



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2024 – 12:22 AM EDT

PDB ID : 1J20
Title : Crystal Structure of Thermus thermophilus HB8 Argininosuccinate Synthetase in complex with product
Authors : Goto, M.; Hirotsu, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-12-24
Resolution : 2.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

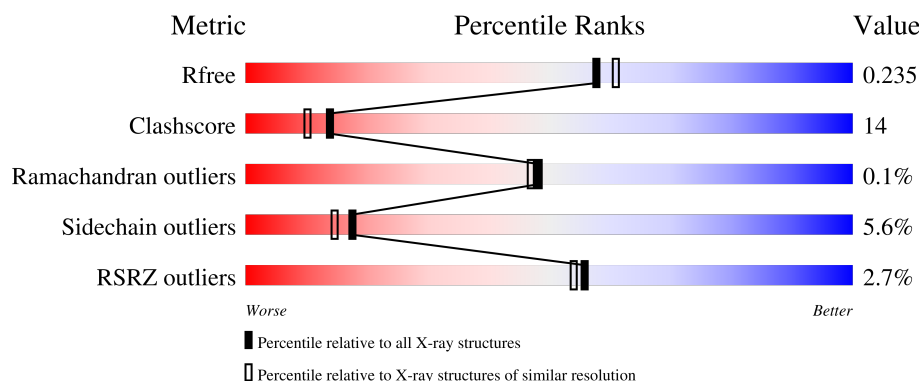
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	400	
1	B	400	
1	C	400	
1	D	400	

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
4	AS1	A	520	X	-	X	-
4	AS1	B	2520	X	X	-	-
4	AS1	C	3520	X	-	X	-
4	AS1	D	4520	X	X	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13318 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 SULFATE ION (three-letter code: SO₄) (formula: O₄S).



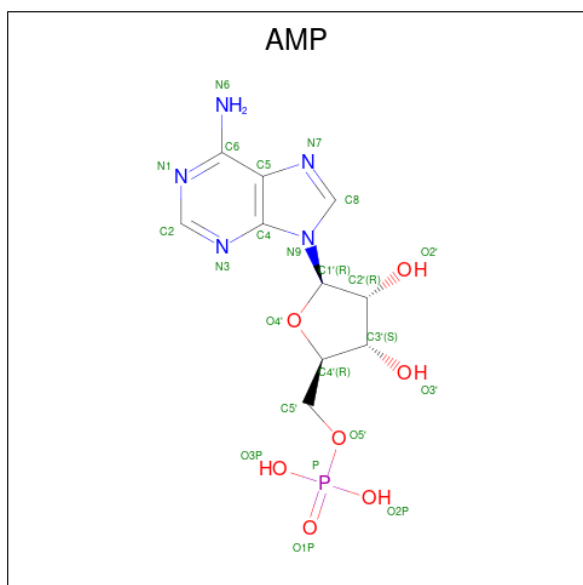
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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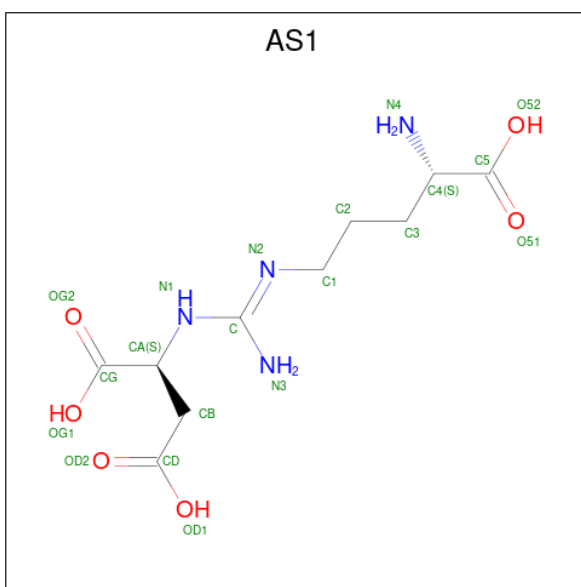
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is ARGININOSUCCINATE (three-letter code: AS1) (formula: $C_{10}H_{18}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 20	C 10	N 4	O 6	0	0
4	B	1	Total 20	C 10	N 4	O 6	0	0
4	C	1	Total 20	C 10	N 4	O 6	0	0
4	D	1	Total 20	C 10	N 4	O 6	0	0

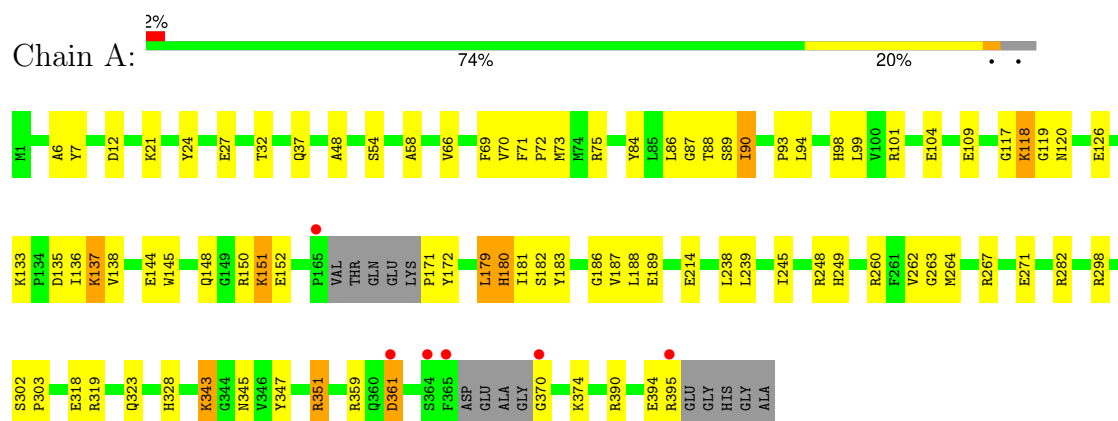
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	230	Total O 230 230	0	0
5	B	238	Total O 238 238	0	0
5	C	194	Total O 194 194	0	0
5	D	200	Total O 200 200	0	0

