G	805	ILE
1	G	811	GLN
1	G	812	GLN
1	G	845	ARG
1	G	849	THR
1	G	855	LYS
1	G	873	SER
1	G	876	GLU
1	G	880	THR
1	G	881	LYS
1	G	891	LYS
1	G	903	VAL
1	G	906	LEU
1	G	912	ARG
1	G	940	LYS
1	G	949	VAL
1	G	950	ARG
1	G	956	ARG
1	G	963	LYS
1	G	967	GLN
1	G	983	GLU
1	G	991	VAL
1	G	1001	ILE
1	G	1004	ARG
1	G	1006	LYS

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Mol	Chain	Res	Type
1	G	1021	ARG
1	G	1026	SER
1	G	1030	ARG
1	G	1061	LYS
1	G	1073	LYS
2	H	2	ILE
2	H	6	LEU
2	H	18	ARG
2	H	50	ARG
2	H	104	ARG
2	H	125	LYS
2	H	153	LEU
2	H	166	GLU
2	H	192	PHE
2	H	216	LEU
2	H	218	ILE
2	H	222	GLN
2	H	223	THR
2	H	257	LYS
2	H	263	ILE
2	H	282	LYS
2	H	301	GLU
2	H	306	MET
2	H	324	ASN
2	H	332	LEU
2	H	372	GLU
2	H	376	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	679	GLN
1	A	689	GLN
1	A	692	ASN
1	A	784	GLN
1	A	803	GLN
1	A	814	GLN
1	A	834	ASN
1	A	835	ASN
1	A	936	ASN
1	A	992	ASN

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Mol	Chain	Res	Type
1	A	1000	HIS
1	A	1007	ASN
1	A	1015	ASN
1	A	1035	GLN
1	A	1039	HIS
1	A	1055	ASN
2	B	51	GLN
2	B	78	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	105	GLN
1	C	266	ASN
1	C	391	GLN
1	C	457	ASN
1	C	645	GLN
1	C	679	GLN
1	C	689	GLN
1	C	784	GLN
1	C	803	GLN
1	C	812	GLN
1	C	827	ASN
1	C	843	ASN
1	C	898	ASN
1	C	936	ASN
1	C	942	HIS
1	C	987	ASN
1	C	992	ASN
1	C	995	HIS
1	C	1007	ASN
1	C	1015	ASN
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	154	ASN
2	D	222	GLN
2	D	273	GLN
2	D	324	ASN
1	E	105	GLN
1	E	266	ASN

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Mol	Chain	Res	Type
1	E	337	ASN
1	E	491	GLN
1	E	679	GLN
1	E	689	GLN
1	E	784	GLN
1	E	803	GLN
1	E	812	GLN
1	E	814	GLN
1	E	827	ASN
1	E	835	ASN
1	E	843	ASN
1	E	898	ASN
1	E	936	ASN
1	E	987	ASN
1	E	992	ASN
1	E	1000	HIS
1	E	1015	ASN
1	E	1035	GLN
1	E	1039	HIS
1	E	1055	ASN
1	E	1071	GLN
2	F	16	HIS
2	F	51	GLN
2	F	154	ASN
2	F	324	ASN
1	G	105	GLN
1	G	150	HIS
1	G	266	ASN
1	G	523	HIS
1	G	679	GLN
1	G	689	GLN
1	G	692	ASN
1	G	784	GLN
1	G	803	GLN
1	G	936	ASN
1	G	942	HIS
1	G	987	ASN
1	G	992	ASN
1	G	995	HIS
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN

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Mol	Chain	Res	Type
2	H	51	GLN
2	H	128	GLN
2	H	222	GLN
2	H	232	ASN
2	H	324	ASN
2	H	351	GLN
2	H	361	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	143	H	269	2	12,16,17	8.37	7 (58%)	5,21,23	7.02	2 (40%)
2	143	B	269	2	12,16,17	5.54	6 (50%)	5,21,23	7.36	3 (60%)
2	143	F	269	2	12,16,17	7.64	6 (50%)	5,21,23	6.89	3 (60%)
2	143	D	269	2	12,16,17	6.74	7 (58%)	5,21,23	6.93	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	143	H	269	2	1/1/5/8	3/9/24/26	0/1/1/1
2	143	B	269	2	1/1/5/8	4/9/24/26	0/1/1/1
2	143	F	269	2	1/1/5/8	4/9/24/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	143	D	269	2	1/1/5/8	3/9/24/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	269	143	CD-NX	-20.68	1.17	1.45
2	F	269	143	CD-NX	-19.40	1.19	1.45
2	D	269	143	CD-NX	-16.99	1.22	1.45
2	B	269	143	CD-NX	-13.21	1.27	1.45
2	H	269	143	CD-CE	-12.26	1.33	1.49
2	F	269	143	CD-SG	-12.02	1.62	1.82
2	H	269	143	CD-SG	-11.80	1.62	1.82
2	D	269	143	CD-SG	-10.70	1.64	1.82
2	B	269	143	CD-SG	-10.02	1.65	1.82
2	F	269	143	CB-SG	-8.35	1.73	1.82
2	H	269	143	CB-SG	-7.35	1.74	1.82
2	H	269	143	OJ2-CJ	7.28	1.43	1.22
2	F	269	143	CD-CE	-7.15	1.40	1.49
2	D	269	143	CB-SG	-6.92	1.75	1.82
2	B	269	143	CB-SG	-6.49	1.75	1.82
2	F	269	143	OJ2-CJ	6.43	1.41	1.22
2	D	269	143	CI-CF	5.74	1.54	1.50
2	D	269	143	OJ2-CJ	5.71	1.39	1.22
2	B	269	143	OJ2-CJ	4.92	1.36	1.22
2	D	269	143	CD-CE	-4.51	1.43	1.49
2	B	269	143	CI-CF	4.30	1.53	1.50
2	F	269	143	CI-CF	3.11	1.52	1.50
2	B	269	143	OJ1-CJ	2.41	1.38	1.30
2	H	269	143	CI-CF	2.27	1.51	1.50
2	H	269	143	OJ1-CJ	2.10	1.37	1.30
2	D	269	143	OJ1-CJ	2.08	1.37	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	143	CI-CF-CE	-15.77	113.57	133.64
2	D	269	143	CI-CF-CE	-15.14	114.36	133.64
2	H	269	143	CI-CF-CE	-14.76	114.85	133.64
2	F	269	143	CI-CF-CE	-13.55	116.39	133.64
2	F	269	143	OF-CF-CI	-6.85	107.98	116.06
2	H	269	143	OF-CF-CI	-4.87	110.31	116.06
2	B	269	143	OF-CF-CI	-3.43	112.01	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	143	OJ1-CJ-OJ2	-2.82	117.68	124.08
2	F	269	143	OJ1-CJ-OJ2	-2.43	118.57	124.08
2	D	269	143	OF-CF-CI	-2.25	113.40	116.06

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	269	143	CD
2	D	269	143	CD
2	F	269	143	CD
2	H	269	143	CD

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	269	143	N-CA-CB-SG
2	B	269	143	OF-CF-CI-CJ
2	D	269	143	N-CA-CB-SG
2	D	269	143	OF-CF-CI-CJ
2	F	269	143	N-CA-CB-SG
2	F	269	143	C-CA-CB-SG
2	F	269	143	OF-CF-CI-CJ
2	H	269	143	N-CA-CB-SG
2	H	269	143	C-CA-CB-SG
2	H	269	143	OF-CF-CI-CJ
2	B	269	143	NI-CI-CJ-OJ1
2	D	269	143	NI-CI-CJ-OJ1
2	F	269	143	NI-CI-CJ-OJ1
2	B	269	143	NI-CI-CJ-OJ2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	269	143	2	0
2	B	269	143	2	0
2	F	269	143	2	0
2	D	269	143	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	PO4	G	2071	3	4,4,4	2.13	2 (50%)	6,6,6	1.10	0
7	ADP	C	2023	3	28,29,29	1.66	5 (17%)	43,45,45	0.95	3 (6%)
8	ORN	C	5033	-	7,8,8	0.90	0	6,9,9	0.86	0
9	NET	G	5077	-	8,8,8	0.87	0	10,10,10	0.37	0
8	ORN	E	5055	-	7,8,8	0.97	0	6,9,9	1.29	1 (16%)
7	ADP	G	2066	3	28,29,29	1.25	5 (17%)	43,45,45	1.02	3 (6%)
9	NET	A	5012	-	8,8,8	0.68	0	10,10,10	0.55	0
8	ORN	G	5076	-	7,8,8	1.00	1 (14%)	6,9,9	0.79	0
7	ADP	A	2001	3	28,29,29	1.39	4 (14%)	43,45,45	1.04	3 (6%)
6	PO4	E	2050	3	4,4,4	2.06	3 (75%)	6,6,6	1.12	0
7	ADP	A	2007	3,4	28,29,29	1.26	3 (10%)	43,45,45	0.88	2 (4%)
9	NET	C	5034	-	8,8,8	0.63	0	10,10,10	0.48	0
7	ADP	C	2029	3,4	28,29,29	1.19	4 (14%)	43,45,45	1.06	3 (6%)
7	ADP	E	2051	3,4	28,29,29	1.20	4 (14%)	43,45,45	0.78	2 (4%)
8	ORN	A	5011	-	7,8,8	0.80	0	6,9,9	1.30	1 (16%)
7	ADP	E	2045	3	28,29,29	1.13	3 (10%)	43,45,45	0.96	2 (4%)
6	PO4	A	2006	3	4,4,4	1.90	2 (50%)	6,6,6	1.34	1 (16%)
9	NET	E	5056	-	8,8,8	0.83	0	10,10,10	0.37	0
6	PO4	C	2028	3	4,4,4	2.35	2 (50%)	6,6,6	1.03	0
7	ADP	G	2072	3,4	28,29,29	1.21	4 (14%)	43,45,45	1.03	3 (6%)

