Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 10:52 PM EST

PDB ID	:	1J1Z
Title	:	Crystal Structure of Thermus thermophilus HB8 Argininosuccinate Synthetase in complex with substrate
Authors	:	Goto, M.; Hirotsu, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2002-12-24
Resolution	:	2.10 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.251
Clashscore		15
Ramachandran outliers		0.3%
Sidechain outliers		4.7%
RSRZ outliers		2.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
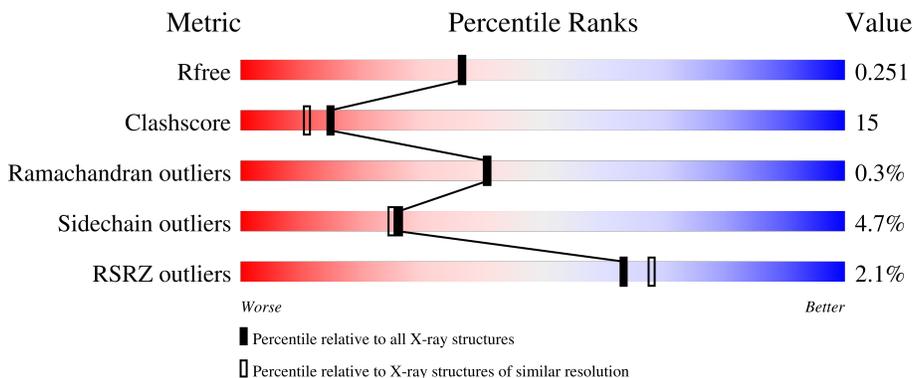
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	400	2% 72% 22% · ·
1	B	400	2% 72% 22% · ·
1	C	400	3% 67% 28% · ·
1	D	400	2% 69% 25% · ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13150 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 Argininosuccinate Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3066	1963	533	561	9			
1	B	386	Total	C	N	O	S	0	0	0
			3066	1963	533	561	9			
1	C	386	Total	C	N	O	S	0	0	0
			3066	1963	533	561	9			
1	D	386	Total	C	N	O	S	0	0	0
			3066	1963	533	561	9			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 3 is CITRULLINE (three-letter code: CIR) (formula: $C_6H_{13}N_3O_3$).

CIR
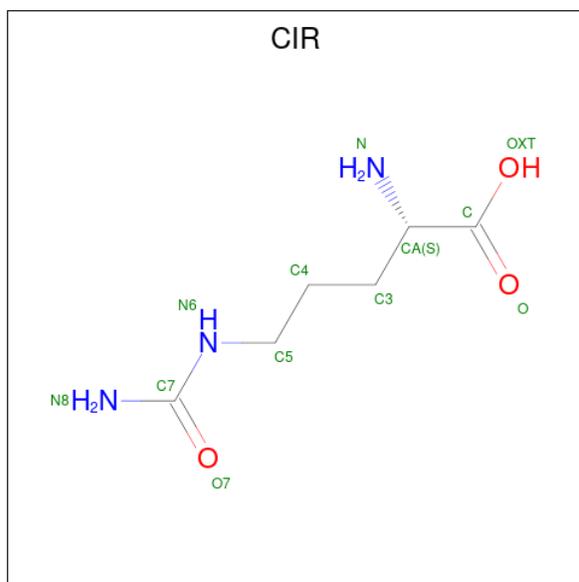
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 12	C 6	N 3	O 3	0	0
3	B	1	Total 12	C 6	N 3	O 3	0	0
3	C	1	Total 12	C 6	N 3	O 3	0	0
3	D	1	Total 12	C 6	N 3	O 3	0	0

- Molecule 4 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).
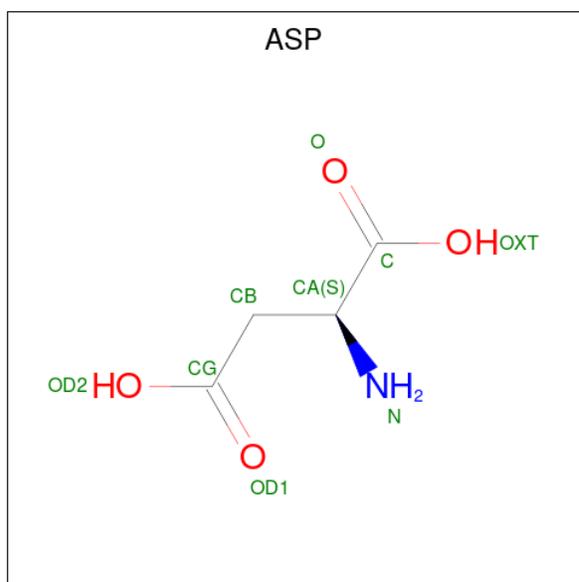
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total C N O				0	0
			9 4 1 4					
4	A	1	Total C N O				0	0
			9 4 1 4					
4	A	1	Total C N O				0	0
			9 4 1 4					
4	A	1	Total C N O				0	0
			9 4 1 4					

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total O		0	0
			186 186			
5	B	186	Total O		0	0
			186 186			
5	C	149	Total O		0	0
			149 149			
5	D	157	Total O		0	0
			157 157			

3 Residue-property plots (i)

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: Argininosuccinate Synthetase
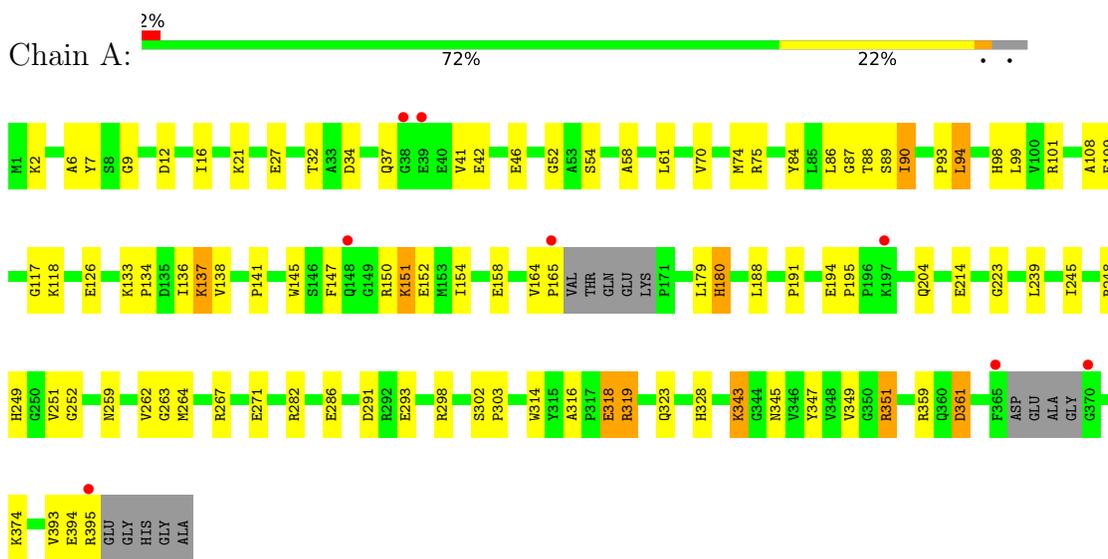
Chain A:

• Molecule 1: Argininosuccinate Synthetase

Chain B:

• Molecule 1: Argininosuccinate Synthetase

Chain C:
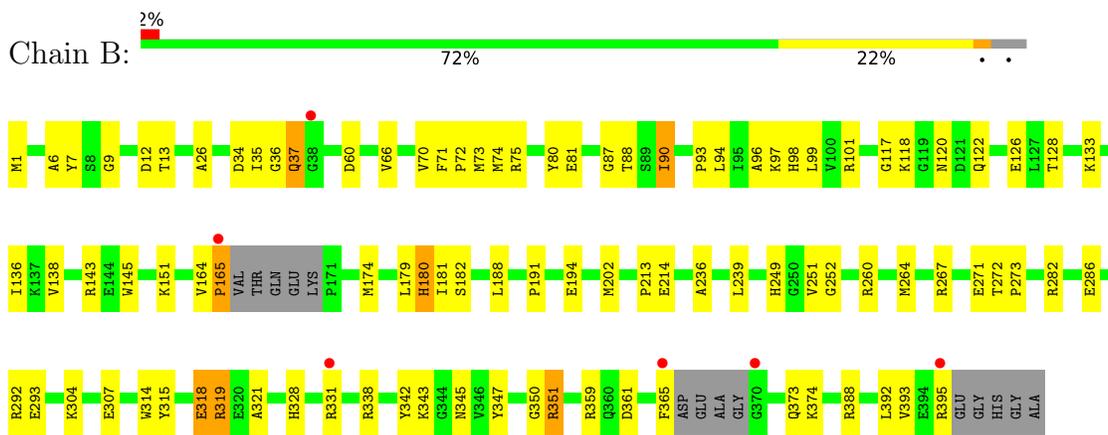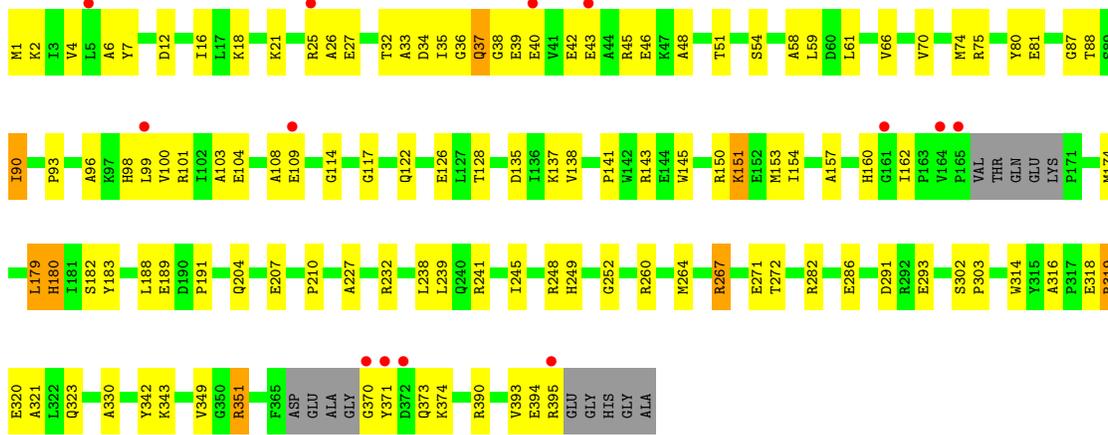
• Molecule 1: Argininosuccinate Synthetase
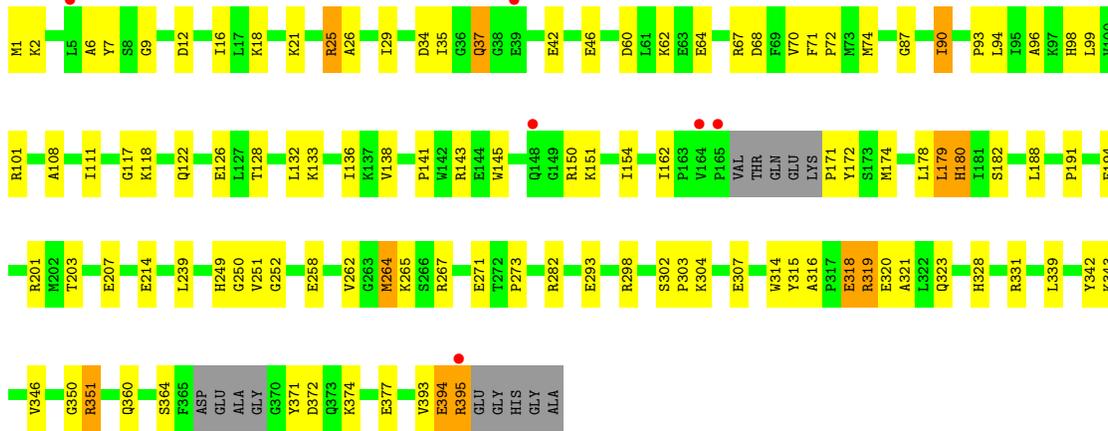
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	229.33Å 229.33Å 159.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10 20.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.10) 97.4 (20.01-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 2.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.257 0.222 , 0.251	Depositor DCC
R_{free} test set	17608 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 56.3	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13150	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: CIR, ATP