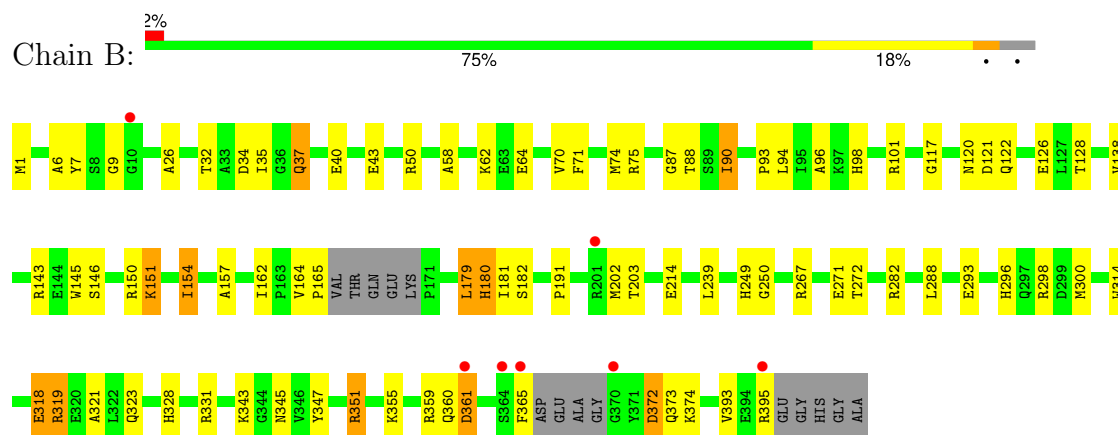
3 Residue-property plots

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.

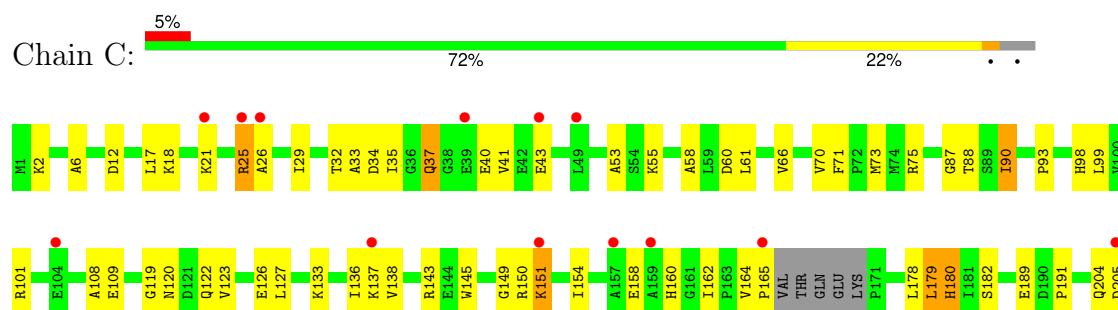
• Molecule 1: Argininosuccinate Synthetase

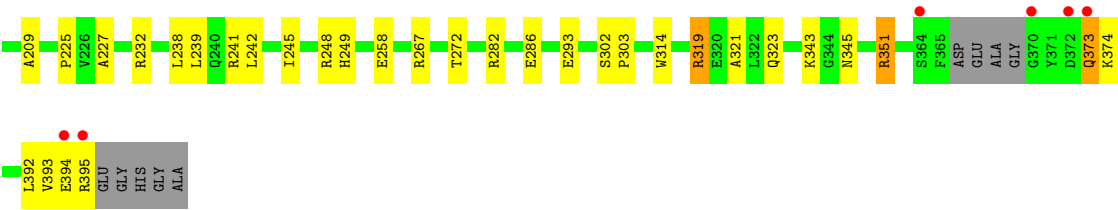


• Molecule 1: Argininosuccinate Synthetase

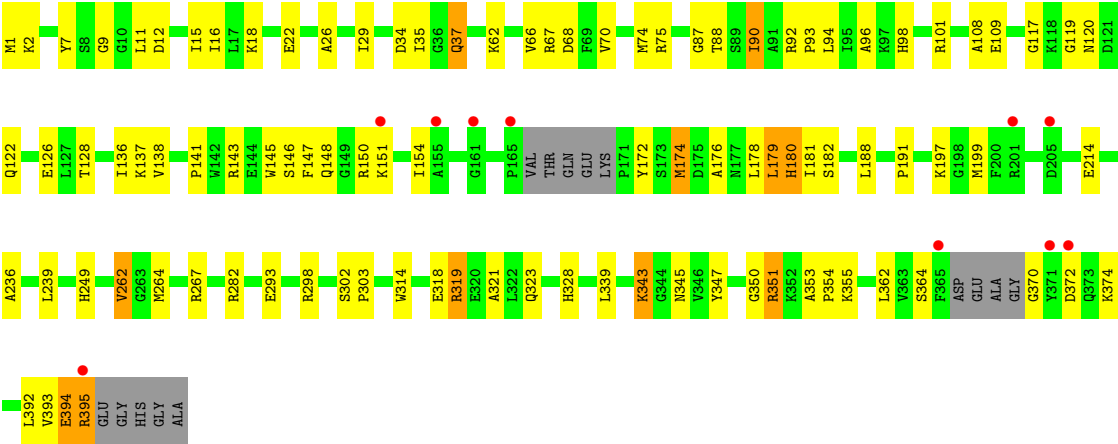


• Molecule 1: Argininosuccinate Synthetase





● 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	228.78Å 228.78Å 159.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 98.8 (10.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.239 0.208 , 0.235	Depositor DCC
R_{free} test set	20669 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.003 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13318	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, AS1, AMP

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	0.40	0/3135	0.66	1/4237 (0.0%)
1	B	0.39	0/3135	0.67	0/4237
1	C	0.41	0/3135	0.67	0/4237
1	D	0.40	0/3135	0.67	0/4237
All	All	0.40	0/12540	0.67	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(°)	Ideal(°)
1	A	263	GLY	N-CA-C	5.16	126.00	113.10

There are no chirality outliers.

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	3066	0	3052	78	0
1	B	3066	0	3052	95	0
1	C	3066	0	3052	103	0
1	D	3066	0	3052	96	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	23	0	12	2	0
3	B	23	0	12	3	0
3	C	23	0	12	1	0
3	D	23	0	12	2	0
4	A	20	0	13	8	0
4	B	20	0	13	6	0
4	C	20	0	13	9	0
4	D	20	0	11	8	0
5	A	230	0	0	12	0
5	B	238	0	0	8	0
5	C	194	0	0	7	0
5	D	200	0	0	5	0
All	All	13318	0	12306	352	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 14.