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	C	5033	-	-	7/8/8/8	-
7	ADP	E	2051	3,4	-	4/16/32/32	0/3/3/3
8	ORN	A	5011	-	-	5/8/8/8	-
7	ADP	A	2001	3	-	0/16/32/32	0/3/3/3
8	ORN	E	5055	-	-	6/8/8/8	-
9	NET	G	5077	-	-	3/12/12/12	-
7	ADP	C	2023	3	-	3/16/32/32	0/3/3/3
7	ADP	G	2066	3	-	0/16/32/32	0/3/3/3
9	NET	A	5012	-	-	11/12/12/12	-
7	ADP	E	2045	3	-	0/16/32/32	0/3/3/3
9	NET	E	5056	-	-	3/12/12/12	-
7	ADP	A	2007	3,4	-	3/16/32/32	0/3/3/3
8	ORN	G	5076	-	-	6/8/8/8	-
7	ADP	G	2072	3,4	-	3/16/32/32	0/3/3/3
9	NET	C	5034	-	-	0/12/12/12	-
7	ADP	C	2029	3,4	-	4/16/32/32	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2023	ADP	PA-O3A	-5.95	1.53	1.59
7	A	2007	ADP	PA-O3A	-3.71	1.55	1.59
7	A	2001	ADP	PA-O3A	-3.71	1.55	1.59
7	C	2029	ADP	O3'-C3'	3.28	1.51	1.43
6	C	2028	PO4	P-O4	-2.91	1.46	1.54
6	G	2071	PO4	P-O2	-2.86	1.46	1.54
7	G	2066	ADP	O2'-C2'	2.85	1.50	1.43
7	A	2001	ADP	O3'-C3'	2.82	1.49	1.43
7	C	2023	ADP	O3'-C3'	2.82	1.49	1.43
7	G	2066	ADP	PA-O3A	-2.81	1.56	1.59
7	G	2072	ADP	PA-O3A	-2.75	1.56	1.59
6	C	2028	PO4	P-O2	-2.68	1.46	1.54
7	E	2051	ADP	PA-O3A	-2.66	1.56	1.59
7	A	2001	ADP	O2'-C2'	2.56	1.49	1.43
7	E	2051	ADP	O2'-C2'	2.50	1.49	1.43
7	A	2007	ADP	C2-N3	-2.49	1.29	1.33
7	G	2066	ADP	O3'-C3'	2.41	1.48	1.43
6	E	2050	PO4	P-O3	-2.41	1.47	1.54
7	C	2023	ADP	O2'-C2'	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2006	PO4	P-O4	-2.36	1.47	1.54
8	G	5076	ORN	O-C	2.35	1.29	1.22
7	C	2029	ADP	O2'-C2'	2.34	1.48	1.43
6	E	2050	PO4	P-O4	-2.31	1.47	1.54
7	C	2029	ADP	PA-O3A	-2.31	1.57	1.59
7	G	2072	ADP	C2-N1	2.30	1.38	1.33
7	E	2045	ADP	O3'-C3'	2.29	1.48	1.43
7	E	2051	ADP	C2-N1	2.27	1.38	1.33
7	C	2023	ADP	C2-N1	2.20	1.37	1.33
6	A	2006	PO4	P-O3	-2.18	1.48	1.54
7	C	2023	ADP	O4'-C1'	-2.17	1.37	1.42
7	E	2045	ADP	O2'-C2'	2.16	1.48	1.43
7	A	2001	ADP	C2-N3	-2.15	1.30	1.33
7	G	2066	ADP	C2-N3	-2.15	1.30	1.33
7	E	2045	ADP	PA-O3A	-2.14	1.57	1.59
6	E	2050	PO4	P-O2	-2.14	1.48	1.54
7	A	2007	ADP	PB-O2B	-2.12	1.46	1.54
7	G	2066	ADP	C2-N1	2.11	1.37	1.33
7	C	2029	ADP	C2-N1	2.07	1.37	1.33
6	G	2071	PO4	P-O4	-2.07	1.48	1.54
7	E	2051	ADP	O3'-C3'	2.06	1.48	1.43
7	G	2072	ADP	O3'-C3'	2.04	1.48	1.43
7	G	2072	ADP	O2'-C2'	2.00	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	2072	ADP	O3B-PB-O3A	3.94	117.86	104.64
7	G	2066	ADP	O2'-C2'-C3'	3.22	122.15	111.82
7	C	2029	ADP	O2A-PA-O3A	3.22	115.97	107.27
7	G	2066	ADP	O3'-C3'-C2'	2.98	121.37	111.82
7	C	2029	ADP	O2'-C2'-C3'	2.88	121.06	111.82
7	G	2072	ADP	O2'-C2'-C3'	2.77	120.70	111.82
7	C	2029	ADP	O3'-C3'-C2'	2.76	120.67	111.82
6	A	2006	PO4	O4-P-O2	2.63	116.08	107.91
7	A	2007	ADP	O2B-PB-O3A	2.62	113.44	104.64
7	C	2023	ADP	O2'-C2'-C3'	2.57	120.04	111.82
7	E	2045	ADP	O2A-PA-O3A	2.54	114.14	107.27
7	C	2023	ADP	O3'-C3'-C2'	2.46	119.72	111.82
8	E	5055	ORN	OXT-C-O	-2.37	118.69	124.08
7	A	2001	ADP	N6-C6-N1	2.32	123.55	118.38
7	G	2066	ADP	O2A-PA-O3A	2.21	113.25	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2001	ADP	O2A-PA-O3A	2.21	113.25	107.27
8	A	5011	ORN	CB-CA-C	-2.19	104.64	110.45
7	E	2051	ADP	O3'-C3'-C2'	2.13	118.63	111.82
7	C	2023	ADP	C2'-C3'-C4'	-2.07	98.61	102.61
7	G	2072	ADP	O3'-C3'-C2'	2.07	118.45	111.82
7	A	2001	ADP	O2'-C2'-C3'	2.03	118.33	111.82
7	E	2045	ADP	O2'-C2'-C3'	2.01	118.25	111.82
7	A	2007	ADP	C3'-C2'-C1'	2.01	105.26	101.46
7	E	2051	ADP	C2'-C3'-C4'	-2.00	98.74	102.61

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2007	ADP	PA-O3A-PB-O3B
7	C	2029	ADP	PA-O3A-PB-O3B
7	E	2051	ADP	PA-O3A-PB-O3B
8	A	5011	ORN	N-CA-CB-CG
8	A	5011	ORN	C-CA-CB-CG
8	C	5033	ORN	N-CA-CB-CG
8	C	5033	ORN	C-CA-CB-CG
8	E	5055	ORN	N-CA-CB-CG
8	E	5055	ORN	C-CA-CB-CG
8	G	5076	ORN	N-CA-CB-CG
8	G	5076	ORN	C-CA-CB-CG
8	G	5076	ORN	O-C-CA-N
9	A	5012	NET	C4-C3-N1-C1
9	A	5012	NET	C4-C3-N1-C7
9	A	5012	NET	C4-C3-N1-C5
9	A	5012	NET	C8-C7-N1-C3
8	C	5033	ORN	OXT-C-CA-N
9	A	5012	NET	C8-C7-N1-C1
9	A	5012	NET	C8-C7-N1-C5
8	G	5076	ORN	OXT-C-CA-N
8	E	5055	ORN	CA-CB-CG-CD
7	E	2051	ADP	PA-O3A-PB-O1B
7	G	2072	ADP	PA-O3A-PB-O1B
9	G	5077	NET	C4-C3-N1-C1
8	G	5076	ORN	CA-CB-CG-CD
8	C	5033	ORN	CA-CB-CG-CD
8	A	5011	ORN	O-C-CA-N
8	C	5033	ORN	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
8	E	5055	ORN	O-C-CA-N
9	E	5056	NET	C4-C3-N1-C7
9	G	5077	NET	C4-C3-N1-C7
9	A	5012	NET	C6-C5-N1-C3
9	G	5077	NET	C4-C3-N1-C5
9	E	5056	NET	C4-C3-N1-C5
7	A	2007	ADP	PB-O3A-PA-O2A
7	C	2023	ADP	PB-O3A-PA-O1A
9	A	5012	NET	C6-C5-N1-C1
9	E	5056	NET	C4-C3-N1-C1
8	A	5011	ORN	NE-CD-CG-CB
8	C	5033	ORN	NE-CD-CG-CB
8	G	5076	ORN	NE-CD-CG-CB
8	E	5055	ORN	O-C-CA-CB
7	C	2023	ADP	C5'-O5'-PA-O1A
9	A	5012	NET	C6-C5-N1-C7
7	C	2029	ADP	PB-O3A-PA-O2A
7	E	2051	ADP	PB-O3A-PA-O2A
8	A	5011	ORN	CA-CB-CG-CD
7	A	2007	ADP	PA-O3A-PB-O1B
7	G	2072	ADP	PB-O3A-PA-O2A
7	C	2029	ADP	PA-O3A-PB-O1B
8	E	5055	ORN	OXT-C-CA-N
8	C	5033	ORN	O-C-CA-CB
9	A	5012	NET	C2-C1-N1-C5
9	A	5012	NET	C2-C1-N1-C7
7	C	2023	ADP	PB-O3A-PA-O2A
7	C	2029	ADP	PB-O3A-PA-O1A
7	E	2051	ADP	PB-O3A-PA-O1A
7	G	2072	ADP	PB-O3A-PA-O1A

There are no ring outliers.