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	0.37	0/3135	0.62	1/4237 (0.0%)
1	B	0.36	0/3135	0.62	0/4237
1	C	0.37	0/3135	0.62	0/4237
1	D	0.36	0/3135	0.63	0/4237
All	All	0.37	0/12540	0.62	1/16948 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	263	GLY	N-CA-C	5.43	126.67	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3066	0	3052	97	0
1	B	3066	0	3052	103	0
1	C	3066	0	3052	115	0
1	D	3066	0	3052	105	0
2	A	31	0	10	1	0
2	B	31	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	10	1	0
2	D	31	0	10	2	0
3	A	12	0	7	1	0
3	B	12	0	7	1	0
3	C	12	0	7	1	0
3	D	12	0	7	0	0
4	A	36	0	12	0	0
5	A	186	0	0	5	0
5	B	186	0	0	8	0
5	C	149	0	0	6	0
5	D	157	0	0	3	0
All	All	13150	0	12288	375	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 (375) 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:C:151:LYS:H	1:C:151:LYS:HD2	1.07	1.09
1:A:151:LYS:H	1:A:151:LYS:HD2	1.01	1.08
1:D:151:LYS:H	1:D:151:LYS:HD2	1.16	1.08
1:B:151:LYS:H	1:B:151:LYS:HD2	1.08	1.08
1:B:98:HIS:HD2	1:B:101:ARG:HH21	1.05	0.95
1:C:35:ILE:H	1:C:37:GLN:NE2	1.65	0.94
1:B:35:ILE:H	1:B:37:GLN:NE2	1.66	0.94
1:C:151:LYS:HD2	1:C:151:LYS:N	1.83	0.93
1:A:151:LYS:HD2	1:A:151:LYS:N	1.84	0.93
1:C:151:LYS:H	1:C:151:LYS:CD	1.81	0.92
1:A:151:LYS:H	1:A:151:LYS:CD	1.83	0.91
1:D:35:ILE:H	1:D:37:GLN:NE2	1.67	0.91
1:D:133:LYS:HD3	1:D:136:ILE:HB	1.55	0.88
1:A:318:GLU:HG2	1:C:293:GLU:HB2	1.54	0.86
1:B:151:LYS:H	1:B:151:LYS:CD	1.88	0.86
1:C:37:GLN:NE2	1:C:37:GLN:H	1.74	0.86
1:A:319:ARG:HH21	1:A:323:GLN:HE21	1.23	0.84
1:D:12:ASP:HB2	2:D:4510:ATP:O2G	1.77	0.84
1:D:351:ARG:HD2	1:D:351:ARG:N	1.92	0.84
1:A:318:GLU:HG2	1:C:293:GLU:CB	2.07	0.84
1:A:351:ARG:HD2	1:A:351:ARG:N	1.93	0.84
1:A:98:HIS:HD2	1:A:101:ARG:HH21	1.24	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:O	1:C:26:ALA:HB1	1.80	0.82
1:B:351:ARG:HD2	1:B:351:ARG:N	1.93	0.82
1:C:109:GLU:O	1:C:137:LYS:HE2	1.79	0.81
1:C:98:HIS:HD2	1:C:101:ARG:HH21	1.26	0.81
1:A:395:ARG:HG3	1:A:395:ARG:HH11	1.46	0.80
1:C:371:TYR:HA	5:C:1606:HOH:O	1.82	0.79
1:B:98:HIS:CD2	1:B:101:ARG:HH21	1.97	0.79
1:B:293:GLU:CB	1:D:318:GLU:HG2	2.13	0.78
1:B:151:LYS:HD2	1:B:151:LYS:N	1.93	0.77
1:B:293:GLU:HB3	1:D:318:GLU:HG2	1.65	0.77
1:A:318:GLU:CG	1:C:293:GLU:HB2	2.15	0.75
1:C:37:GLN:H	1:C:37:GLN:HE21	1.32	0.75
1:D:37:GLN:NE2	1:D:37:GLN:H	1.86	0.74
1:C:371:TYR:OH	1:D:262:VAL:HG21	1.87	0.73
1:C:122:GLN:HE21	1:C:143:ARG:HH11	1.37	0.73
1:A:223:GLY:O	1:A:282:ARG:NH2	2.22	0.72
1:C:109:GLU:HG2	1:C:137:LYS:HE3	1.72	0.72
1:A:98:HIS:CD2	1:A:101:ARG:HH21	2.07	0.71
1:D:151:LYS:HD2	1:D:151:LYS:N	2.00	0.71
1:C:314:TRP:O	1:C:319:ARG:HD3	1.91	0.71
1:B:37:GLN:NE2	1:B:37:GLN:H	1.89	0.71
1:B:388:ARG:HH12	1:C:370:GLY:CA	2.04	0.70
1:B:388:ARG:HH12	1:C:370:GLY:HA2	1.57	0.70
1:B:93:PRO:HG3	5:B:1181:HOH:O	1.90	0.70
1:D:35:ILE:H	1:D:37:GLN:HE22	1.39	0.69
1:D:1:MET:O	1:D:26:ALA:HB1	1.93	0.69
1:B:314:TRP:O	1:B:319:ARG:HD3	1.91	0.69
1:D:126:GLU:HG2	1:D:138:VAL:HG11	1.74	0.69
1:B:318:GLU:CG	1:D:293:GLU:HB2	2.22	0.69
1:C:21:LYS:O	1:C:25:ARG:HA	1.92	0.69
1:C:351:ARG:HD2	1:C:351:ARG:N	2.07	0.69
1:A:293:GLU:HB2	1:C:318:GLU:HG3	1.74	0.69
1:D:87:GLY:HA2	1:D:179:LEU:HD13	1.75	0.69
1:A:41:VAL:HG12	1:A:58:ALA:HB1	1.75	0.68
1:A:293:GLU:HB2	1:C:318:GLU:CG	2.24	0.68
1:D:111:ILE:HG23	1:D:136:ILE:HD11	1.74	0.68
1:A:126:GLU:HG2	1:A:138:VAL:HG11	1.74	0.68
1:C:35:ILE:N	1:C:37:GLN:NE2	2.42	0.67
1:C:227:ALA:HB2	1:C:232:ARG:HD2	1.76	0.67
1:A:319:ARG:HH21	1:A:323:GLN:NE2	1.92	0.67
1:B:318:GLU:HG2	1:D:293:GLU:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLN:NE2	1:C:143:ARG:HH11	1.94	0.66
1:B:318:GLU:HG3	1:D:293:GLU:HB2	1.77	0.66
1:B:359:ARG:HB3	1:B:361:ASP:OD1	1.96	0.66
1:C:27:GLU:HG3	1:C:54:SER:OG	1.96	0.66
1:C:58:ALA:O	1:C:59:LEU:HD23	1.95	0.66
1:B:318:GLU:HG2	1:D:293:GLU:HB3	1.77	0.65
1:B:35:ILE:N	1:B:37:GLN:NE2	2.43	0.64
1:C:150:ARG:HA	1:C:153:MET:HE3	1.79	0.64
1:C:2:LYS:HB2	1:C:108:ALA:HA	1.79	0.64
1:D:29:ILE:HD12	1:D:29:ILE:N	2.12	0.64
1:A:109:GLU:O	1:A:137:LYS:HE2	1.98	0.64
1:A:314:TRP:O	1:A:319:ARG:HD3	1.97	0.64
1:C:40:GLU:HB3	1:C:43:GLU:HG3	1.80	0.64
1:C:373:GLN:HE22	1:D:117:GLY:HA3	1.63	0.63
1:C:21:LYS:HD2	1:C:26:ALA:O	1.99	0.63
1:B:1:MET:O	1:B:26:ALA:HB1	1.99	0.63
1:B:314:TRP:CE3	1:B:319:ARG:HD2	2.34	0.62
1:D:6:ALA:HB2	1:D:99:LEU:HD11	1.81	0.62
1:D:339:LEU:N	1:D:339:LEU:HD12	2.14	0.62
1:D:37:GLN:H	1:D:37:GLN:HE21	1.45	0.62
1:D:42:GLU:O	1:D:46:GLU:HG3	1.99	0.62
1:A:154:ILE:O	1:A:158:GLU:HG3	1.99	0.62
1:B:293:GLU:HB2	1:D:318:GLU:CG	2.28	0.62
1:A:118:LYS:HD3	1:B:365:PHE:CE2	2.34	0.62
1:B:328:HIS:CE1	1:B:331:ARG:HH22	2.18	0.62
1:D:214:GLU:OE1	1:D:249:HIS:HE1	1.81	0.62
1:B:37:GLN:H	1:B:37:GLN:HE21	1.46	0.62
1:C:314:TRP:CE3	1:C:319:ARG:HD2	2.34	0.62
1:D:151:LYS:H	1:D:151:LYS:CD	1.93	0.61
1:C:12:ASP:OD1	1:C:150:ARG:NH2	2.26	0.61
1:C:100:VAL:O	1:C:104:GLU:HG3	2.01	0.61
1:B:126:GLU:HG2	1:B:138:VAL:HG11	1.81	0.61
1:B:374:LYS:HD3	1:C:374:LYS:CE	2.31	0.61
1:A:293:GLU:HB3	1:C:318:GLU:HG2	1.82	0.60
1:C:245:ILE:O	1:C:248:ARG:HG2	2.01	0.60
1:C:189:GLU:O	1:C:191:PRO:HD3	2.01	0.60
1:C:204:GLN:HG2	5:C:1505:HOH:O	2.01	0.60
1:A:293:GLU:CB	1:C:318:GLU:HG2	2.32	0.60
1:D:150:ARG:O	1:D:154:ILE:HD13	2.00	0.60
1:B:122:GLN:HE21	1:B:143:ARG:HH11	1.48	0.60
1:A:41:VAL:CG1	1:A:58:ALA:HB1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLU:CG	1:C:137:LYS:HE3	2.32	0.60
1:A:345:ASN:HB3	1:A:347:TYR:CE1	2.36	0.60
1:A:90:ILE:HD11	1:A:179:LEU:HD23	1.84	0.59
1:B:359:ARG:HD2	5:B:1444:HOH:O	2.02	0.59
1:A:21:LYS:HE2	1:A:52:GLY:O	2.03	0.59
1:C:150:ARG:O	1:C:154:ILE:HG13	2.01	0.59
1:A:318:GLU:HG2	1:C:293:GLU:HB3	1.83	0.59
1:D:282:ARG:HD2	5:D:1547:HOH:O	2.02	0.59
1:A:154:ILE:HG23	1:A:164:VAL:HG11	1.84	0.59
1:B:374:LYS:HD3	1:C:374:LYS:HE3	1.85	0.59
1:B:293:GLU:HB2	1:D:318:GLU:HG2	1.82	0.59