All (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:520:AS1:CB	4:A:520:AS1:CA	1.80	1.59
4:C:3520:AS1:CB	4:C:3520:AS1:CA	1.80	1.56
4:B:2520:AS1:CB	4:B:2520:AS1:CA	1.80	1.55
4:D:4520:AS1:CB	4:D:4520:AS1:CA	1.81	1.54
1:A:151:LYS:H	1:A:151:LYS:HD2	0.99	1.11
1:B:151:LYS:H	1:B:151:LYS:HD2	1.18	1.09
1:D:151:LYS:H	1:D:151:LYS:HD2	1.12	1.07
1:B:98:HIS:HD2	1:B:101:ARG:HH21	1.05	1.03
1:B:35:ILE:H	1:B:37:GLN:NE2	1.60	0.99
1:C:154:ILE:HG23	1:C:164:VAL:HG11	1.44	0.98
1:A:151:LYS:H	1:A:151:LYS:CD	1.79	0.94
1:A:151:LYS:HD2	1:A:151:LYS:N	1.81	0.92
1:A:98:HIS:HD2	1:A:101:ARG:HH21	1.15	0.90
1:D:351:ARG:HD2	1:D:351:ARG:N	1.87	0.89
1:C:35:ILE:H	1:C:37:GLN:NE2	1.69	0.88
1:A:359:ARG:NH2	5:A:1286:HOH:O	2.06	0.87
1:B:318:GLU:HG3	1:D:293:GLU:HB2	1.55	0.86
1:D:35:ILE:H	1:D:37:GLN:NE2	1.76	0.84
1:C:37:GLN:NE2	1:C:37:GLN:H	1.75	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:LYS:H	1:D:151:LYS:CD	1.91	0.83
1:B:181:ILE:HG13	1:B:202:MET:HE1	1.61	0.82
1:B:151:LYS:H	1:B:151:LYS:CD	1.93	0.82
1:A:351:ARG:HD2	1:A:351:ARG:N	1.95	0.80
1:C:37:GLN:H	1:C:37:GLN:HE21	1.28	0.80
1:B:98:HIS:CD2	1:B:101:ARG:HH21	1.97	0.79
1:B:126:GLU:HG2	1:B:138:VAL:HG11	1.65	0.78
1:C:18:LYS:HG3	1:C:162:ILE:HD11	1.66	0.78
1:B:318:GLU:HG3	1:D:293:GLU:CB	2.13	0.78
1:C:319:ARG:HH21	1:C:323:GLN:HE21	1.31	0.78
1:A:126:GLU:HG2	1:A:138:VAL:HG11	1.67	0.77
1:D:395:ARG:HG3	1:D:395:ARG:HH11	1.51	0.76
1:C:245:ILE:O	1:C:248:ARG:HG2	1.86	0.76
1:D:37:GLN:NE2	1:D:37:GLN:H	1.84	0.76
1:A:319:ARG:HH11	1:A:323:GLN:HE21	1.30	0.75
1:B:37:GLN:NE2	1:B:37:GLN:H	1.84	0.75
1:C:343:LYS:HD2	1:D:343:LYS:HD2	1.67	0.75
1:D:151:LYS:HD2	1:D:151:LYS:N	1.97	0.75
1:B:293:GLU:HB3	1:D:318:GLU:HG2	1.68	0.74
1:D:98:HIS:HD2	1:D:101:ARG:HH21	1.33	0.74
1:C:164:VAL:HG12	1:C:165:PRO:HD2	1.69	0.73
1:B:314:TRP:O	1:B:319:ARG:HD3	1.88	0.73
1:B:40:GLU:HG3	1:B:43:GLU:HG3	1.72	0.72
1:B:181:ILE:HG13	1:B:202:MET:CE	2.19	0.71
1:C:151:LYS:CD	1:C:151:LYS:H	2.04	0.70
1:B:35:ILE:H	1:B:37:GLN:HE22	1.40	0.70
1:D:109:GLU:O	1:D:137:LYS:HE2	1.91	0.70
4:A:520:AS1:CB	4:A:520:AS1:HA	2.17	0.70
4:C:3520:AS1:CB	4:C:3520:AS1:HA	2.17	0.69
1:C:351:ARG:HD2	1:C:351:ARG:N	2.07	0.69
1:A:318:GLU:CG	1:C:293:GLU:HB2	2.23	0.68
1:D:137:LYS:HD3	1:D:137:LYS:N	2.08	0.68
1:C:109:GLU:O	1:C:137:LYS:HE2	1.93	0.67
1:A:98:HIS:CD2	1:A:101:ARG:HH21	2.06	0.67
1:D:75:ARG:NH2	5:D:1529:HOH:O	2.26	0.67
1:C:40:GLU:CG	1:C:43:GLU:HG3	2.25	0.67
1:D:319:ARG:HH21	1:D:323:GLN:HE21	1.40	0.67
1:B:40:GLU:CG	1:B:43:GLU:HG3	2.25	0.67
1:B:319:ARG:HH21	1:B:323:GLN:HE21	1.42	0.67
1:D:37:GLN:H	1:D:37:GLN:HE21	1.42	0.67
3:B:2510:AMP:H5'1	3:B:2510:AMP:H8	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:O	1:A:248:ARG:HG2	1.96	0.65
1:D:282:ARG:HD2	5:D:1355:HOH:O	1.94	0.65
1:C:314:TRP:O	1:C:319:ARG:HD3	1.96	0.65
1:B:93:PRO:HG3	5:B:1181:HOH:O	1.97	0.65
1:C:351:ARG:HD3	1:D:191:PRO:HB2	1.78	0.65
5:A:1694:HOH:O	1:B:345:ASN:HB2	1.96	0.65
1:A:318:GLU:HG2	1:C:293:GLU:HB3	1.78	0.64
1:B:293:GLU:CB	1:D:318:GLU:HG2	2.28	0.64
5:A:1272:HOH:O	1:B:191:PRO:HG2	1.98	0.64
1:D:314:TRP:O	1:D:319:ARG:HD3	1.97	0.63
1:A:318:GLU:HG2	1:C:293:GLU:CB	2.29	0.63