14 monomers are involved in 21 short contacts:

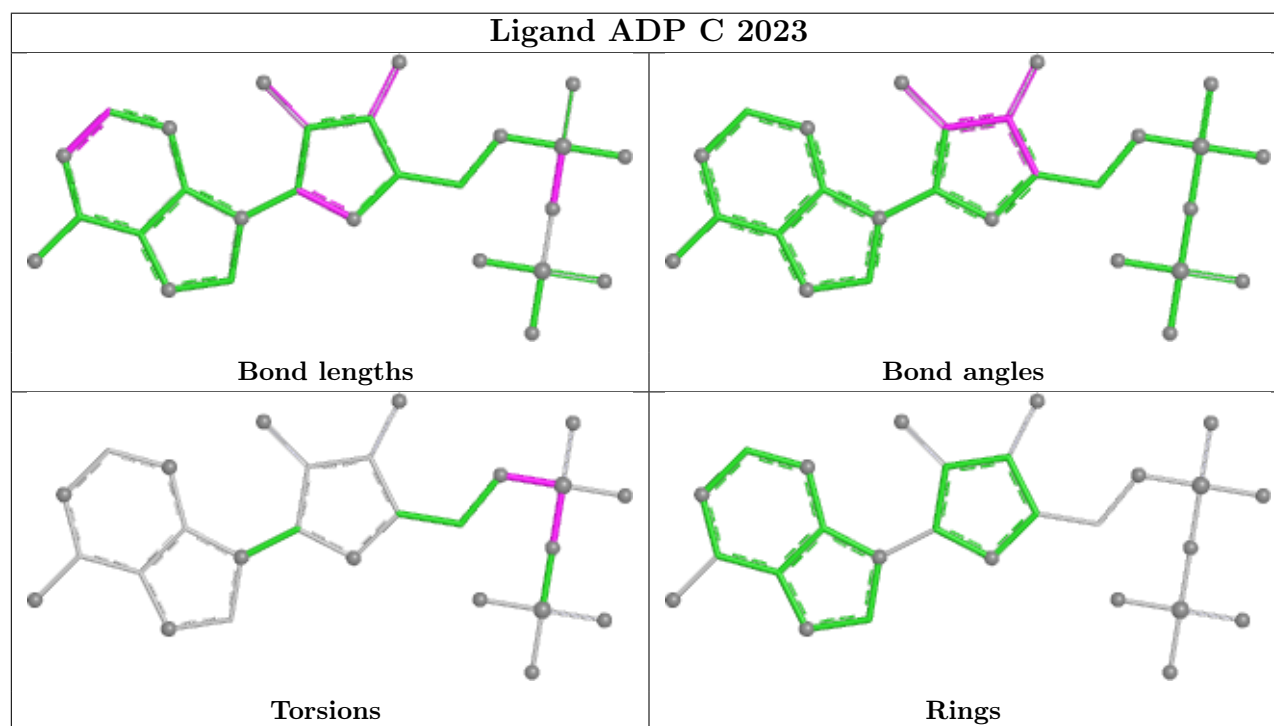
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	2071	PO4	1	0
7	C	2023	ADP	1	0
8	C	5033	ORN	1	0
9	G	5077	NET	1	0
8	E	5055	ORN	1	0
7	G	2066	ADP	1	0
9	A	5012	NET	4	0

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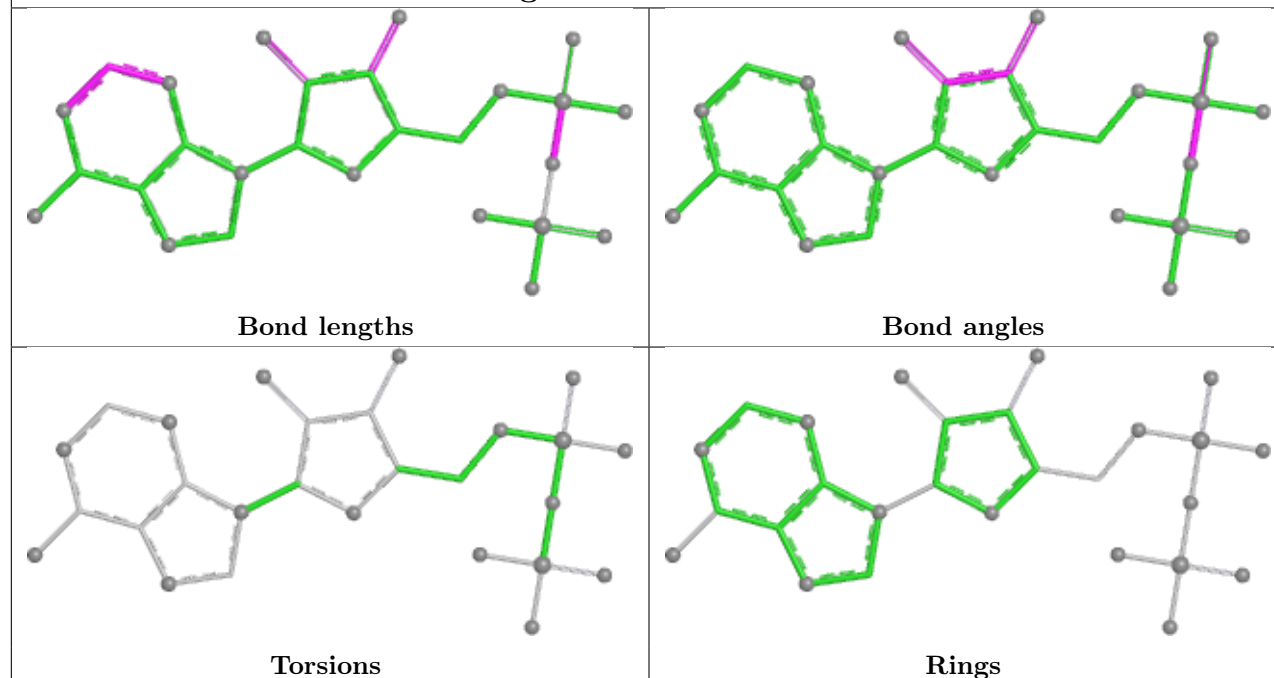
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	5076	ORN	2	0
7	A	2001	ADP	1	0
7	E	2051	ADP	2	0
7	E	2045	ADP	2	0
9	E	5056	NET	1	0
6	C	2028	PO4	1	0
7	G	2072	ADP	2	0

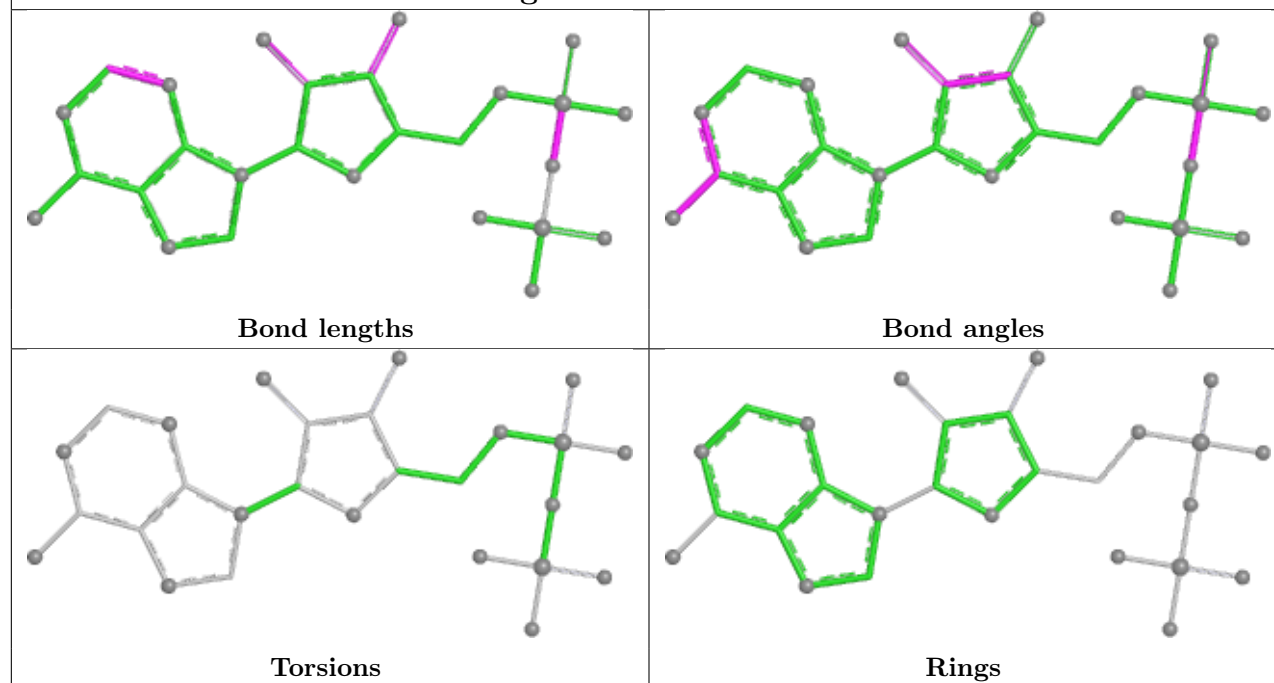
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