1:B:318:GLU:CG	1:D:293:GLU:CB	2.82	0.57
1:C:93:PRO:HG3	5:C:1407:HOH:O	2.04	0.57
1:D:314:TRP:CE3	1:D:319:ARG:HD2	2.38	0.57
1:C:35:ILE:H	1:C:37:GLN:HE22	1.50	0.57
1:D:18:LYS:HG3	1:D:162:ILE:HD11	1.86	0.57
1:A:147:PHE:HD2	1:A:152:GLU:HG2	1.69	0.57
1:A:316:ALA:HB1	1:A:318:GLU:OE2	2.04	0.57
1:C:16:ILE:HG23	1:C:141:PRO:HG2	1.87	0.57
1:A:87:GLY:HA2	1:A:179:LEU:HD23	1.88	0.56
1:A:118:LYS:HD3	1:B:365:PHE:CZ	2.40	0.56
1:D:262:VAL:HG22	1:D:262:VAL:O	2.06	0.56
1:A:293:GLU:CB	1:C:318:GLU:CG	2.83	0.56
1:B:6:ALA:HB2	1:B:99:LEU:HD11	1.88	0.56
1:D:93:PRO:HG3	5:D:1235:HOH:O	2.05	0.55
1:A:319:ARG:NH2	1:A:323:GLN:HE21	2.00	0.55
1:D:16:ILE:HG23	1:D:141:PRO:HG2	1.89	0.55
1:D:395:ARG:HG3	1:D:395:ARG:HH11	1.72	0.55
1:B:393:VAL:C	1:B:395:ARG:H	2.11	0.55
1:D:394:GLU:O	1:D:395:ARG:C	2.46	0.55
1:A:393:VAL:O	1:A:395:ARG:NH1	2.40	0.55
1:D:35:ILE:N	1:D:37:GLN:NE2	2.46	0.55
1:D:118:LYS:O	1:D:264:MET:HE1	2.07	0.54
1:D:350:GLY:C	1:D:351:ARG:HD2	2.27	0.54
1:D:35:ILE:N	1:D:37:GLN:HE22	2.05	0.54
1:D:351:ARG:N	1:D:351:ARG:CD	2.69	0.54
1:B:90:ILE:HD11	1:B:179:LEU:HD23	1.88	0.54
1:D:393:VAL:O	1:D:395:ARG:HG3	2.07	0.54
1:A:75:ARG:HA	1:A:282:ARG:CZ	2.38	0.54
1:A:93:PRO:HG3	5:A:1238:HOH:O	2.08	0.53
1:B:34:ASP:HA	1:B:37:GLN:HE22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:THR:HG21	3:C:3520:CIR:H42	1.90	0.53
1:D:70:VAL:O	1:D:74:MET:HG3	2.07	0.53
1:D:314:TRP:O	1:D:319:ARG:HD3	2.08	0.53
1:B:98:HIS:HD2	1:B:101:ARG:NH2	1.88	0.53
1:C:98:HIS:CD2	1:C:101:ARG:HH21	2.16	0.53
1:B:96:ALA:HB3	1:B:128:THR:HG21	1.90	0.53
1:B:35:ILE:H	1:B:37:GLN:HE22	1.50	0.53
1:C:18:LYS:HE3	1:C:160:HIS:HB3	1.91	0.53
1:A:343:LYS:HD2	1:B:343:LYS:HD3	1.91	0.53
1:C:126:GLU:HG2	1:C:138:VAL:HG11	1.91	0.52
1:C:33:ALA:HB1	1:C:61:LEU:HD12	1.90	0.52
1:C:122:GLN:HE21	1:C:143:ARG:NH1	2.05	0.52
1:C:45:ARG:NH1	1:C:45:ARG:HG2	2.25	0.52
1:A:133:LYS:HG2	1:A:136:ILE:HB	1.92	0.52
1:B:70:VAL:O	1:B:74:MET:HG3	2.10	0.52
1:B:122:GLN:NE2	1:B:143:ARG:HH11	2.08	0.51
1:C:45:ARG:HG2	1:C:45:ARG:HH11	1.75	0.51
1:C:393:VAL:C	1:C:395:ARG:H	2.13	0.51
1:A:117:GLY:H	1:B:373:GLN:HE22	1.58	0.51
1:A:245:ILE:O	1:A:248:ARG:HG2	2.09	0.51
5:A:1274:HOH:O	1:B:191:PRO:HG2	2.09	0.51
1:A:314:TRP:CE3	1:A:319:ARG:HD2	2.45	0.51
1:D:67:ARG:HD2	1:D:68:ASP:OD1	2.11	0.51
1:B:37:GLN:HG2	5:B:1506:HOH:O	2.10	0.51
1:B:164:VAL:HG13	1:B:165:PRO:HD2	1.92	0.51
1:D:90:ILE:HD11	1:D:179:LEU:HD12	1.92	0.51
1:A:164:VAL:HG12	1:A:164:VAL:O	2.11	0.51
1:D:395:ARG:HG3	1:D:395:ARG:NH1	2.26	0.51
1:A:214:GLU:OE1	1:A:249:HIS:HE1	1.93	0.50
1:B:75:ARG:NH2	5:B:1250:HOH:O	2.45	0.50
1:D:98:HIS:HD2	1:D:101:ARG:NH1	2.09	0.50
1:C:302:SER:HB2	1:C:303:PRO:HD3	1.93	0.50
1:C:179:LEU:O	1:C:272:THR:HG23	2.12	0.50
1:B:321:ALA:HA	1:D:328:HIS:CD2	2.47	0.50
1:D:262:VAL:CG1	1:D:264:MET:HE1	2.42	0.49
1:A:191:PRO:HB2	1:B:351:ARG:HD3	1.92	0.49
1:B:338:ARG:HD3	5:B:1305:HOH:O	2.12	0.49
1:C:40:GLU:CG	1:C:43:GLU:HG3	2.42	0.49
1:B:13:THR:HG23	2:B:2510:ATP:O2G	2.12	0.49
1:C:37:GLN:HE21	1:C:37:GLN:N	2.05	0.49
1:D:111:ILE:CG2	1:D:136:ILE:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLY:HA2	1:B:179:LEU:HD23	1.95	0.49
1:C:150:ARG:N	1:C:151:LYS:HD2	2.27	0.49
1:C:316:ALA:O	1:C:320:GLU:HG3	2.13	0.49
1:C:42:GLU:OE1	1:C:45:ARG:HD3	2.13	0.49
1:B:374:LYS:HD3	1:C:374:LYS:HE2	1.95	0.48
1:B:393:VAL:C	1:B:395:ARG:N	2.64	0.48
1:C:75:ARG:HG2	1:C:330:ALA:CB	2.42	0.48
1:A:150:ARG:HG3	1:A:154:ILE:HD13	1.95	0.48
1:A:302:SER:HB2	1:A:303:PRO:HD3	1.94	0.48
1:D:6:ALA:HB3	2:D:4510:ATP:O2'	2.12	0.48
1:A:42:GLU:O	1:A:46:GLU:HG3	2.12	0.48
1:B:88:THR:HG21	3:B:2520:CIR:H42	1.96	0.48
1:C:7:TYR:CE2	1:C:48:ALA:HB2	2.48	0.48
1:C:248:ARG:HG3	1:C:249:HIS:CD2	2.47	0.48
1:A:86:LEU:HB3	1:A:89:SER:HB2	1.96	0.48
1:C:6:ALA:HB2	1:C:99:LEU:HD11	1.95	0.48
1:C:319:ARG:HH21	1:C:323:GLN:HE21	1.61	0.48
1:A:117:GLY:H	1:B:373:GLN:NE2	2.12	0.48
1:A:282:ARG:O	1:A:286:GLU:HG3	2.13	0.48
1:A:395:ARG:HG3	1:A:395:ARG:NH1	2.19	0.48
1:D:96:ALA:HB3	1:D:128:THR:HG21	1.96	0.48
1:A:6:ALA:HB2	1:A:99:LEU:HD11	1.95	0.48
1:D:328:HIS:CE1	1:D:331:ARG:HH22	2.31	0.48
1:C:210:PRO:O	1:C:343:LYS:NZ	2.47	0.48
1:A:12:ASP:OD1	1:A:150:ARG:NH2	2.46	0.47
1:B:73:MET:CE	1:B:90:ILE:HG12	2.44	0.47
1:C:35:ILE:N	1:C:37:GLN:HE22	2.08	0.47
1:A:194:GLU:HG3	1:A:195:PRO:HD2	1.97	0.47
1:A:328:HIS:CD2	1:C:321:ALA:HA	2.50	0.47
1:D:302:SER:HB2	1:D:303:PRO:HD3	1.96	0.47
5:C:1130:HOH:O	1:D:191:PRO:HG2	2.13	0.47
1:C:117:GLY:HA2	1:C:122:GLN:NE2	2.29	0.47
1:D:262:VAL:HG11	1:D:264:MET:HE1	1.97	0.47
1:A:150:ARG:HG3	1:A:154:ILE:CD1	2.45	0.47
1:B:35:ILE:N	1:B:37:GLN:HE22	2.11	0.47
1:C:260:ARG:HD2	1:C:264:MET:SD	2.54	0.47
1:B:260:ARG:HD2	1:B:264:MET:SD	2.54	0.47
1:C:21:LYS:O	1:C:25:ARG:CA	2.61	0.47
1:A:27:GLU:HG3	1:A:54:SER:HB3	1.97	0.47
1:A:298:ARG:C	1:A:298:ARG:HD2	2.35	0.47
1:A:191:PRO:HG2	5:B:1163:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:HD3	1:B:191:PRO:HB2	1.97	0.46
1:B:117:GLY:HA2	1:B:122:GLN:NE2	2.30	0.46
1:C:4:VAL:HG21	1:C:103:ALA:HA	1.97	0.46
1:D:298:ARG:O	1:D:298:ARG:HD2	2.15	0.46
1:D:319:ARG:HH21	1:D:323:GLN:HE21	1.62	0.46
1:A:180:HIS:C	1:A:180:HIS:ND1	2.67	0.46
1:C:1:MET:HG2	1:C:26:ALA:HB2	1.97	0.46
1:C:4:VAL:HG12	1:C:99:LEU:HD23	1.96	0.46
1:A:154:ILE:HG13	1:A:164:VAL:CG1	2.45	0.46
1:B:174:MET:HA	1:B:182:SER:O	2.16	0.46
1:B:180:HIS:ND1	1:B:180:HIS:C	2.68	0.46
1:D:122:GLN:HE21	1:D:143:ARG:HH11	1.62	0.46
1:D:171:PRO:HG2	1:D:172:TYR:CD2	2.51	0.46
1:C:42:GLU:O	1:C:46:GLU:HG3	2.15	0.46
1:B:80:TYR:CD2	1:B:81:GLU:HG3	2.50	0.46
1:C:114:GLY:CA	2:C:3510:ATP:O3'	2.64	0.46
1:D:174:MET:HA	1:D:182:SER:O	2.16	0.46
1:B:97:LYS:HD2	1:B:315:TYR:OH	2.15	0.46
1:B:328:HIS:CD2	1:D:321:ALA:HA	2.51	0.46
1:D:374:LYS:HD2	1:D:377:GLU:HB3	1.98	0.46
1:B:249:HIS:HD2	5:B:1103:HOH:O	1.98	0.46
1:A:259:ASN:HB2	1:B:292:ARG:HG3	1.98	0.46