1:B:151:LYS:HD2	1:B:151:LYS:N	2.01	0.63
1:C:12:ASP:OD1	1:C:150:ARG:NH2	2.31	0.63
1:B:37:GLN:H	1:B:37:GLN:HE21	1.45	0.63
1:D:395:ARG:HG3	1:D:395:ARG:NH1	2.12	0.63
1:C:35:ILE:H	1:C:37:GLN:HE22	1.43	0.62
1:C:119:GLY:HA3	4:C:3520:AS1:OD1	1.99	0.62
1:D:126:GLU:HG2	1:D:138:VAL:HG11	1.82	0.62
1:C:122:GLN:HE21	1:C:143:ARG:HH11	1.46	0.62
1:D:35:ILE:H	1:D:37:GLN:HE22	1.47	0.62
1:D:197:LYS:HG3	5:D:1447:HOH:O	1.98	0.62
1:A:214:GLU:OE1	1:A:249:HIS:HE1	1.83	0.62
1:B:293:GLU:HB2	1:D:318:GLU:CG	2.30	0.62
1:B:202:MET:HE2	5:B:1479:HOH:O	2.00	0.62
1:A:87:GLY:HA2	1:A:179:LEU:HD13	1.82	0.61
1:D:87:GLY:HA2	1:D:179:LEU:HD13	1.82	0.61
1:B:120:ASN:H	4:B:2520:AS1:CD	2.13	0.61
1:B:122:GLN:HE21	1:B:143:ARG:HH11	1.46	0.61
1:C:395:ARG:HG3	1:C:395:ARG:HH11	1.64	0.61
1:B:35:ILE:N	1:B:37:GLN:NE2	2.40	0.61
1:B:318:GLU:CG	1:D:293:GLU:CB	2.79	0.61
1:D:120:ASN:N	4:D:4520:AS1:OD2	2.35	0.60
1:C:88:THR:HG21	4:C:3520:AS1:H12	1.84	0.60
1:A:119:GLY:HA3	4:A:520:AS1:OD2	2.02	0.60
3:B:2510:AMP:H5'1	3:B:2510:AMP:C8	2.38	0.59
1:D:29:ILE:HD12	1:D:29:ILE:N	2.17	0.59
1:B:150:ARG:O	1:B:154:ILE:HD12	2.02	0.59
1:B:282:ARG:NH2	5:B:1160:HOH:O	2.36	0.59
4:D:4520:AS1:CB	4:D:4520:AS1:HA	2.19	0.59
1:C:248:ARG:HG3	1:C:249:HIS:CD2	2.37	0.59
1:C:35:ILE:N	1:C:37:GLN:NE2	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:GLU:OE1	1:D:249:HIS:HE1	1.86	0.59
1:A:318:GLU:HG3	1:C:293:GLU:HB2	1.84	0.58
1:A:374:LYS:NZ	1:D:374:LYS:HE3	2.18	0.58
1:B:293:GLU:CB	1:D:318:GLU:CG	2.81	0.58
1:C:98:HIS:HD2	1:C:101:ARG:NH1	2.02	0.58
1:A:27:GLU:HG2	1:A:54:SER:OG	2.02	0.58
5:C:1151:HOH:O	1:D:191:PRO:HG2	2.04	0.57
1:D:1:MET:O	1:D:26:ALA:HB1	2.04	0.57
1:C:41:VAL:HG12	1:C:58:ALA:HB1	1.85	0.57
1:C:151:LYS:H	1:C:151:LYS:HD2	1.68	0.57
1:A:88:THR:HG21	4:A:520:AS1:H12	1.87	0.57
1:D:394:GLU:O	1:D:395:ARG:C	2.43	0.57
1:B:88:THR:HG21	4:B:2520:AS1:H12	1.86	0.57
1:D:67:ARG:HD2	1:D:68:ASP:OD1	2.04	0.57
1:A:109:GLU:O	1:A:137:LYS:HE2	2.05	0.57
1:D:119:GLY:HA3	4:D:4520:AS1:OD2	2.04	0.57
1:C:120:ASN:N	4:C:3520:AS1:OD1	2.38	0.56
1:B:122:GLN:NE2	1:B:143:ARG:HH11	2.03	0.56
1:B:214:GLU:OE1	1:B:249:HIS:HE1	1.88	0.56
1:B:293:GLU:HB2	1:D:318:GLU:HG3	1.87	0.56
1:C:98:HIS:CD2	1:C:101:ARG:NH1	2.74	0.56
1:D:74:MET:HE2	5:D:1833:HOH:O	2.05	0.56
1:B:314:TRP:CE3	1:B:319:ARG:HD2	2.41	0.56
1:C:164:VAL:CG1	1:C:165:PRO:HD2	2.34	0.56
1:D:136:ILE:C	1:D:137:LYS:HD3	2.25	0.56
1:C:343:LYS:HD2	1:D:343:LYS:CD	2.35	0.56
1:D:122:GLN:HE21	1:D:143:ARG:HH11	1.52	0.56
1:C:162:ILE:O	1:C:164:VAL:HG23	2.07	0.55
1:C:319:ARG:HH21	1:C:323:GLN:NE2	2.02	0.55
1:A:90:ILE:HD11	1:A:179:LEU:HD12	1.88	0.55
1:A:318:GLU:CG	1:C:293:GLU:CB	2.84	0.55
1:C:21:LYS:HD2	1:C:26:ALA:O	2.06	0.55
1:A:120:ASN:N	4:A:520:AS1:OD2	2.39	0.55
1:C:133:LYS:HD3	1:C:136:ILE:HD13	1.86	0.55
1:C:33:ALA:HB1	1:C:61:LEU:HD12	1.88	0.55
1:C:122:GLN:NE2	1:C:143:ARG:HH11	2.05	0.55
1:D:7:TYR:CZ	1:D:9:GLY:HA2	2.42	0.54
1:B:87:GLY:HA2	1:B:179:LEU:HD13	1.88	0.54
1:C:343:LYS:CD	1:D:343:LYS:HD2	2.36	0.54
1:C:2:LYS:HB2	1:C:108:ALA:HA	1.90	0.54
1:B:374:LYS:HG2	1:B:374:LYS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASN:H	4:D:4520:AS1:CD	2.21	0.54