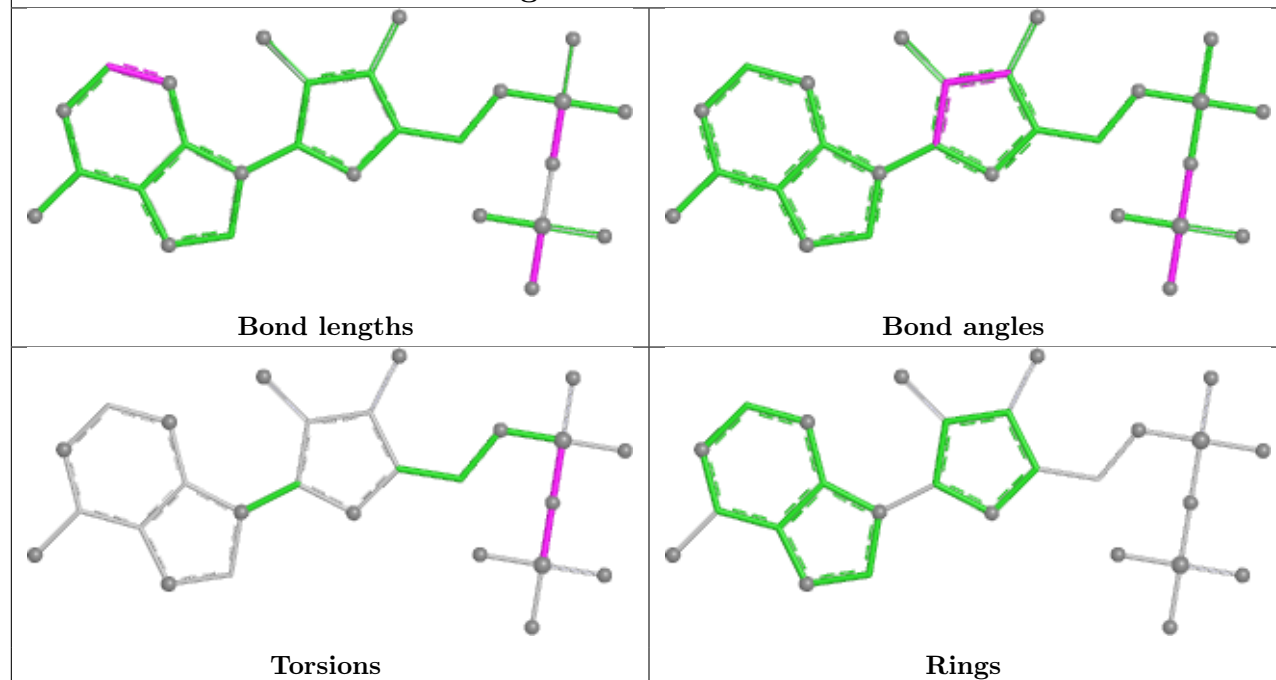
Ligand ADP G 2066



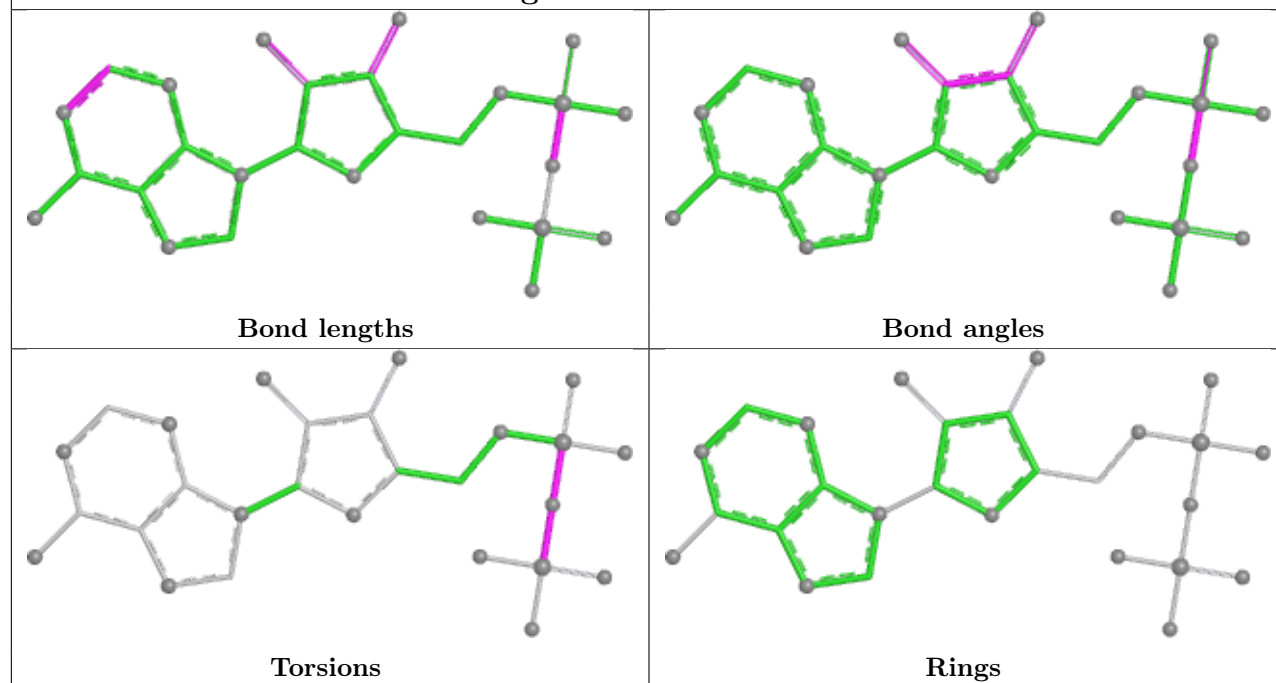
Ligand ADP A 2001

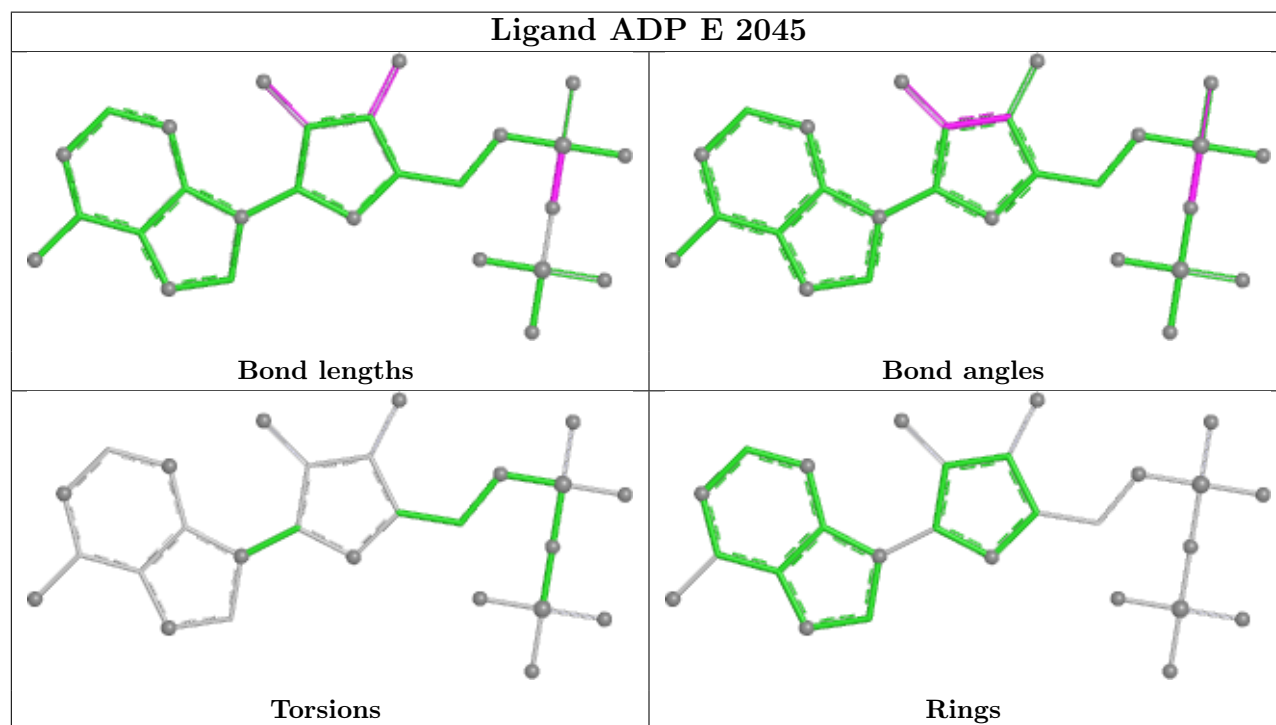
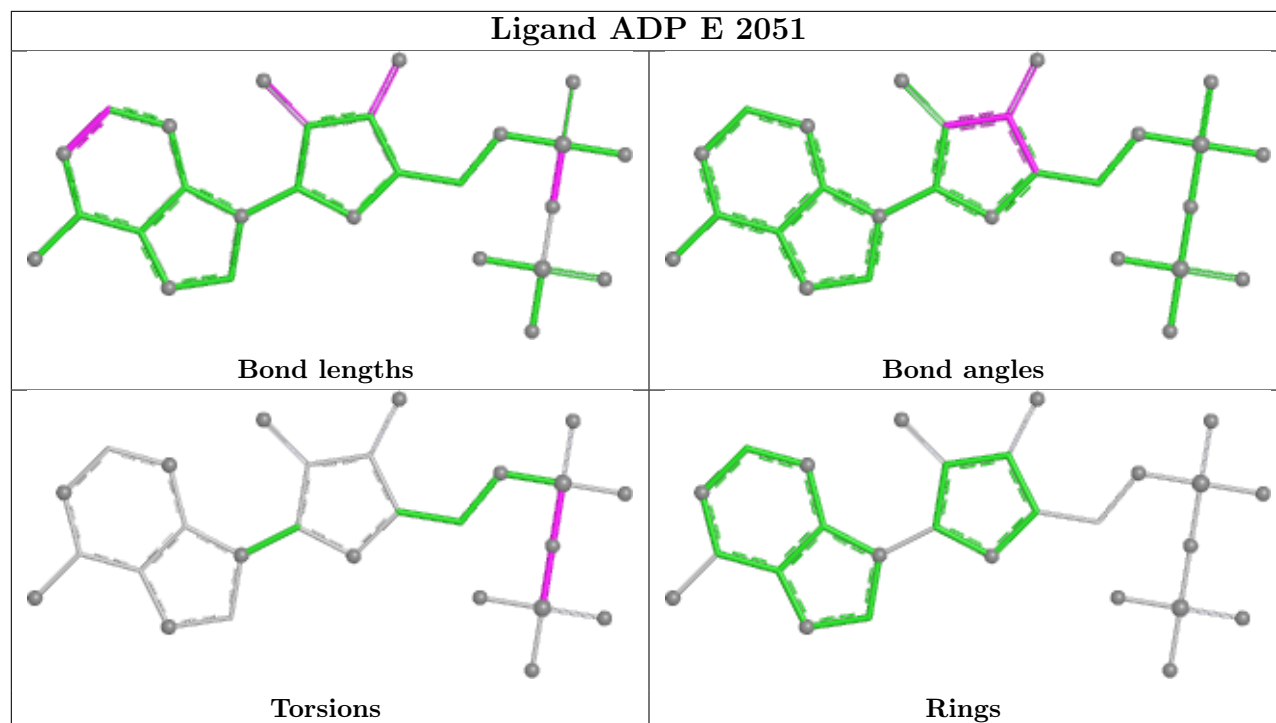