1:B:282:ARG:O	1:B:286:GLU:HG3	2.17	0.46
1:C:351:ARG:HD3	1:D:191:PRO:HB2	1.97	0.46
1:D:251:VAL:HG11	1:D:346:VAL:CG2	2.46	0.46
1:C:38:GLY:C	1:C:39:GLU:HG3	2.36	0.45
1:C:154:ILE:O	1:C:157:ALA:HB3	2.16	0.45
1:D:21:LYS:O	1:D:25:ARG:HA	2.16	0.45
1:C:40:GLU:CB	1:C:43:GLU:HG3	2.46	0.45
1:D:18:LYS:CG	1:D:162:ILE:HD11	2.47	0.45
1:B:6:ALA:HB1	2:B:2510:ATP:N3	2.31	0.45
1:C:80:TYR:CD2	1:C:81:GLU:HG3	2.52	0.45
1:A:249:HIS:HD2	5:A:1138:HOH:O	1.98	0.45
1:B:388:ARG:HH12	1:C:370:GLY:HA3	1.80	0.45
1:D:133:LYS:O	1:D:136:ILE:HG22	2.17	0.45
1:B:36:GLY:HA2	5:B:1497:HOH:O	2.17	0.45
1:B:87:GLY:HA3	1:B:180:HIS:CD2	2.51	0.45
1:D:128:THR:O	1:D:132:LEU:HG	2.17	0.45
1:A:34:ASP:HB2	1:A:41:VAL:HG21	1.98	0.44
1:A:180:HIS:HB2	1:A:271:GLU:O	2.17	0.44
1:C:390:ARG:O	1:C:394:GLU:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:LYS:HB2	1:D:108:ALA:HA	1.98	0.44
1:A:351:ARG:N	1:A:351:ARG:CD	2.75	0.44
1:C:96:ALA:HB3	1:C:128:THR:HG21	1.98	0.44
1:C:241:ARG:NH2	5:C:1529:HOH:O	2.50	0.44
1:A:7:TYR:CE2	1:A:9:GLY:HA2	2.53	0.44
1:B:345:ASN:HB2	1:B:347:TYR:CE1	2.52	0.44
1:B:350:GLY:C	1:B:351:ARG:HD2	2.38	0.44
1:A:204:GLN:HG2	5:A:1576:HOH:O	2.16	0.44
1:C:180:HIS:ND1	1:C:180:HIS:C	2.70	0.44
1:D:298:ARG:HD2	1:D:298:ARG:C	2.38	0.44
1:B:179:LEU:O	1:B:272:THR:HG23	2.18	0.44
1:D:128:THR:HG23	1:D:315:TYR:CD1	2.53	0.44
1:A:248:ARG:HG3	1:A:249:HIS:ND1	2.32	0.44
1:D:249:HIS:HD2	5:D:1491:HOH:O	2.01	0.44
1:A:88:THR:HG21	3:A:520:CIR:H42	1.99	0.44
1:A:262:VAL:HG13	5:A:1668:HOH:O	2.18	0.44
1:B:181:ILE:HD12	1:B:202:MET:HB2	1.99	0.44
1:D:180:HIS:HB2	1:D:271:GLU:O	2.18	0.44
1:B:304:LYS:O	1:B:307:GLU:HG2	2.17	0.43
1:B:392:LEU:O	1:B:395:ARG:HA	2.17	0.43
1:D:251:VAL:CG1	1:D:252:GLY:N	2.81	0.43
1:A:27:GLU:HG3	1:A:54:SER:CB	2.48	0.43
1:A:349:VAL:HB	1:B:194:GLU:HG3	2.00	0.43
1:B:7:TYR:CE2	1:B:9:GLY:HA2	2.52	0.43
1:B:66:VAL:HG21	1:B:236:ALA:HA	2.00	0.43
1:C:282:ARG:HD2	5:C:1333:HOH:O	2.17	0.43
1:C:342:TYR:CZ	1:D:207:GLU:HG2	2.53	0.43
1:C:36:GLY:N	1:C:37:GLN:HE21	2.16	0.43
1:A:150:ARG:O	1:A:154:ILE:HD13	2.18	0.43
1:C:135:ASP:O	1:C:137:LYS:HD3	2.19	0.43
1:D:128:THR:HG23	1:D:315:TYR:HD1	1.83	0.43
1:B:117:GLY:HA2	1:B:122:GLN:HE22	1.83	0.43
1:A:32:THR:O	1:A:58:ALA:HA	2.19	0.43
1:A:84:TYR:CE2	1:A:86:LEU:HA	2.53	0.43
1:D:318:GLU:H	1:D:318:GLU:CD	2.21	0.43
1:A:61:LEU:HD13	1:A:94:LEU:CD2	2.49	0.43
1:A:298:ARG:HD2	1:A:298:ARG:O	2.19	0.43
1:C:34:ASP:HA	1:C:37:GLN:HE22	1.83	0.43
1:D:154:ILE:HD12	1:D:154:ILE:N	2.33	0.43
1:C:4:VAL:HG21	1:C:103:ALA:CA	2.49	0.43
1:D:374:LYS:HE2	1:D:377:GLU:OE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:NZ	1:D:374:LYS:HG2	2.33	0.42
1:C:174:MET:HG2	1:C:183:TYR:CD2	2.53	0.42
1:A:70:VAL:O	1:A:74:MET:HG3	2.19	0.42
1:A:259:ASN:CB	1:B:292:ARG:HG3	2.50	0.42
1:A:343:LYS:HD2	1:B:343:LYS:CD	2.48	0.42
1:B:80:TYR:CE2	1:B:81:GLU:HG3	2.54	0.42
1:C:174:MET:HA	1:C:182:SER:O	2.18	0.42
1:C:151:LYS:N	1:C:151:LYS:CD	2.58	0.42
1:B:71:PHE:HB2	1:B:72:PRO:HD3	2.01	0.42
1:B:345:ASN:CB	1:B:347:TYR:CE1	3.03	0.42
1:D:34:ASP:HB3	1:D:60:ASP:HA	2.02	0.42
1:B:1:MET:HB3	1:B:26:ALA:HB2	2.02	0.42
1:C:90:ILE:HD11	1:C:179:LEU:HD12	2.00	0.42
1:C:238:LEU:C	1:C:238:LEU:HD23	2.39	0.42
1:D:316:ALA:O	1:D:320:GLU:HG3	2.19	0.42
1:A:16:ILE:HG23	1:A:141:PRO:HG2	2.01	0.42
1:D:117:GLY:HA2	1:D:122:GLN:NE2	2.35	0.42
1:B:34:ASP:HB3	1:B:60:ASP:HA	2.02	0.42
1:C:393:VAL:C	1:C:395:ARG:N	2.73	0.42
1:D:34:ASP:HA	1:D:37:GLN:HE22	1.84	0.42
1:B:120:ASN:HD21	1:B:260:ARG:HG2	1.85	0.42
1:D:7:TYR:CE2	1:D:9:GLY:HA2	2.54	0.42
1:D:203:THR:HB	1:D:250:GLY:HA2	2.02	0.42
1:C:207:GLU:HA	1:D:342:TYR:OH	2.20	0.42
1:C:282:ARG:O	1:C:286:GLU:HG3	2.20	0.42
1:D:331:ARG:HE	1:D:331:ARG:HB3	1.42	0.42
1:A:394:GLU:O	1:A:395:ARG:HB2	2.19	0.41
1:B:12:ASP:HB2	2:B:2510:ATP:O3G	2.20	0.41
1:D:29:ILE:N	1:D:29:ILE:CD1	2.82	0.41
1:D:304:LYS:O	1:D:307:GLU:HG2	2.21	0.41
1:B:213:PRO:HB3	1:B:342:TYR:HB2	2.03	0.41
1:A:6:ALA:HB3	2:A:510:ATP:O2'	2.21	0.41
1:B:180:HIS:HB2	1:B:271:GLU:O	2.21	0.41
1:B:252:GLY:O	1:B:271:GLU:HA	2.20	0.41
1:C:18:LYS:HG3	1:C:162:ILE:HD11	2.02	0.41
1:C:252:GLY:O	1:C:271:GLU:HA	2.21	0.41
1:A:61:LEU:HD13	1:A:94:LEU:HD21	2.03	0.41
1:A:359:ARG:C	1:A:361:ASP:N	2.74	0.41
1:C:32:THR:O	1:C:58:ALA:HA	2.21	0.41
1:D:64:GLU:OE1	1:D:98:HIS:HE1	2.03	0.41
1:D:174:MET:HE3	1:D:201:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:HB2	1:A:108:ALA:HA	2.03	0.41
1:B:133:LYS:O	1:B:136:ILE:HG22	2.21	0.41
1:B:351:ARG:N	1:B:351:ARG:CD	2.74	0.41
1:C:70:VAL:O	1:C:74:MET:HG3	2.21	0.41
1:D:12:ASP:O	1:D:16:ILE:HG13	2.20	0.41
1:D:150:ARG:HG3	1:D:154:ILE:CD1	2.51	0.41
1:A:164:VAL:O	1:A:165:PRO:C	2.59	0.41
1:B:251:VAL:HG23	1:B:273:PRO:HA	2.03	0.41
1:B:328:HIS:CE1	1:B:331:ARG:NH2	2.86	0.41
1:C:66:VAL:HA	1:C:70:VAL:HB	2.03	0.41
1:C:349:VAL:HB	1:D:194:GLU:HG3	2.02	0.41
1:D:360:GLN:HG2	1:D:364:SER:OG	2.21	0.41
1:D:371:TYR:HD1	1:D:372:ASP:O	2.04	0.41
1:A:154:ILE:HG13	1:A:164:VAL:HG11	2.03	0.41
1:D:71:PHE:HB2	1:D:72:PRO:HD3	2.03	0.41
1:A:395:ARG:NH1	1:A:395:ARG:CG	2.82	0.40
1:D:171:PRO:HG2	1:D:172:TYR:CE2	2.56	0.40
1:B:214:GLU:OE1	1:B:249:HIS:HE1	2.04	0.40
1:C:87:GLY:HA3	1:C:180:HIS:CD2	2.55	0.40
1:A:133:LYS:HA	1:A:134:PRO:HD2	1.89	0.40
1:A:147:PHE:CD2	1:A:152:GLU:HG2	2.52	0.40
1:A:251:VAL:CG1	1:A:252:GLY:N	2.85	0.40
1:B:118:LYS:HE2	1:B:118:LYS:HB3	1.92	0.40
1:D:258:GLU:O	1:D:265:LYS:HA	2.21	0.40
1:C:267:ARG:C	1:C:267:ARG:HD3	2.42	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	380/400 (95%)	372 (98%)	7 (2%)	1 (0%)	41	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	380/400 (95%)	368 (97%)	12 (3%)	0	100	100
1	C	380/400 (95%)	365 (96%)	14 (4%)	1 (0%)	41	41
1	D	380/400 (95%)	373 (98%)	5 (1%)	2 (0%)	29	26
All	All	1520/1600 (95%)	1478 (97%)	38 (2%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	THR
1	D	343	LYS
1	A	343	LYS
1	D	273	PRO