1:A:319:ARG:NH1	1:A:323:GLN:HE21	2.04	0.53
1:B:70:VAL:O	1:B:74:MET:HG3	2.09	0.53
1:C:164:VAL:HG12	1:C:165:PRO:CD	2.36	0.53
1:C:189:GLU:O	1:C:191:PRO:HD3	2.08	0.53
1:C:40:GLU:HG2	1:C:43:GLU:HG3	1.91	0.53
1:B:318:GLU:CG	1:D:293:GLU:HB3	2.37	0.53
1:C:126:GLU:HG2	1:C:138:VAL:HG11	1.91	0.53
1:D:88:THR:HG21	4:D:4520:AS1:H12	1.90	0.53
1:A:120:ASN:H	4:A:520:AS1:CD	2.22	0.53
1:B:40:GLU:HB3	1:B:43:GLU:HG3	1.91	0.52
1:D:351:ARG:N	1:D:351:ARG:CD	2.67	0.52
1:A:395:ARG:NH1	5:A:1722:HOH:O	2.41	0.52
1:C:21:LYS:O	1:C:25:ARG:HA	2.08	0.52
1:D:146:SER:O	1:D:148:GLN:HG3	2.10	0.52
1:C:32:THR:CG2	1:C:41:VAL:HG13	2.39	0.52
1:C:374:LYS:HE2	5:C:1586:HOH:O	2.08	0.52
1:A:343:LYS:HD2	1:B:343:LYS:HD3	1.90	0.52
1:B:372:ASP:OD2	1:B:372:ASP:C	2.48	0.52
1:C:151:LYS:HD2	1:C:151:LYS:N	2.24	0.52
1:D:345:ASN:HB3	1:D:347:TYR:CE1	2.44	0.52
1:D:98:HIS:CD2	1:D:101:ARG:HH21	2.23	0.52
1:C:373:GLN:HG3	1:D:117:GLY:HA3	1.92	0.52
1:D:18:LYS:O	1:D:22:GLU:HG3	2.09	0.52
1:B:1:MET:O	1:B:26:ALA:HB1	2.10	0.52
1:B:35:ILE:N	1:B:37:GLN:HE22	2.04	0.52
1:A:395:ARG:HH22	1:D:355:LYS:HE3	1.75	0.51
1:C:37:GLN:HE21	1:C:37:GLN:N	2.03	0.51
1:C:18:LYS:HE3	1:C:160:HIS:HB3	1.92	0.51
1:D:350:GLY:C	1:D:351:ARG:HD2	2.29	0.51
1:C:209:ALA:O	1:C:343:LYS:NZ	2.42	0.51
1:A:374:LYS:HZ2	1:D:374:LYS:HE3	1.75	0.51
1:B:359:ARG:HB3	1:B:361:ASP:HB2	1.93	0.51
1:B:318:GLU:HG3	1:D:293:GLU:HB3	1.93	0.51
1:B:179:LEU:O	1:B:272:THR:HG23	2.11	0.51
1:A:93:PRO:HG3	5:A:1256:HOH:O	2.10	0.50
1:D:393:VAL:O	1:D:395:ARG:HG3	2.11	0.50
1:C:180:HIS:ND1	1:C:180:HIS:C	2.64	0.50
1:C:227:ALA:HB2	1:C:232:ARG:HD2	1.92	0.50
1:D:93:PRO:HG3	5:D:1293:HOH:O	2.11	0.50
1:A:302:SER:HB2	1:A:303:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:HD3	1:B:191:PRO:HB2	1.93	0.50
1:C:35:ILE:N	1:C:37:GLN:HE22	2.06	0.50
1:A:180:HIS:C	1:A:180:HIS:ND1	2.64	0.50
1:A:12:ASP:OD1	1:A:150:ARG:NH2	2.33	0.50
1:A:119:GLY:HA3	4:A:520:AS1:CD	2.41	0.50
1:A:249:HIS:HD2	5:A:1159:HOH:O	1.94	0.50
1:C:73:MET:CE	1:C:90:ILE:HG12	2.42	0.49
1:C:154:ILE:HG23	1:C:164:VAL:CG1	2.30	0.49
1:C:90:ILE:HD11	1:C:179:LEU:HD12	1.94	0.49
1:B:249:HIS:HD2	5:B:1825:HOH:O	1.95	0.49
1:C:164:VAL:CG1	1:C:165:PRO:CD	2.89	0.49
1:B:34:ASP:HA	1:B:37:GLN:HE22	1.76	0.49
1:B:122:GLN:HE22	1:B:143:ARG:HD3	1.78	0.49
1:D:12:ASP:OD1	1:D:150:ARG:NH2	2.37	0.49
1:B:318:GLU:CG	1:D:293:GLU:HB2	2.35	0.49
1:C:179:LEU:O	1:C:272:THR:HG23	2.12	0.49
1:C:93:PRO:HG3	5:C:1406:HOH:O	2.12	0.48
1:B:202:MET:CE	5:B:1479:HOH:O	2.60	0.48
1:A:6:ALA:HB1	3:A:510:AMP:N3	2.29	0.48
1:C:6:ALA:HB2	1:C:99:LEU:HD11	1.96	0.48
1:C:204:GLN:HG2	5:C:1667:HOH:O	2.13	0.48
1:A:117:GLY:H	1:B:373:GLN:NE2	2.11	0.48
1:C:149:GLY:HA3	1:C:151:LYS:HE3	1.95	0.48
1:B:296:HIS:O	1:B:300:MET:HE2	2.14	0.48
1:C:302:SER:HB2	1:C:303:PRO:HD3	1.94	0.47
1:B:121:ASP:N	4:B:2520:AS1:OD2	2.28	0.47
1:B:328:HIS:CE1	1:B:331:ARG:HH22	2.32	0.47
1:C:151:LYS:CD	1:C:151:LYS:N	2.76	0.47
1:D:11:LEU:O	1:D:15:ILE:HG13	2.14	0.47
1:D:16:ILE:HG23	1:D:141:PRO:HG2	1.97	0.47
1:A:148:GLN:HB2	1:A:152:GLU:OE2	2.14	0.47
1:B:87:GLY:HA3	1:B:180:HIS:CD2	2.49	0.47