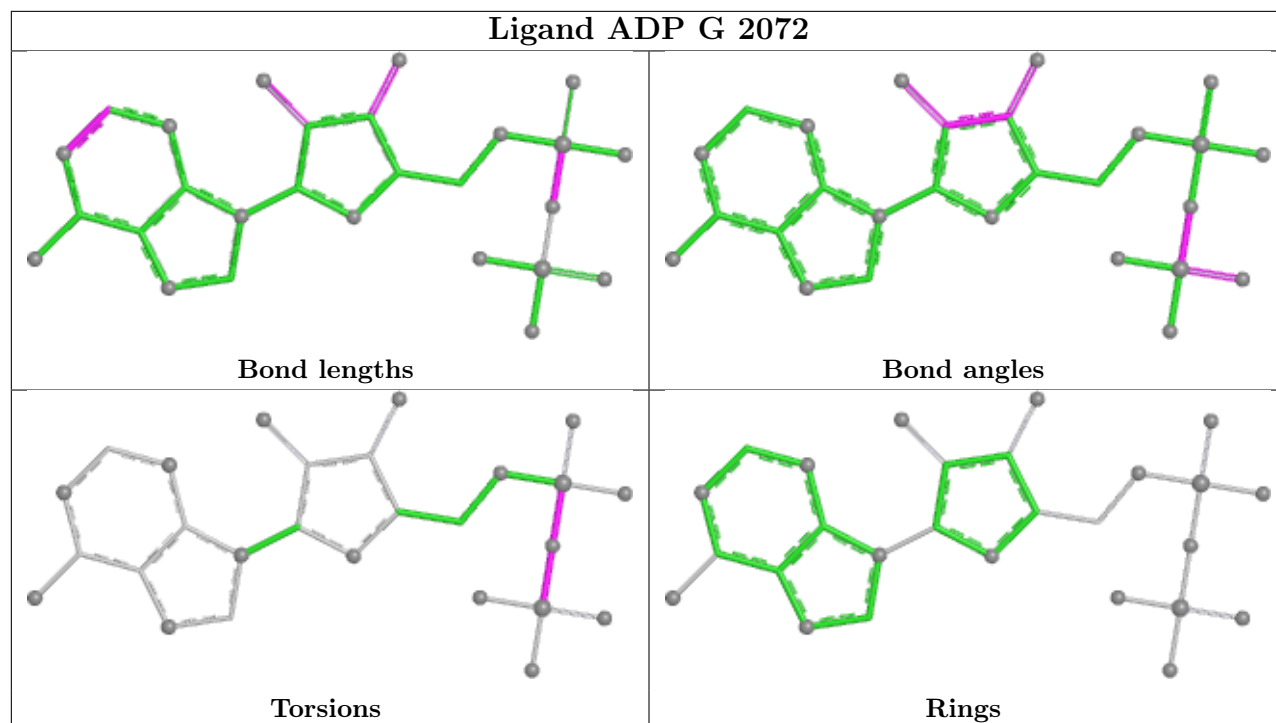
Ligand ADP A 2007



Ligand ADP C 2029







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	1058/1073 (98%)	-0.25	43 (4%)	41	43	15, 32, 80, 100	5 (0%)
1	C	1058/1073 (98%)	-0.29	29 (2%)	56	59	15, 33, 81, 100	2 (0%)
1	E	1058/1073 (98%)	-0.36	35 (3%)	49	51	16, 29, 81, 100	8 (0%)
1	G	1058/1073 (98%)	-0.06	41 (3%)	43	45	16, 37, 87, 100	0
2	B	378/382 (98%)	-0.15	4 (1%)	78	80	19, 40, 75, 100	1 (0%)
2	D	378/382 (98%)	-0.31	3 (0%)	82	84	18, 33, 63, 92	1 (0%)
2	F	378/382 (98%)	-0.15	4 (1%)	78	80	18, 35, 74, 99	0
2	H	378/382 (98%)	0.13	6 (1%)	70	73	25, 45, 78, 98	0
All	All	5744/5820 (98%)	-0.21	165 (2%)	53	56	15, 34, 80, 100	17 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	693	ALA	5.9
1	A	750	VAL	5.6
1	A	729	TYR	5.5
1	A	716	PRO	5.4
1	A	710	TYR	5.2
1	G	1	MET	5.2
1	A	1	MET	4.9
1	C	738	PHE	4.9
1	A	738	PHE	4.7
1	A	714	VAL	4.7
1	A	999	PRO	4.5
1	G	678	PHE	4.4
1	A	752	LEU	4.3
1	C	999	PRO	4.3
1	A	46	LEU	4.2
1	C	695	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	698	ILE	4.1
1	E	2	PRO	4.1
1	E	1	MET	4.0
1	C	750	VAL	4.0
1	C	729	TYR	4.0
1	E	750	VAL	4.0
1	G	729	TYR	3.9
1	A	728	VAL	3.9
1	G	738	PHE	3.9
1	A	724	ALA	3.8
1	A	695	VAL	3.8
1	E	738	PHE	3.7
2	D	2	ILE	3.7
1	E	729	TYR	3.7
1	E	46	LEU	3.6
1	A	751	LEU	3.6
1	G	750	VAL	3.6
1	A	712	LEU	3.6
1	E	751	LEU	3.6
1	A	368	ALA	3.5
1	G	751	LEU	3.5
1	G	714	VAL	3.5
2	B	2	ILE	3.5
1	G	694	THR	3.5
1	E	695	VAL	3.4
1	A	737	TYR	3.4
2	F	195	VAL	3.4
1	C	698	ILE	3.4
1	C	709	GLY	3.3
1	G	162	VAL	3.3
1	E	368	ALA	3.3
1	C	1	MET	3.3
1	A	727	ILE	3.3
1	E	728	VAL	3.2
1	A	678	PHE	3.2
1	A	679	GLN	3.2
1	C	725	MET	3.2
1	E	740	THR	3.2
1	A	739	GLN	3.2
1	E	1001	ILE	3.2
1	A	694	THR	3.1
1	A	732	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	695	VAL	3.1
1	C	710	TYR	3.1
1	E	732	ALA	3.1
1	C	724	ALA	3.0
1	G	368	ALA	3.0
1	A	680	HIS	3.0
1	G	188	PHE	3.0
1	A	741	ALA	3.0
1	E	741	ALA	3.0
1	G	46	LEU	3.0
2	H	188	ASP	3.0
1	E	724	ALA	2.9
1	A	844	PRO	2.9
1	E	737	TYR	2.9
1	G	183	TYR	2.9
1	G	740	THR	2.9
2	F	2	ILE	2.9
1	G	734	LEU	2.8
1	A	725	MET	2.8
1	A	696	THR	2.8
1	G	5	THR	2.8
1	A	736	ARG	2.8
2	H	319	ALA	2.8
1	A	740	THR	2.8
1	C	677	ARG	2.8
1	E	675	ARG	2.8
1	C	678	PHE	2.8
1	C	694	THR	2.8
2	B	380	THR	2.8
1	C	740	THR	2.7
1	C	716	PRO	2.7
1	G	715	ARG	2.7
1	E	710	TYR	2.7
1	C	751	LEU	2.7
1	E	418	PRO	2.7
2	H	232	ASN	2.6
2	F	377	TYR	2.6
2	H	2	ILE	2.6
1	G	716	PRO	2.6
1	G	724	ALA	2.6
1	E	716	PRO	2.6
1	C	736	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	696	THR	2.6
1	E	1018	SER	2.5
1	E	673	GLU	2.5
1	A	700	MET	2.5
1	G	710	TYR	2.5
1	C	730	ASP	2.5
1	A	730	ASP	2.5
1	A	697	ALA	2.5
1	E	518	ASP	2.4
1	G	693	ALA	2.4
1	C	733	ASP	2.4
1	E	998[A]	ARG	2.4
2	D	141	ALA	2.4
1	E	342	GLY	2.4
1	G	179	GLY	2.4