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/319 (97%)	294 (95%)	16 (5%)	23	21
1	B	310/319 (97%)	298 (96%)	12 (4%)	32	33
1	C	310/319 (97%)	298 (96%)	12 (4%)	32	33
1	D	310/319 (97%)	292 (94%)	18 (6%)	20	17
All	All	1240/1276 (97%)	1182 (95%)	58 (5%)	26	25

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	90	ILE
1	A	94	LEU
1	A	137	LYS
1	A	145	TRP
1	A	151	LYS
1	A	180	HIS

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type
1	A	188	LEU
1	A	239	LEU
1	A	264	MET
1	A	267	ARG
1	A	291	ASP
1	A	318	GLU
1	A	319	ARG
1	A	351	ARG
1	A	361	ASP
1	B	37	GLN
1	B	90	ILE
1	B	94	LEU
1	B	145	TRP
1	B	165	PRO
1	B	180	HIS
1	B	188	LEU
1	B	239	LEU
1	B	267	ARG
1	B	318	GLU
1	B	319	ARG
1	B	351	ARG
1	C	37	GLN
1	C	90	ILE
1	C	145	TRP
1	C	151	LYS
1	C	179	LEU
1	C	180	HIS
1	C	188	LEU
1	C	239	LEU
1	C	267	ARG
1	C	291	ASP
1	C	319	ARG
1	C	351	ARG
1	D	25	ARG
1	D	37	GLN
1	D	62	LYS
1	D	90	ILE
1	D	94	LEU
1	D	145	TRP
1	D	178	LEU
1	D	179	LEU
1	D	180	HIS

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Mol	Chain	Res	Type
1	D	188	LEU
1	D	239	LEU
1	D	264	MET
1	D	267	ARG
1	D	318	GLU
1	D	319	ARG
1	D	351	ARG
1	D	394	GLU
1	D	395	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	148	GLN
1	A	249	HIS
1	A	323	GLN
1	A	345	ASN
1	A	360	GLN
1	A	373	GLN
1	B	37	GLN
1	B	98	HIS
1	B	122	GLN
1	B	148	GLN
1	B	180	HIS
1	B	249	HIS
1	B	297	GLN
1	B	360	GLN
1	B	373	GLN
1	C	37	GLN
1	C	98	HIS
1	C	122	GLN
1	C	180	HIS
1	C	323	GLN
1	C	360	GLN
1	C	373	GLN
1	D	37	GLN
1	D	98	HIS
1	D	122	GLN
1	D	148	GLN
1	D	204	GLN
1	D	249	HIS

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Mol	Chain	Res	Type
1	D	297	GLN
1	D	323	GLN
1	D	360	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	ATP	B	2510	-	26,33,33	2.62	10 (38%)	31,52,52	3.60	9 (29%)
3	CIR	C	3520	-	10,11,11	1.51	2 (20%)	12,13,13	1.38	1 (8%)
3	CIR	D	4520	-	10,11,11	1.45	2 (20%)	12,13,13	1.45	1 (8%)
4	ASP	A	3530	-	6,8,8	1.20	0	8,10,10	0.86	0
3	CIR	B	2520	-	10,11,11	1.47	2 (20%)	12,13,13	1.56	4 (33%)
2	ATP	D	4510	-	26,33,33	2.43	9 (34%)	31,52,52	3.37	8 (25%)
2	ATP	C	3510	-	26,33,33	2.49	9 (34%)	31,52,52	3.61	9 (29%)
3	CIR	A	520	-	10,11,11	1.45	2 (20%)	12,13,13	1.37	1 (8%)
4	ASP	A	530	-	6,8,8	1.28	0	8,10,10	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	ASP	A	2530	-	6,8,8	1.18	0	8,10,10	0.89	0
2	ATP	A	510	-	26,33,33	2.60	10 (38%)	31,52,52	3.71	8 (25%)
4	ASP	A	4530	-	6,8,8	1.18	0	8,10,10	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	2510	-	-	1/18/38/38	0/3/3/3
3	CIR	C	3520	-	-	2/11/11/11	-
3	CIR	D	4520	-	-	4/11/11/11	-
4	ASP	A	3530	-	-	0/8/8/8	-
3	CIR	B	2520	-	-	4/11/11/11	-
2	ATP	D	4510	-	-	2/18/38/38	0/3/3/3
2	ATP	C	3510	-	-	3/18/38/38	0/3/3/3
3	CIR	A	520	-	-	4/11/11/11	-
4	ASP	A	530	-	-	0/8/8/8	-
4	ASP	A	2530	-	-	0/8/8/8	-
2	ATP	A	510	-	-	4/18/38/38	0/3/3/3
4	ASP	A	4530	-	-	0/8/8/8	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2510	ATP	O5'-C5'	-6.06	1.21	1.44
2	A	510	ATP	O5'-C5'	-5.80	1.22	1.44
2	B	2510	ATP	O4'-C1'	5.75	1.49	1.41
2	A	510	ATP	C4-N3	5.60	1.43	1.35
2	A	510	ATP	O4'-C1'	5.60	1.48	1.41
2	C	3510	ATP	O5'-C5'	-5.54	1.23	1.44
2	D	4510	ATP	C4-N3	5.52	1.43	1.35
2	D	4510	ATP	O5'-C5'	-5.36	1.24	1.44
2	B	2510	ATP	C4-N3	5.32	1.43	1.35
2	D	4510	ATP	O4'-C1'	5.32	1.48	1.41
2	C	3510	ATP	C4-N3	5.32	1.43	1.35
2	C	3510	ATP	O4'-C1'	5.30	1.48	1.41
2	B	2510	ATP	PA-O5'	-4.37	1.41	1.59
2	A	510	ATP	PA-O5'	-4.08	1.42	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3510	ATP	PA-O5'	-3.79	1.44	1.59
2	D	4510	ATP	PA-O5'	-3.68	1.44	1.59
2	B	2510	ATP	C2'-C1'	3.67	1.59	1.53
2	A	510	ATP	C2'-C1'	3.57	1.59	1.53
3	A	520	CIR	C7-N6	-3.35	1.30	1.34
2	C	3510	ATP	C2'-C1'	3.26	1.58	1.53
3	C	3520	CIR	C7-N6	-3.19	1.30	1.34
3	D	4520	CIR	C7-N6	-3.14	1.30	1.34
2	B	2510	ATP	C3'-C4'	-3.11	1.45	1.53
2	B	2510	ATP	C5'-C4'	-3.02	1.42	1.51
2	D	4510	ATP	C3'-C4'	-2.98	1.45	1.53
2	A	510	ATP	C5'-C4'	-2.86	1.42	1.51
3	B	2520	CIR	C7-N6	-2.86	1.31	1.34
2	D	4510	ATP	C2'-C1'	2.81	1.58	1.53
2	A	510	ATP	C3'-C4'	-2.73	1.46	1.53
3	B	2520	CIR	OXT-C	-2.69	1.21	1.30
2	C	3510	ATP	C8-N7	-2.63	1.30	1.34
2	C	3510	ATP	C5'-C4'	-2.60	1.43	1.51
3	C	3520	CIR	OXT-C	-2.58	1.22	1.30
2	D	4510	ATP	C2-N3	2.57	1.36	1.32
3	D	4520	CIR	OXT-C	-2.56	1.22	1.30
3	A	520	CIR	OXT-C	-2.54	1.22	1.30
2	A	510	ATP	C8-N7	-2.44	1.30	1.34
2	C	3510	ATP	C3'-C4'	-2.42	1.46	1.53
2	C	3510	ATP	C2-N3	2.36	1.35	1.32
2	A	510	ATP	PB-O1B	-2.31	1.42	1.50
2	B	2510	ATP	C2-N3	2.28	1.35	1.32
2	D	4510	ATP	C5'-C4'	-2.27	1.44	1.51
2	D	4510	ATP	C8-N7	-2.24	1.30	1.34
2	A	510	ATP	C2-N3	2.23	1.35	1.32
2	B	2510	ATP	C8-N7	-2.06	1.31	1.34
2	B	2510	ATP	PA-O2A	-2.02	1.45	1.55