1:C:258:GLU:OE2	4:C:3520:AS1:N4	2.48	0.47
1:B:180:HIS:ND1	1:B:180:HIS:C	2.66	0.47
1:A:24:TYR:OH	1:A:144:GLU:OE2	2.28	0.47
1:D:176:ALA:CB	1:D:181:ILE:HG12	2.45	0.47
1:D:122:GLN:NE2	1:D:143:ARG:HH11	2.13	0.47
1:A:137:LYS:N	1:A:137:LYS:HD3	2.30	0.46
1:A:171:PRO:HB2	1:A:187:VAL:HG13	1.96	0.46
1:A:189:GLU:OE2	1:B:360:GLN:OE1	2.33	0.46
1:B:96:ALA:HB3	1:B:128:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLY:HA3	4:C:3520:AS1:CD	2.44	0.46
1:A:71:PHE:O	1:A:75:ARG:HG3	2.14	0.46
1:B:321:ALA:HA	1:D:328:HIS:CD2	2.50	0.46
1:C:71:PHE:O	1:C:75:ARG:HG3	2.14	0.46
1:B:90:ILE:HD11	1:B:179:LEU:HD12	1.97	0.46
1:C:154:ILE:CG2	1:C:164:VAL:HG11	2.31	0.46
1:D:302:SER:HB2	1:D:303:PRO:HD3	1.97	0.46
1:B:164:VAL:HG13	1:B:165:PRO:HD2	1.96	0.46
1:A:359:ARG:NH1	1:A:361:ASP:OD2	2.48	0.46
1:D:2:LYS:HB2	1:D:108:ALA:HA	1.98	0.46
1:D:180:HIS:ND1	1:D:180:HIS:C	2.69	0.46
1:A:395:ARG:NH1	5:A:1382:HOH:O	2.49	0.46
1:A:328:HIS:CD2	1:C:321:ALA:HA	2.51	0.46
3:C:3510:AMP:H5'1	3:C:3510:AMP:H8	1.79	0.46
1:B:180:HIS:CD2	5:B:1074:HOH:O	2.69	0.45
4:B:2520:AS1:CB	4:B:2520:AS1:C	2.94	0.45
1:D:150:ARG:O	1:D:154:ILE:HD12	2.16	0.45
1:A:370:GLY:N	5:A:1286:HOH:O	2.49	0.45
1:B:6:ALA:HB1	3:B:2510:AMP:N3	2.31	0.45
1:D:90:ILE:HD11	1:D:179:LEU:HD12	1.98	0.45
1:D:96:ALA:HB3	1:D:128:THR:HG21	1.98	0.45
1:D:262:VAL:O	1:D:262:VAL:HG13	2.16	0.45
1:A:282:ARG:HD2	5:A:1351:HOH:O	2.17	0.45
1:B:151:LYS:CD	1:B:151:LYS:N	2.71	0.45
4:B:2520:AS1:CB	4:B:2520:AS1:HA	2.21	0.45
1:C:392:LEU:O	1:C:395:ARG:N	2.48	0.45
1:D:174:MET:HA	1:D:182:SER:O	2.16	0.45
1:A:118:LYS:HD3	1:B:365:PHE:CE2	2.51	0.45
1:C:393:VAL:O	1:C:395:ARG:NH1	2.49	0.45
1:A:6:ALA:HB2	1:A:99:LEU:HD11	1.99	0.45
1:B:40:GLU:CB	1:B:43:GLU:HG3	2.46	0.45
1:B:71:PHE:O	1:B:75:ARG:HG3	2.15	0.45
1:B:355:LYS:NZ	1:C:394:GLU:OE1	2.49	0.45
1:A:73:MET:CE	1:A:90:ILE:HG12	2.46	0.45
1:C:40:GLU:HG3	1:C:43:GLU:HG3	1.99	0.45
1:C:395:ARG:HG3	1:C:395:ARG:NH1	2.32	0.45
1:D:66:VAL:HA	1:D:70:VAL:HB	1.97	0.45
1:A:66:VAL:HA	1:A:70:VAL:HB	1.98	0.45
1:A:298:ARG:C	1:A:298:ARG:HD2	2.37	0.45
1:C:34:ASP:HB3	1:C:60:ASP:HA	1.99	0.45
1:C:393:VAL:C	1:C:395:ARG:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:CZ	1:A:86:LEU:HA	2.52	0.44
1:D:66:VAL:HG21	1:D:236:ALA:HA	1.99	0.44
1:B:319:ARG:HH21	1:B:323:GLN:NE2	2.11	0.44
3:A:510:AMP:H5'1	3:A:510:AMP:H8	1.82	0.44
1:B:180:HIS:HD2	5:B:1074:HOH:O	2.00	0.44
1:B:393:VAL:C	1:B:395:ARG:H	2.20	0.44
1:C:101:ARG:HD3	5:C:1261:HOH:O	2.17	0.44
1:D:117:GLY:HA2	1:D:122:GLN:NE2	2.32	0.44
1:B:393:VAL:C	1:B:395:ARG:N	2.69	0.44
1:C:17:LEU:O	1:C:17:LEU:HD23	2.17	0.44
1:A:238:LEU:C	1:A:238:LEU:HD23	2.38	0.44
1:C:120:ASN:H	4:C:3520:AS1:CD	2.30	0.44
3:D:4510:AMP:O2P	4:D:4520:AS1:C	2.66	0.44
1:A:117:GLY:HA3	1:B:373:GLN:NE2	2.32	0.44
1:D:92:ARG:NH2	3:D:4510:AMP:H5'2	2.33	0.44
1:B:32:THR:O	1:B:58:ALA:HA	2.17	0.44
1:C:241:ARG:NH2	5:C:1653:HOH:O	2.47	0.44
4:C:3520:AS1:CB	4:C:3520:AS1:C	2.95	0.44
1:A:345:ASN:HB3	1:A:347:TYR:CE1	2.53	0.43
1:B:318:GLU:HG2	1:D:293:GLU:HB3	1.99	0.43
1:D:146:SER:O	1:D:147:PHE:C	2.56	0.43
1:B:117:GLY:HA2	1:B:122:GLN:NE2	2.33	0.43
1:A:260:ARG:HD2	1:A:264:MET:SD	2.58	0.43