1	A	726	GLU	2.4
1	E	694	THR	2.4
1	E	954	LYS	2.4
2	H	233	PRO	2.4
1	A	701	ALA	2.4
1	A	117	GLY	2.4
1	E	730	ASP	2.4
1	A	711	PRO	2.4
1	G	170	PRO	2.4
1	G	737	TYR	2.3
1	G	732	ALA	2.3
1	E	739	GLN	2.3
1	G	184	ASN	2.3
1	A	559	ARG	2.3
1	G	1001	ILE	2.3
1	G	158	VAL	2.3
1	C	711	PRO	2.3
1	C	737	TYR	2.3
1	E	1007	ASN	2.3
2	D	380	THR	2.3
2	B	319	ALA	2.3
1	E	198	LEU	2.3
2	B	379	LYS	2.3
1	C	994	VAL	2.3
1	C	732	ALA	2.3
1	C	46	LEU	2.3
1	E	703	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	191	ILE	2.2
1	A	675	ARG	2.2
1	G	954	LYS	2.2
1	C	368	ALA	2.2
1	A	734	LEU	2.2
1	E	698	ILE	2.2
2	F	366	LEU	2.2
1	G	991	VAL	2.2
1	G	160	ALA	2.2
1	G	205	LEU	2.2
1	G	1020	ARG	2.1
1	G	733	ASP	2.1
1	G	164	PHE	2.1
1	E	727	ILE	2.1
2	H	288	PHE	2.1
1	E	118	ALA	2.1
1	G	157	ALA	2.1
1	G	199	SER	2.1
1	G	741	ALA	2.1
1	C	884	ILE	2.0
1	G	840	ILE	2.0
1	C	680	HIS	2.0
1	A	5	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	143	H	269	16/17	0.89	0.15	29,71,100,100	0
2	143	F	269	16/17	0.90	0.13	25,46,100,100	0
2	143	B	269	16/17	0.90	0.12	34,46,87,90	0
2	143	D	269	16/17	0.95	0.09	21,32,100,100	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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(Å ²)	Q<0.9
4	K	C	5031	1/1	0.95	0.06	52,52,52,52	0
4	K	E	5057	1/1	0.95	0.07	59,59,59,59	0
5	CL	A	5020	1/1	0.95	0.10	61,61,61,61	0
8	ORN	A	5011	9/9	0.95	0.07	21,24,31,40	0
9	NET	G	5077	9/9	0.95	0.10	23,39,55,64	0
5	CL	C	5042	1/1	0.96	0.09	55,55,55,55	0
5	CL	E	5062	1/1	0.96	0.09	59,59,59,59	0
5	CL	G	5084	1/1	0.96	0.13	65,65,65,65	0
6	PO4	A	2006	5/5	0.96	0.08	22,25,39,50	0
4	K	A	5009	1/1	0.96	0.07	38,38,38,38	0
8	ORN	C	5033	9/9	0.96	0.07	12,21,37,46	0
8	ORN	G	5076	9/9	0.96	0.08	18,27,35,49	0
9	NET	A	5012	9/9	0.96	0.07	20,29,37,45	0
9	NET	E	5056	9/9	0.96	0.08	19,29,41,43	0
4	K	C	5035	1/1	0.96	0.07	48,48,48,48	0
6	PO4	G	2071	5/5	0.97	0.07	20,28,40,56	0
5	CL	A	5022	1/1	0.97	0.13	74,74,74,74	0
4	K	A	5015	1/1	0.97	0.07	54,54,54,54	0
8	ORN	E	5055	9/9	0.97	0.07	21,23,35,53	0
4	K	G	5074	1/1	0.97	0.10	67,67,67,67	0
4	K	H	5081	1/1	0.97	0.08	57,57,57,57	0
5	CL	G	5085	1/1	0.97	0.09	68,68,68,68	0
4	K	C	5037	1/1	0.97	0.10	62,62,62,62	0
4	K	E	5058	1/1	0.98	0.20	53,53,53,53	0
5	CL	E	5064	1/1	0.98	0.06	54,54,54,54	0
5	CL	G	5082	1/1	0.98	0.05	39,39,39,39	0
5	CL	G	5083	1/1	0.98	0.06	40,40,40,40	0
4	K	E	5059	1/1	0.98	0.05	43,43,43,43	0
4	K	C	5036	1/1	0.98	0.14	56,56,56,56	0
5	CL	H	5086	1/1	0.98	0.05	47,47,47,47	0
4	K	G	5079	1/1	0.98	0.26	71,71,71,71	0
6	PO4	E	2050	5/5	0.98	0.10	22,25,48,48	0
4	K	G	5080	1/1	0.98	0.05	43,43,43,43	0
7	ADP	A	2007	27/27	0.98	0.05	17,26,37,45	0
7	ADP	C	2029	27/27	0.98	0.05	16,35,60,82	0
7	ADP	E	2051	27/27	0.98	0.05	20,32,49,89	0
7	ADP	G	2072	27/27	0.98	0.06	24,38,60,83	0