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	510	ATP	O5'-C5'-C4'	16.90	167.15	108.99
2	C	3510	ATP	O5'-C5'-C4'	16.33	165.19	108.99
2	B	2510	ATP	O5'-C5'-C4'	15.79	163.33	108.99
2	D	4510	ATP	O5'-C5'-C4'	14.61	159.29	108.99
2	B	2510	ATP	C5'-C4'-C3'	-7.21	88.16	115.18
2	A	510	ATP	C5'-C4'-C3'	-6.96	89.11	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3510	ATP	C5'-C4'-C3'	-6.81	89.67	115.18
2	D	4510	ATP	C5'-C4'-C3'	-6.42	91.11	115.18
2	D	4510	ATP	PA-O5'-C5'	5.94	156.53	121.68
2	B	2510	ATP	PA-O5'-C5'	5.34	153.00	121.68
2	A	510	ATP	PA-O5'-C5'	5.02	151.14	121.68
2	C	3510	ATP	PA-O5'-C5'	4.68	149.11	121.68
2	B	2510	ATP	O4'-C4'-C3'	3.68	112.40	105.11
2	A	510	ATP	O4'-C4'-C3'	3.54	112.12	105.11
2	C	3510	ATP	O4'-C4'-C3'	3.30	111.65	105.11
2	D	4510	ATP	O4'-C4'-C3'	3.30	111.64	105.11
3	B	2520	CIR	N8-C7-N6	3.15	120.17	116.85
2	B	2510	ATP	O2A-PA-O5'	-2.96	93.99	107.75
2	D	4510	ATP	O2A-PA-O5'	-2.91	94.25	107.75
2	C	3510	ATP	C4-C5-N7	2.79	112.31	109.40
2	C	3510	ATP	O2A-PA-O5'	-2.73	95.05	107.75
2	A	510	ATP	C4-C5-N7	2.71	112.23	109.40
3	D	4520	CIR	N8-C7-N6	2.69	119.69	116.85
2	A	510	ATP	O3'-C3'-C4'	2.65	118.71	111.05
2	C	3510	ATP	O3'-C3'-C4'	2.59	118.52	111.05
3	C	3520	CIR	N8-C7-N6	2.56	119.56	116.85
2	B	2510	ATP	C4-C5-N7	2.48	111.98	109.40
2	D	4510	ATP	C4-C5-N7	2.46	111.97	109.40
3	A	520	CIR	N8-C7-N6	2.39	119.37	116.85
2	C	3510	ATP	PA-O3A-PB	2.36	140.94	132.83
2	B	2510	ATP	O3'-C3'-C4'	2.28	117.64	111.05
2	B	2510	ATP	O3'-C3'-C2'	2.25	119.08	111.82
2	B	2510	ATP	O5'-PA-O1A	-2.22	100.39	109.07
2	A	510	ATP	O5'-PA-O1A	-2.18	100.56	109.07
2	D	4510	ATP	O5'-PA-O1A	-2.17	100.58	109.07
2	C	3510	ATP	C3'-C2'-C1'	2.14	104.20	100.98
2	D	4510	ATP	C3'-C2'-C1'	2.13	104.18	100.98
3	B	2520	CIR	O7-C7-N6	-2.11	120.18	121.74
3	B	2520	CIR	C5-N6-C7	-2.10	120.23	122.73
2	A	510	ATP	O3'-C3'-C2'	2.09	118.57	111.82
3	B	2520	CIR	O7-C7-N8	-2.08	119.65	123.22

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3510	ATP	PB-O3B-PG-O2G
3	A	520	CIR	O7-C7-N6-C5

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Mol	Chain	Res	Type	Atoms
3	A	520	CIR	N8-C7-N6-C5
3	B	2520	CIR	O7-C7-N6-C5
3	B	2520	CIR	N8-C7-N6-C5
3	C	3520	CIR	O7-C7-N6-C5
3	C	3520	CIR	N8-C7-N6-C5
3	D	4520	CIR	C4-C3-CA-N
3	D	4520	CIR	O7-C7-N6-C5
3	D	4520	CIR	N8-C7-N6-C5
2	A	510	ATP	PB-O3B-PG-O1G
3	D	4520	CIR	C4-C3-CA-C
2	A	510	ATP	PG-O3B-PB-O2B
2	B	2510	ATP	PG-O3B-PB-O2B
2	C	3510	ATP	PG-O3B-PB-O2B
2	D	4510	ATP	PG-O3B-PB-O2B
3	A	520	CIR	C4-C3-CA-N
3	B	2520	CIR	C4-C3-CA-N
2	A	510	ATP	PB-O3B-PG-O2G
2	A	510	ATP	PB-O3B-PG-O3G
2	C	3510	ATP	PB-O3B-PG-O3G
3	A	520	CIR	C4-C3-CA-C
3	B	2520	CIR	C4-C3-CA-C
2	D	4510	ATP	PB-O3B-PG-O1G

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2510	ATP	3	0
3	C	3520	CIR	1	0
3	B	2520	CIR	1	0
2	D	4510	ATP	2	0
2	C	3510	ATP	1	0
3	A	520	CIR	1	0
2	A	510	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 ATP B 2510