1:B:157:ALA:HB1	1:B:162:ILE:HB	2.00	0.43
1:C:238:LEU:C	1:C:238:LEU:HD23	2.38	0.43
1:D:34:ASP:HA	1:D:37:GLN:HE22	1.83	0.43
1:A:104:GLU:OE1	1:A:133:LYS:NZ	2.51	0.43
1:D:339:LEU:N	1:D:339:LEU:HD12	2.33	0.43
4:A:520:AS1:CB	4:A:520:AS1:C	2.97	0.43
1:B:298:ARG:HD2	1:B:298:ARG:O	2.18	0.43
1:A:282:ARG:NH2	5:A:1218:HOH:O	2.51	0.43
1:B:37:GLN:HE21	1:B:37:GLN:N	2.14	0.43
1:B:180:HIS:HB2	1:B:271:GLU:O	2.19	0.43
1:B:288:LEU:HG	1:B:351:ARG:HG3	1.99	0.43
1:A:171:PRO:O	1:A:186:GLY:HA3	2.18	0.43
1:D:35:ILE:N	1:D:37:GLN:NE2	2.56	0.43
1:A:86:LEU:HB3	1:A:89:SER:HB2	2.01	0.43
1:C:17:LEU:HD11	1:C:53:ALA:HB2	2.01	0.43
1:A:390:ARG:O	1:A:394:GLU:HG2	2.19	0.42
1:B:98:HIS:HD2	1:B:101:ARG:NH2	1.90	0.42
1:A:69:PHE:C	1:A:72:PRO:HD2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ALA:HA	1:D:354:PRO:HD3	1.89	0.42
1:A:180:HIS:HB2	1:A:271:GLU:O	2.20	0.42
1:C:29:ILE:HD12	1:C:55:LYS:HB3	2.02	0.42
1:A:171:PRO:HG2	1:A:172:TYR:CD2	2.54	0.42
1:D:117:GLY:HA2	1:D:122:GLN:HE22	1.85	0.42
1:D:314:TRP:CE3	1:D:319:ARG:HD2	2.55	0.42
1:B:50:ARG:NH1	5:B:1836:HOH:O	2.53	0.42
1:A:248:ARG:HG3	1:A:249:HIS:ND1	2.35	0.41
1:D:7:TYR:CE2	1:D:9:GLY:HA2	2.55	0.41
1:A:7:TYR:CE2	1:A:48:ALA:HB2	2.56	0.41
1:A:136:ILE:HG13	1:A:137:LYS:N	2.35	0.41
1:A:118:LYS:HD3	1:B:365:PHE:CZ	2.56	0.41
1:A:359:ARG:HG2	5:A:1609:HOH:O	2.20	0.41
1:C:122:GLN:HE21	1:C:143:ARG:NH1	2.17	0.41
1:D:395:ARG:NH1	1:D:395:ARG:CG	2.80	0.41
1:A:262:VAL:HG13	5:A:1759:HOH:O	2.20	0.41
1:A:298:ARG:HD2	1:A:298:ARG:O	2.21	0.41
1:B:328:HIS:CD2	1:D:321:ALA:HA	2.56	0.41
1:C:393:VAL:C	1:C:395:ARG:N	2.74	0.41
1:D:362:LEU:CD2	1:D:370:GLY:HA3	2.50	0.41
1:D:392:LEU:O	1:D:395:ARG:N	2.54	0.41
1:C:123:VAL:HG12	1:C:127:LEU:CD1	2.51	0.41
1:D:197:LYS:HE2	1:D:197:LYS:HB3	1.92	0.41
1:D:319:ARG:HH21	1:D:323:GLN:NE2	2.11	0.41
1:A:181:ILE:HG22	1:A:183:TYR:CE1	2.56	0.41
1:B:345:ASN:HB3	1:B:347:TYR:CE1	2.55	0.41
1:C:71:PHE:CZ	1:C:225:PRO:HG2	2.56	0.41
1:C:158:GLU:HG3	1:C:164:VAL:HG21	2.03	0.41
1:C:314:TRP:O	1:C:319:ARG:CD	2.67	0.41
1:C:314:TRP:HA	1:C:319:ARG:HD2	2.03	0.41
4:D:4520:AS1:CB	4:D:4520:AS1:C	2.98	0.41
1:B:355:LYS:CE	1:C:394:GLU:OE1	2.69	0.41
1:A:32:THR:O	1:A:58:ALA:HA	2.21	0.40
1:D:172:TYR:CZ	1:D:199:MET:HG3	2.57	0.40
1:B:203:THR:HB	1:B:250:GLY:HA2	2.03	0.40
1:C:66:VAL:HA	1:C:70:VAL:HB	2.03	0.40
1:C:101:ARG:NH2	5:C:1507:HOH:O	2.49	0.40
1:C:282:ARG:O	1:C:286:GLU:HG3	2.22	0.40
1:A:394:GLU:O	1:A:395:ARG:HB2	2.22	0.40
1:C:204:GLN:HG3	1:C:205:ASP:N	2.36	0.40
1:C:392:LEU:O	1:C:395:ARG:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ARG:O	1:D:298:ARG:HD2	2.21	0.40
1:B:7:TYR:CE2	1:B:9:GLY:HA2	2.55	0.40
1:B:64:GLU:OE1	1:B:98:HIS:HE1	2.05	0.40
1:C:242:LEU:HD23	1:C:242:LEU:HA	1.92	0.40
1:C:87:GLY:HA3	1:C:180:HIS:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/400 (95%)	373 (98%)	6 (2%)	1 (0%)	37	35
1	B	380/400 (95%)	369 (97%)	11 (3%)	0	100	100
1	C	380/400 (95%)	372 (98%)	8 (2%)	0	100	100
1	D	380/400 (95%)	372 (98%)	7 (2%)	1 (0%)	37	35
All	All	1520/1600 (95%)	1486 (98%)	32 (2%)	2 (0%)	48	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	LYS
1	D	343	LYS