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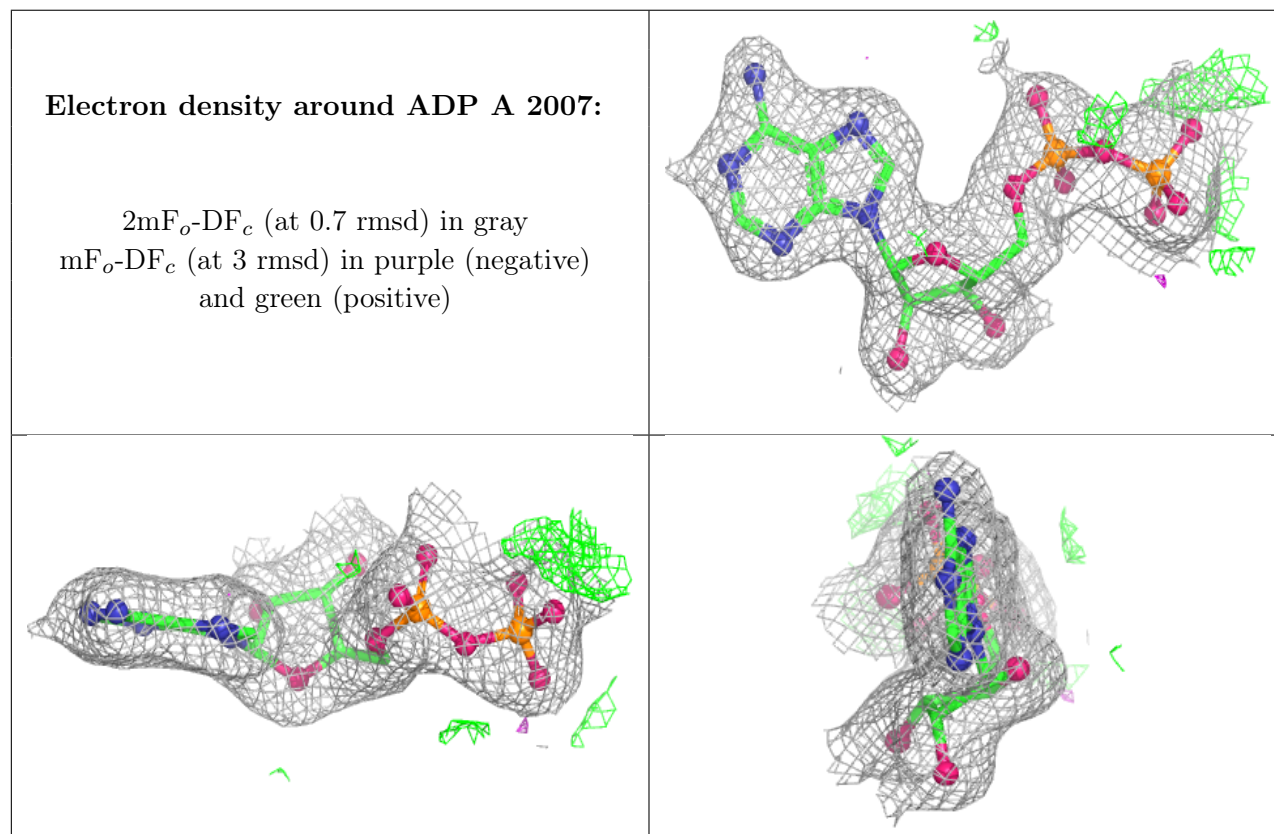
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	A	5014	1/1	0.98	0.16	52,52,52,52	0
4	K	D	5038	1/1	0.98	0.04	37,37,37,37	0
4	K	E	5053	1/1	0.98	0.04	51,51,51,51	0
5	CL	C	5040	1/1	0.98	0.04	35,35,35,35	0
4	K	A	5013	1/1	0.98	0.07	59,59,59,59	0
9	NET	C	5034	9/9	0.98	0.05	17,19,27,30	0
5	CL	C	5044	1/1	0.98	0.16	39,39,39,39	0
5	CL	D	5043	1/1	0.98	0.05	30,30,30,30	0
5	CL	F	5065	1/1	0.99	0.03	31,31,31,31	0
3	MN	G	2067	1/1	0.99	0.03	36,36,36,36	0
4	K	G	5078	1/1	0.99	0.05	54,54,54,54	0
3	MN	G	2073	1/1	0.99	0.02	42,42,42,42	0
4	K	A	5005	1/1	0.99	0.02	27,27,27,27	0
4	K	E	2048	1/1	0.99	0.03	24,24,24,24	0
5	CL	A	5017	1/1	0.99	0.03	29,29,29,29	0
6	PO4	C	2028	5/5	0.99	0.06	13,16,31,35	0
5	CL	A	5018	1/1	0.99	0.04	34,34,34,34	0
5	CL	A	5019	1/1	0.99	0.06	40,40,40,40	0
7	ADP	A	2001	27/27	0.99	0.04	16,25,33,41	0
4	K	E	5049	1/1	0.99	0.02	30,30,30,30	0
7	ADP	C	2023	27/27	0.99	0.04	13,21,23,26	0
4	K	B	5016	1/1	0.99	0.05	45,45,45,45	0
7	ADP	E	2045	27/27	0.99	0.04	16,27,43,64	0
5	CL	B	5021	1/1	0.99	0.03	33,33,33,33	0
7	ADP	G	2066	27/27	0.99	0.04	15,21,36,38	0
4	K	E	5054	1/1	0.99	0.02	24,24,24,24	0
5	CL	C	5041	1/1	0.99	0.03	36,36,36,36	0
4	K	C	5027	1/1	0.99	0.02	29,29,29,29	0
3	MN	C	2024	1/1	0.99	0.02	28,28,28,28	0
4	K	A	5010	1/1	0.99	0.03	24,24,24,24	0
5	CL	E	5061	1/1	0.99	0.03	30,30,30,30	0
4	K	G	2069	1/1	0.99	0.02	23,23,23,23	0
5	CL	E	5063	1/1	0.99	0.03	45,45,45,45	0
4	K	G	5070	1/1	0.99	0.03	36,36,36,36	0
3	MN	C	2030	1/1	1.00	0.01	38,38,38,38	0
3	MN	E	2046	1/1	1.00	0.02	34,34,34,34	0
3	MN	E	2047	1/1	1.00	0.02	27,27,27,27	0
3	MN	E	2052	1/1	1.00	0.01	34,34,34,34	0
3	MN	A	2003	1/1	1.00	0.02	25,25,25,25	0
4	K	C	5026	1/1	1.00	0.03	18,18,18,18	0
3	MN	G	2068	1/1	1.00	0.01	25,25,25,25	0
3	MN	A	5008	1/1	1.00	0.02	28,28,28,28	0

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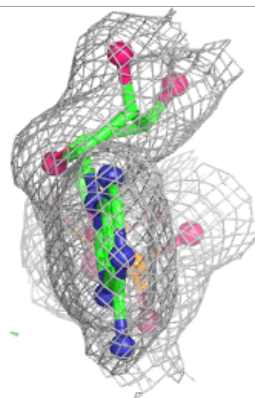
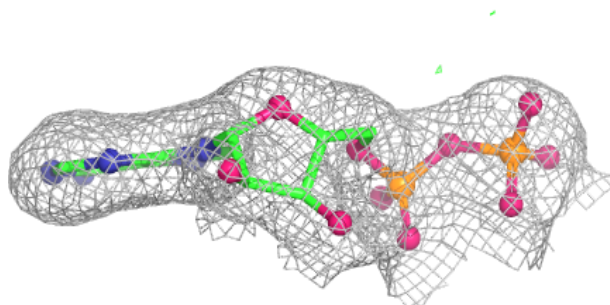
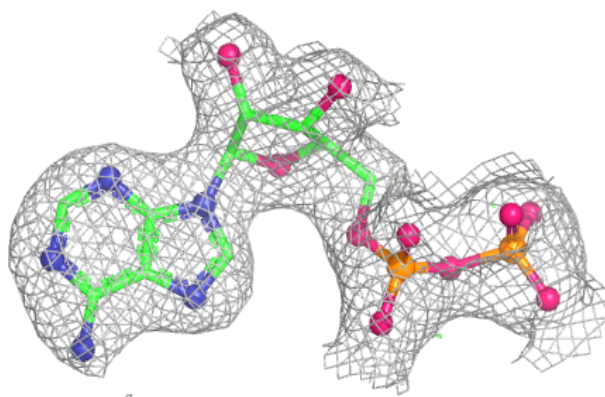
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	F	5060	1/1	1.00	0.03	42,42,42,42	0
5	CL	C	5039	1/1	1.00	0.02	27,27,27,27	0
4	K	C	5032	1/1	1.00	0.03	31,31,31,31	0
4	K	A	5004	1/1	1.00	0.02	24,24,24,24	0
3	MN	A	2002	1/1	1.00	0.01	31,31,31,31	0
4	K	G	5075	1/1	1.00	0.01	29,29,29,29	0
3	MN	C	2025	1/1	1.00	0.01	22,22,22,22	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.

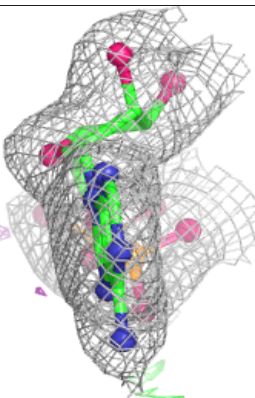
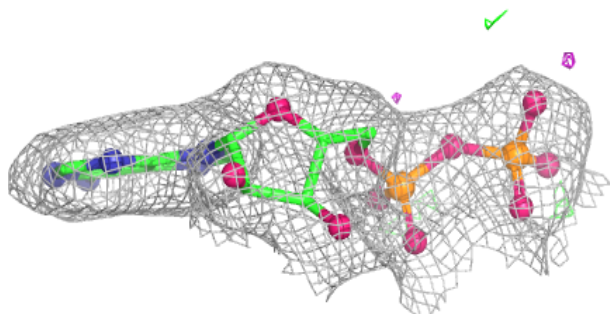
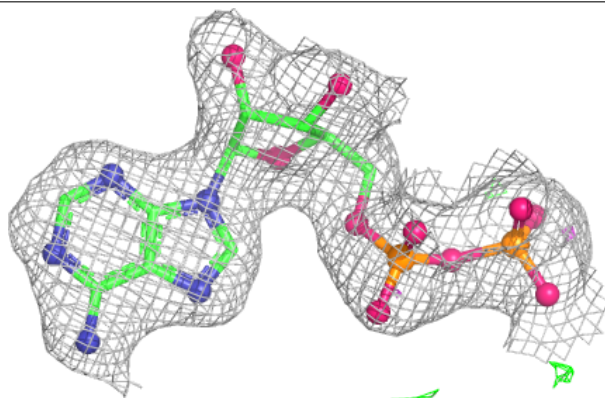


Electron density around ADP C 2029:

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

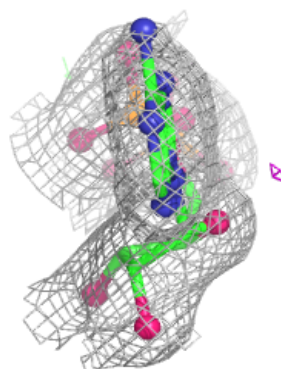
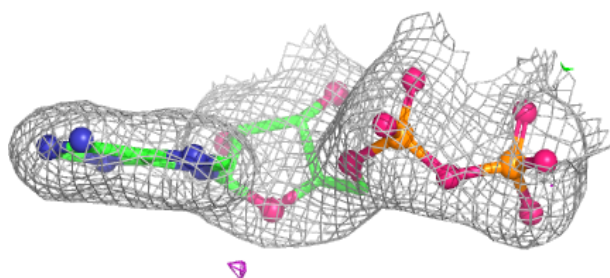
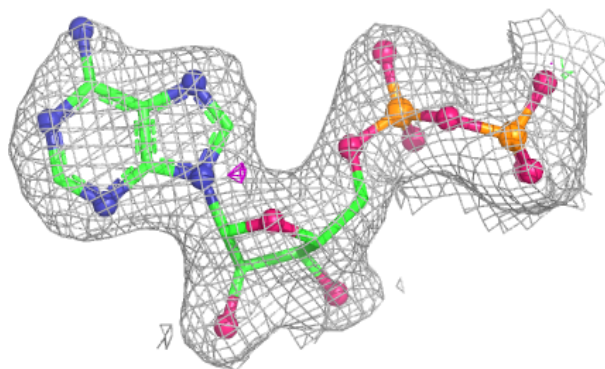
**Electron density around ADP E 2051:**

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

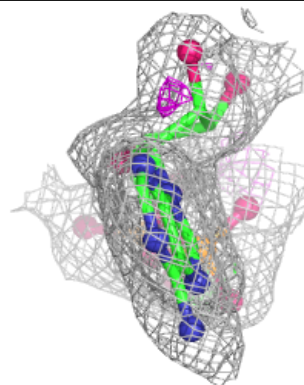
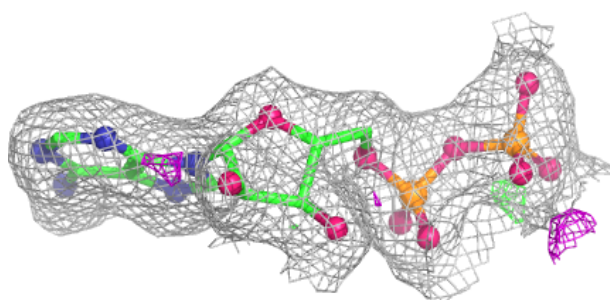
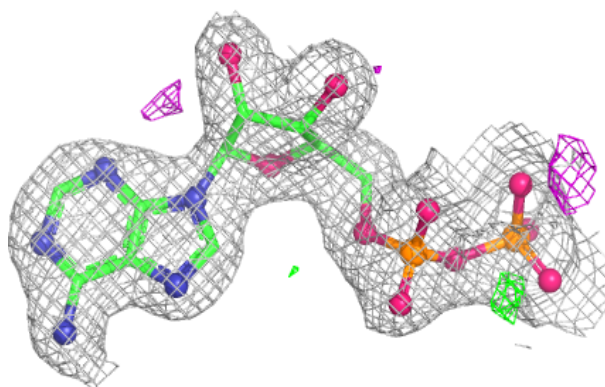


Electron density around ADP G 2072:

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

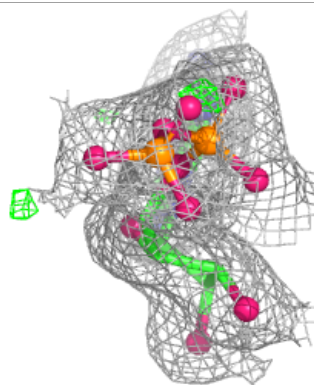
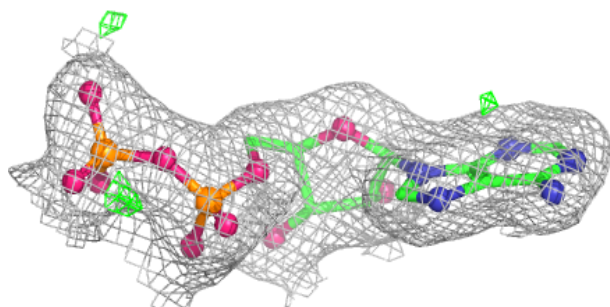
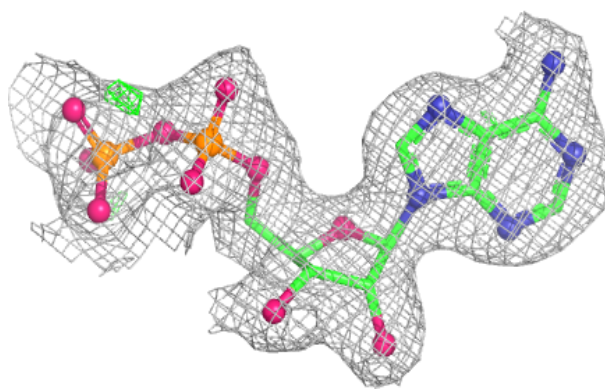
**Electron density around ADP A 2001:**

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

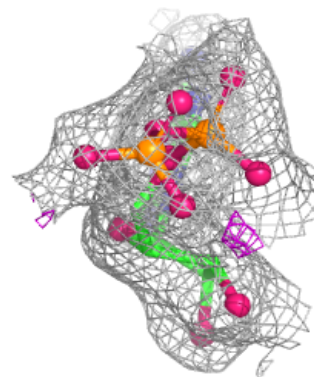
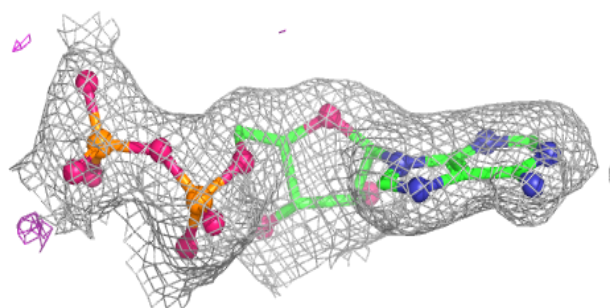
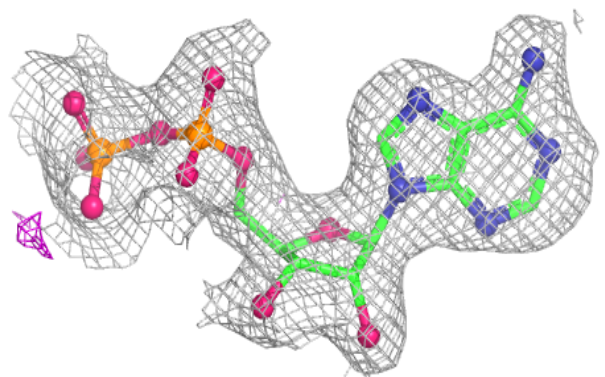


Electron density around ADP C 2023:

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

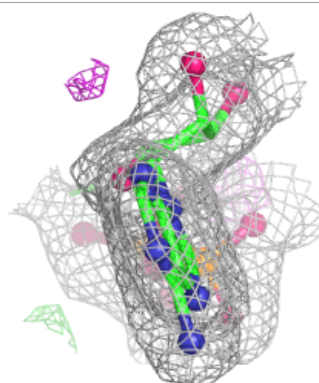
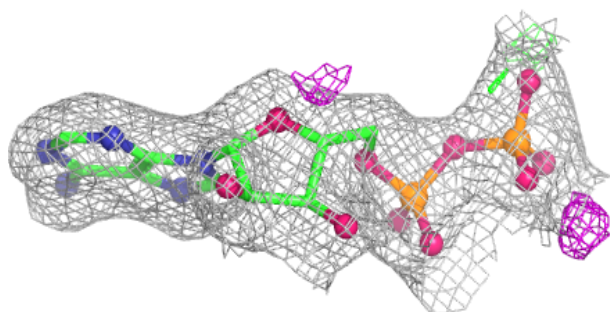
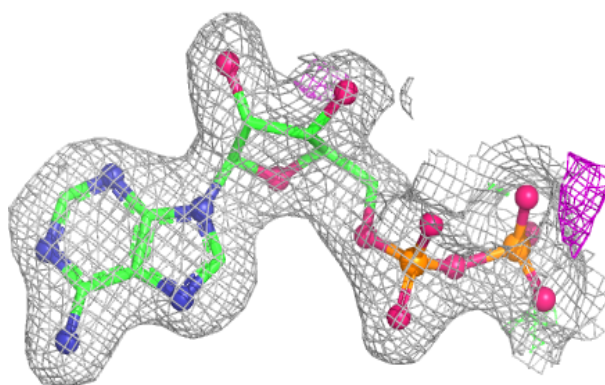
**Electron density around ADP E 2045:**

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



Electron density around ADP G 2066:

$2mF_o - DF_c$ (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.