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 4510

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 3510

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 510

Bond lengths

Bond angles

Torsions

Rings
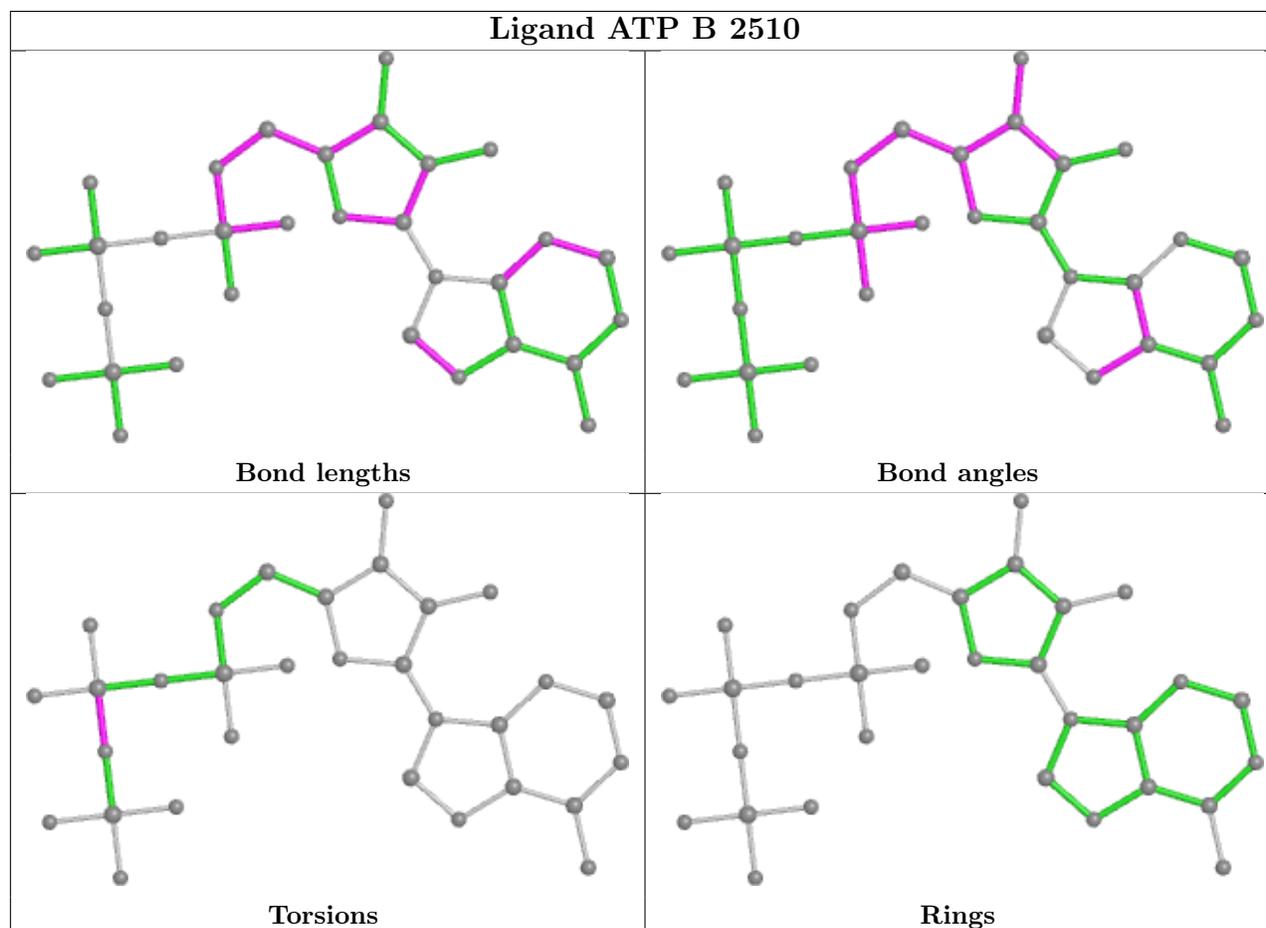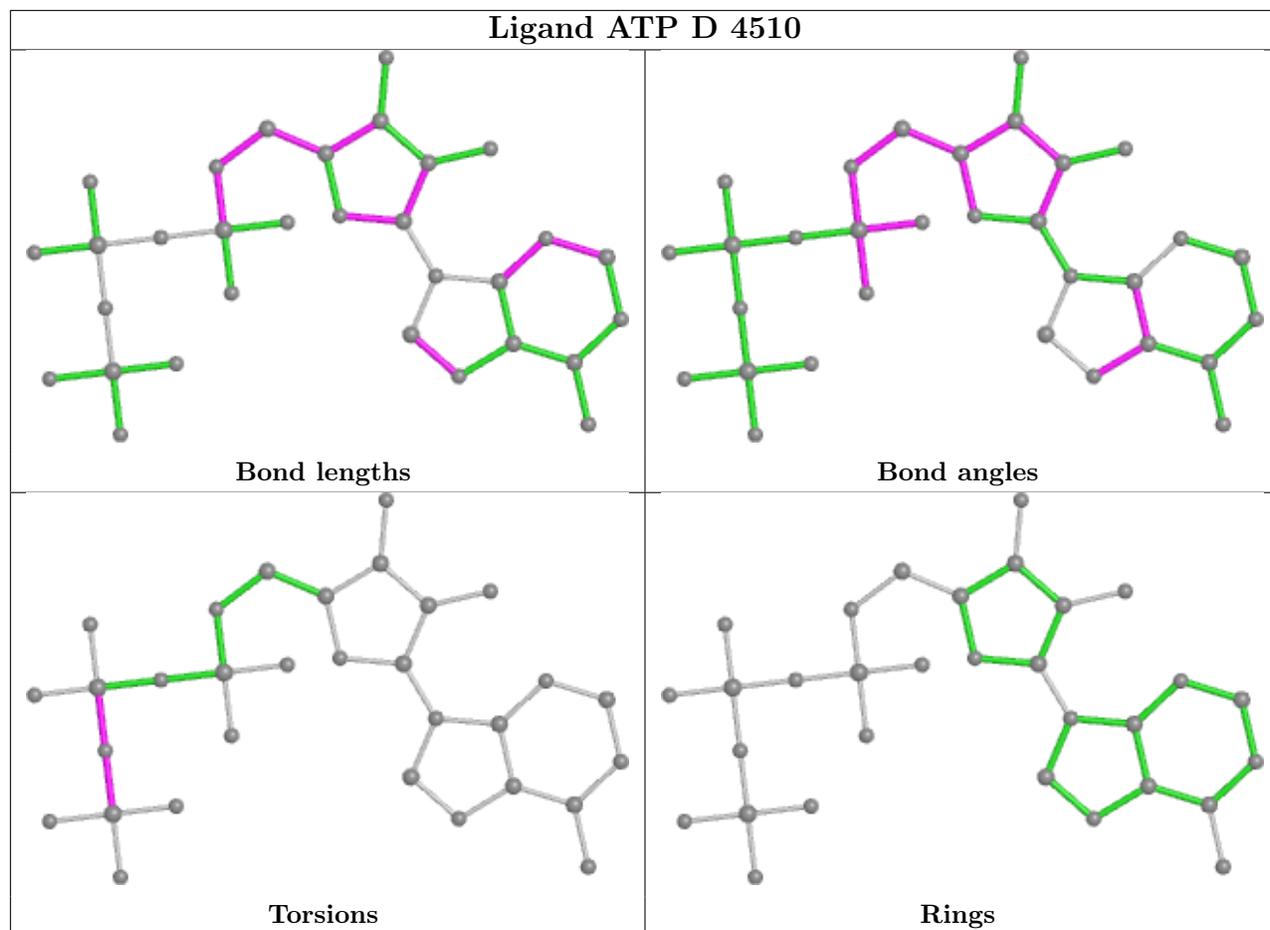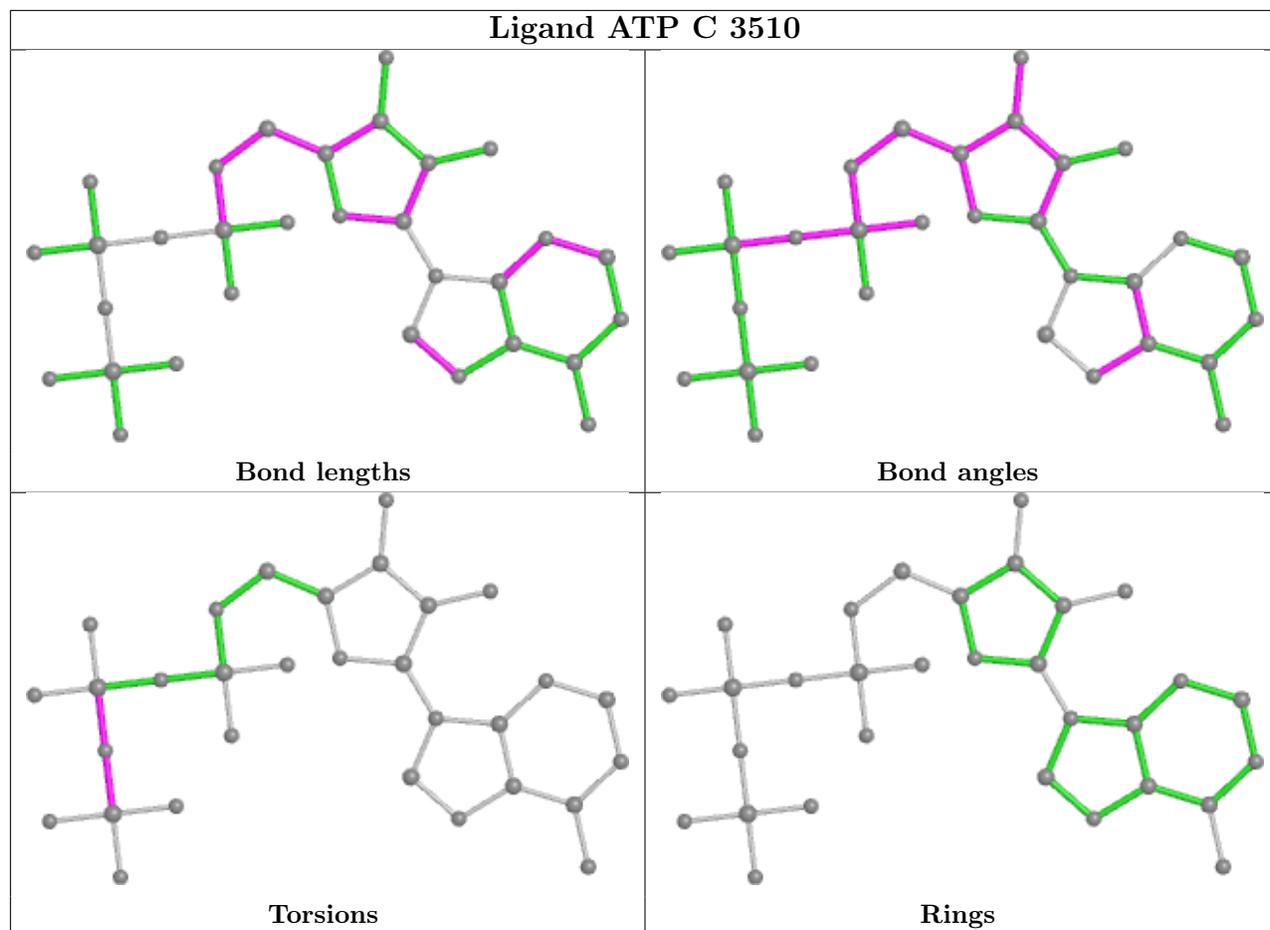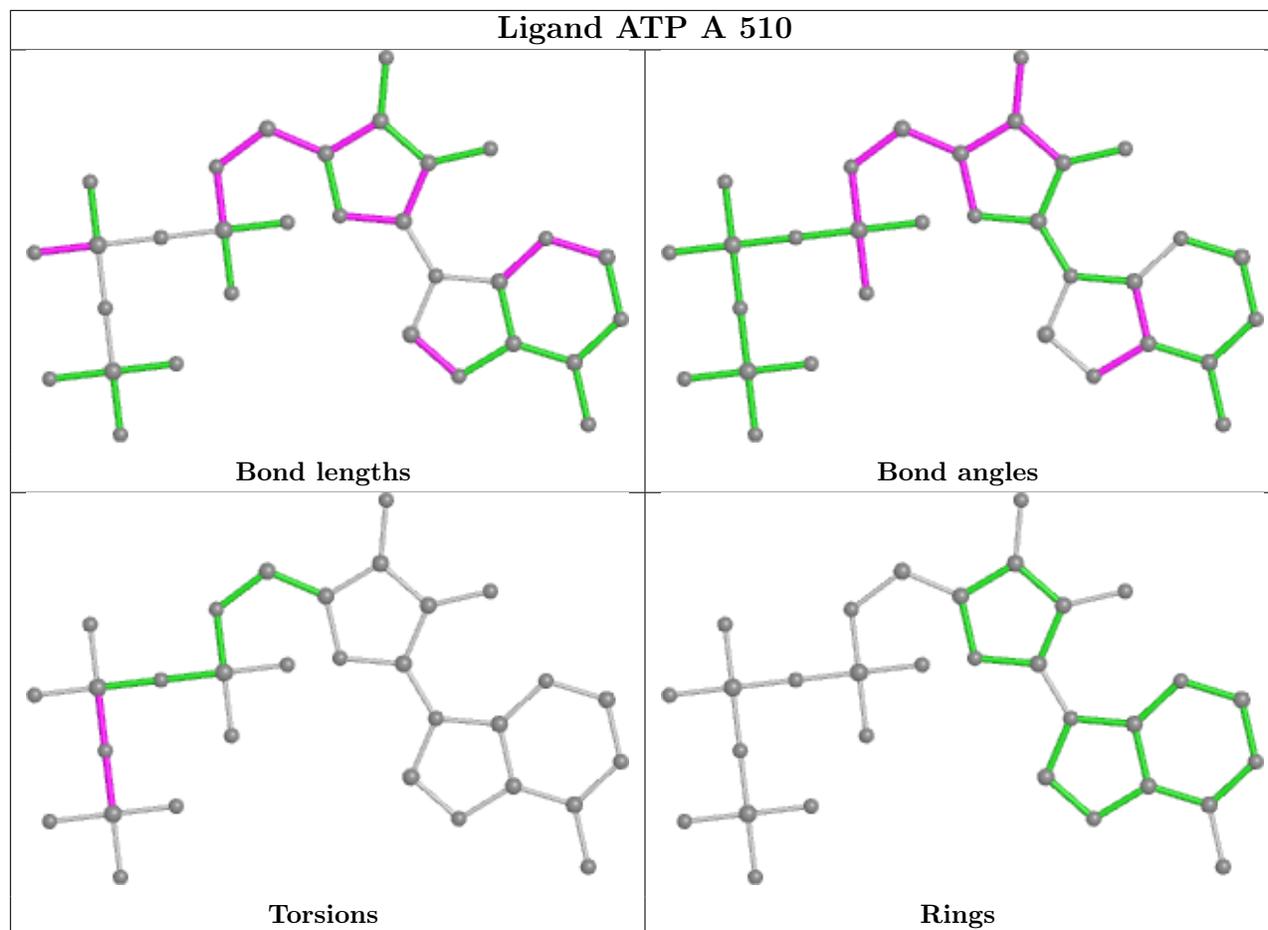
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	386/400 (96%)	-0.30	8 (2%)	63	68	23, 30, 51, 76	0
1	B	386/400 (96%)	-0.36	6 (1%)	72	75	22, 30, 47, 67	0
1	C	386/400 (96%)	-0.09	13 (3%)	45	51	23, 33, 60, 82	0
1	D	386/400 (96%)	-0.17	6 (1%)	72	75	22, 34, 57, 76	0
All	All	1544/1600 (96%)	-0.23	33 (2%)	63	68	22, 32, 56, 82	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	PRO	6.5
1	B	370	GLY	5.9
1	A	370	GLY	5.6
1	C	370	GLY	5.2
1	A	165	PRO	4.8
1	B	165	PRO	3.7
1	D	165	PRO	3.6
1	C	161	GLY	3.5
1	D	395	ARG	2.9
1	A	38	GLY	2.8
1	A	365	PHE	2.8
1	C	25	ARG	2.8
1	C	164	VAL	2.7
1	C	371	TYR	2.6
1	A	197	LYS	2.5
1	C	43	GLU	2.5
1	C	40	GLU	2.4
1	A	148	GLN	2.4
1	D	148	GLN	2.4
1	D	5	LEU	2.3
1	C	372	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	109	GLU	2.3
1	B	38	GLY	2.2
1	D	39	GLU	2.2
1	C	5	LEU	2.2
1	B	365	PHE	2.2
1	D	164	VAL	2.1
1	C	99	LEU	2.1
1	C	395	ARG	2.1
1	B	331	ARG	2.1
1	A	39	GLU	2.0
1	A	395	ARG	2.0
1	B	395	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
2	ATP	D	4510	31/31	0.75	0.20	50,55,79,80	0
2	ATP	B	2510	31/31	0.84	0.16	33,39,67,69	0
2	ATP	A	510	31/31	0.84	0.17	35,40,70,71	31
2	ATP	C	3510	31/31	0.85	0.17	43,47,68,70	0
3	CIR	C	3520	12/12	0.87	0.15	26,31,39,43	0
3	CIR	B	2520	12/12	0.89	0.13	22,27,34,40	0
3	CIR	A	520	12/12	0.90	0.14	24,30,36,45	0
3	CIR	D	4520	12/12	0.90	0.16	25,29,41,43	0
4	ASP	A	3530	9/9	0.95	0.10	25,27,29,30	0
4	ASP	A	4530	9/9	0.95	0.08	23,27,29,30	0
4	ASP	A	530	9/9	0.96	0.07	24,27,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ASP	A	2530	9/9	0.97	0.07	23,25,27,29	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 ATP D 4510:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
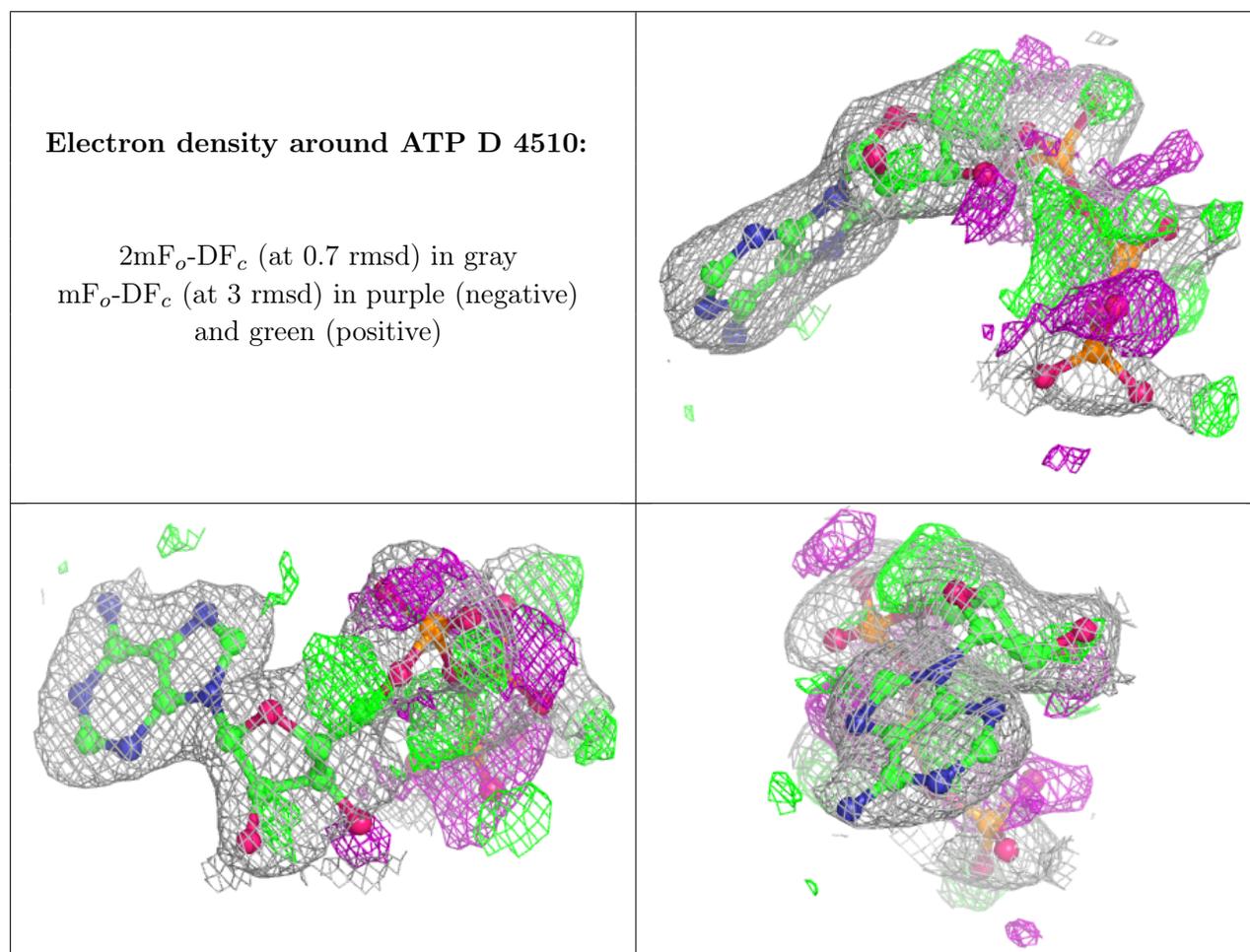
Electron density around ATP B 2510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
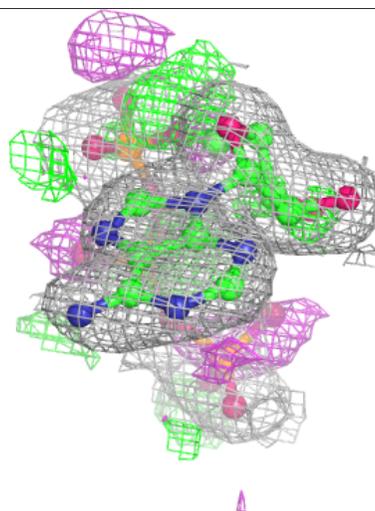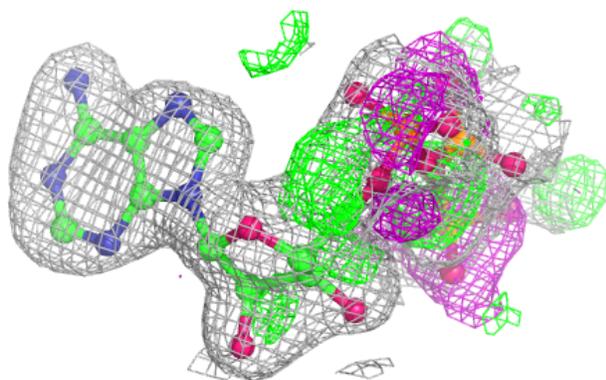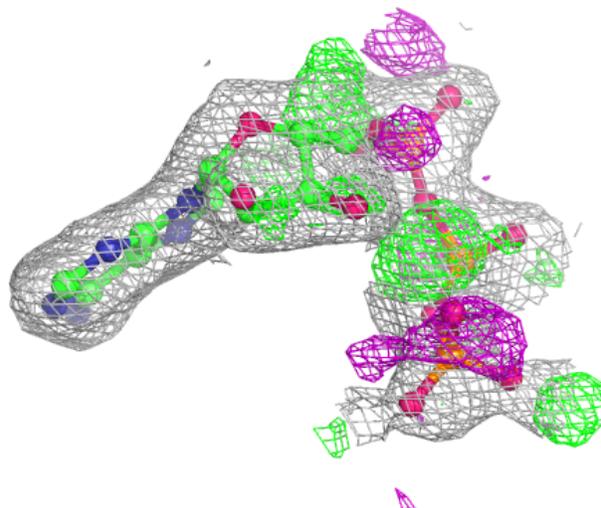
Electron density around ATP A 510:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
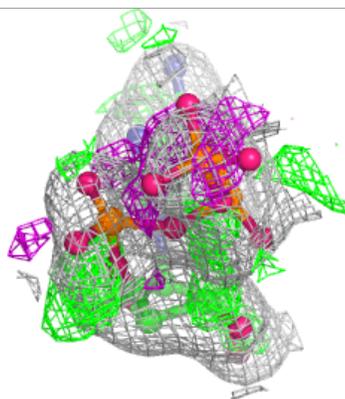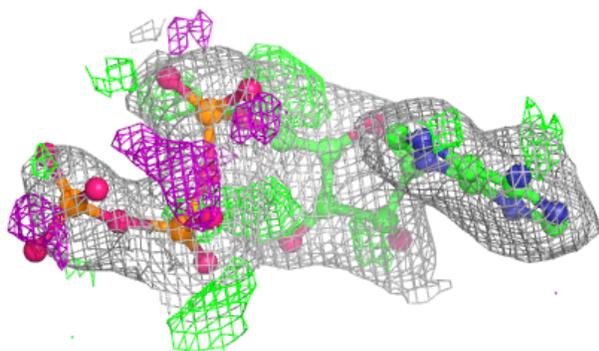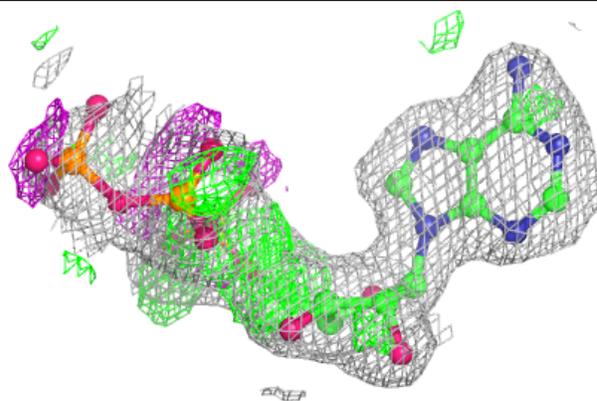
Electron density around ATP C 3510:

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 ⓘ

There are no such residues in this entry.