5.3.2 Protein sidechains [i](#)

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%)	293 (94%)	17 (6%)	18	15
1	B	310/319 (97%)	292 (94%)	18 (6%)	17	14
1	C	310/319 (97%)	295 (95%)	15 (5%)	21	19
1	D	310/319 (97%)	290 (94%)	20 (6%)	14	11
All	All	1240/1276 (97%)	1170 (94%)	70 (6%)	17	15

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	37	GLN
1	A	90	ILE
1	A	94	LEU
1	A	118	LYS
1	A	135	ASP
1	A	137	LYS
1	A	145	TRP
1	A	151	LYS
1	A	179	LEU
1	A	180	HIS
1	A	182	SER
1	A	188	LEU
1	A	239	LEU
1	A	267	ARG
1	A	351	ARG
1	A	361	ASP
1	B	37	GLN
1	B	62	LYS
1	B	90	ILE
1	B	94	LEU
1	B	145	TRP
1	B	146	SER
1	B	151	LYS
1	B	154	ILE
1	B	179	LEU
1	B	180	HIS
1	B	182	SER
1	B	239	LEU
1	B	267	ARG
1	B	318	GLU

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Mol	Chain	Res	Type
1	B	319	ARG
1	B	351	ARG
1	B	361	ASP
1	B	372	ASP
1	C	25	ARG
1	C	37	GLN
1	C	90	ILE
1	C	145	TRP
1	C	151	LYS
1	C	178	LEU
1	C	179	LEU
1	C	180	HIS
1	C	182	SER
1	C	239	LEU
1	C	267	ARG
1	C	319	ARG
1	C	345	ASN
1	C	351	ARG
1	C	373	GLN
1	D	37	GLN
1	D	62	LYS
1	D	90	ILE
1	D	94	LEU
1	D	145	TRP
1	D	174	MET
1	D	178	LEU
1	D	179	LEU
1	D	180	HIS
1	D	188	LEU
1	D	239	LEU
1	D	262	VAL
1	D	264	MET
1	D	267	ARG
1	D	319	ARG
1	D	351	ARG
1	D	364	SER
1	D	372	ASP
1	D	394	GLU
1	D	395	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	180	HIS
1	A	249	HIS
1	A	323	GLN
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	323	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	345	ASN
1	C	360	GLN
1	C	373	GLN
1	D	37	GLN
1	D	98	HIS
1	D	122	GLN
1	D	180	HIS
1	D	249	HIS
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 oligosaccharides 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	SO4	C	3540	-	4,4,4	1.73	1 (25%)	6,6,6	0.89	0
3	AMP	B	2510	-	21,25,25	3.12	14 (66%)	23,38,38	2.31	9 (39%)
2	SO4	B	2540	-	4,4,4	1.79	1 (25%)	6,6,6	0.80	0
3	AMP	D	4510	-	21,25,25	2.78	12 (57%)	23,38,38	2.24	10 (43%)
3	AMP	A	510	-	21,25,25	2.96	12 (57%)	23,38,38	2.21	8 (34%)
4	AS1	B	2520	-	18,19,19	3.88	6 (33%)	19,24,24	7.09	13 (68%)
4	AS1	C	3520	-	18,19,19	3.80	5 (27%)	19,24,24	7.11	11 (57%)
4	AS1	A	520	-	18,19,19	3.88	5 (27%)	19,24,24	7.17	11 (57%)
3	AMP	C	3510	-	21,25,25	2.83	12 (57%)	23,38,38	2.35	10 (43%)
2	SO4	A	540	-	4,4,4	1.52	1 (25%)	6,6,6	0.91	0
4	AS1	D	4520	-	18,19,19	3.91	5 (27%)	19,24,24	7.78	13 (68%)
2	SO4	D	4540	-	4,4,4	1.69	1 (25%)	6,6,6	0.86	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
3	AMP	B	2510	-	-	1/6/26/26	0/3/3/3
3	AMP	D	4510	-	-	0/6/26/26	0/3/3/3
3	AMP	A	510	-	-	0/6/26/26	0/3/3/3
4	AS1	C	3520	-	1/1/6/7	10/21/23/23	-
4	AS1	A	520	-	1/1/6/7	10/21/23/23	-
3	AMP	C	3510	-	-	1/6/26/26	0/3/3/3
4	AS1	B	2520	-	1/1/6/7	10/21/23/23	-
4	AS1	D	4520	-	1/1/6/7	9/21/23/23	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4520	AS1	CB-CA	13.28	1.81	1.53
4	A	520	AS1	CB-CA	12.89	1.80	1.53
4	B	2520	AS1	CB-CA	12.89	1.80	1.53
4	C	3520	AS1	CB-CA	12.77	1.80	1.53
4	A	520	AS1	CA-N1	-6.33	1.32	1.45
3	B	2510	AMP	O4'-C1'	6.30	1.49	1.40
4	D	4520	AS1	CA-N1	-6.08	1.33	1.45
4	B	2520	AS1	C1-N2	6.01	1.63	1.46
4	B	2520	AS1	CA-N1	-5.94	1.33	1.45
3	A	510	AMP	O4'-C1'	5.92	1.48	1.40
4	A	520	AS1	C1-N2	5.80	1.62	1.46
4	C	3520	AS1	CA-N1	-5.66	1.34	1.45
4	C	3520	AS1	C1-N2	5.45	1.61	1.46
4	D	4520	AS1	C1-N2	5.41	1.61	1.46
3	C	3510	AMP	O4'-C1'	5.38	1.48	1.40
3	A	510	AMP	C3'-C4'	5.04	1.65	1.53
3	A	510	AMP	P-O1P	4.90	1.65	1.50
3	D	4510	AMP	P-O1P	4.81	1.65	1.50
3	C	3510	AMP	P-O1P	4.74	1.65	1.50
3	B	2510	AMP	C3'-C4'	4.71	1.64	1.53
3	C	3510	AMP	C3'-C4'	4.70	1.64	1.53
3	D	4510	AMP	C3'-C4'	4.64	1.64	1.53
3	B	2510	AMP	P-O3P	-4.63	1.37	1.54
3	B	2510	AMP	P-O1P	4.62	1.64	1.50
3	A	510	AMP	P-O3P	-4.29	1.38	1.54
3	A	510	AMP	P-O5'	-4.25	1.46	1.60
3	D	4510	AMP	P-O3P	-4.25	1.39	1.54
3	D	4510	AMP	O4'-C1'	4.08	1.46	1.40
3	B	2510	AMP	P-O5'	-3.95	1.47	1.60
3	B	2510	AMP	P-O2P	3.85	1.69	1.54
4	C	3520	AS1	C-N3	3.83	1.43	1.34
3	C	3510	AMP	C2-N3	3.80	1.38	1.32
3	D	4510	AMP	P-O5'	-3.74	1.48	1.60
3	B	2510	AMP	C2-N3	3.63	1.37	1.32
3	C	3510	AMP	P-O3P	-3.61	1.41	1.54
4	B	2520	AS1	C-N3	3.50	1.42	1.34
3	D	4510	AMP	O5'-C5'	3.44	1.57	1.44
4	A	520	AS1	C-N3	3.43	1.42	1.34
3	B	2510	AMP	O5'-C5'	3.41	1.57	1.44
4	D	4520	AS1	C-N3	3.34	1.42	1.34
3	B	2510	AMP	C2-N1	3.33	1.39	1.33
3	C	3510	AMP	P-O5'	-3.32	1.49	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	510	AMP	C2-N3	3.31	1.37	1.32
2	B	2540	SO4	O1-S	3.20	1.63	1.44
3	D	4510	AMP	C2-N3	3.18	1.37	1.32
3	C	3510	AMP	O5'-C5'	3.16	1.56	1.44
3	C	3510	AMP	C2-N1	3.16	1.39	1.33
3	A	510	AMP	C1'-N9	3.07	1.57	1.49
3	D	4510	AMP	O3'-C3'	3.03	1.50	1.43
3	A	510	AMP	O3'-C3'	2.99	1.50	1.43
3	A	510	AMP	C2-N1	2.98	1.39	1.33
2	C	3540	SO4	O1-S	2.94	1.62	1.44
2	D	4540	SO4	O1-S	2.93	1.62	1.44
4	D	4520	AS1	OG1-CG	-2.82	1.21	1.30
3	D	4510	AMP	C2-N1	2.82	1.38	1.33
4	C	3520	AS1	OG1-CG	-2.79	1.21	1.30
3	C	3510	AMP	P-O2P	2.79	1.65	1.54
3	A	510	AMP	O5'-C5'	2.73	1.55	1.44
4	A	520	AS1	OG1-CG	-2.61	1.22	1.30
3	C	3510	AMP	C4-N3	2.59	1.39	1.35
2	A	540	SO4	O1-S	2.58	1.60	1.44
3	D	4510	AMP	C1'-N9	2.54	1.56	1.49
3	B	2510	AMP	O3'-C3'	2.40	1.48	1.43
4	B	2520	AS1	OG1-CG	-2.35	1.23	1.30
3	B	2510	AMP	C2'-C3'	2.32	1.59	1.53
3	B	2510	AMP	C1'-N9	2.32	1.55	1.49
3	A	510	AMP	C2'-C3'	2.30	1.59	1.53
3	C	3510	AMP	C1'-N9	2.29	1.55	1.49
3	D	4510	AMP	P-O2P	2.23	1.63	1.54
3	D	4510	AMP	C2'-C3'	2.21	1.59	1.53
3	C	3510	AMP	O3'-C3'	2.20	1.48	1.43
3	B	2510	AMP	C5'-C4'	2.17	1.58	1.51
3	B	2510	AMP	O4'-C4'	2.07	1.49	1.45
3	A	510	AMP	P-O2P	2.05	1.62	1.54
4	B	2520	AS1	O52-C5	-2.01	1.24	1.30

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4520	AS1	C2-C1-N2	30.76	165.14	110.67
4	A	520	AS1	C2-C1-N2	27.64	159.61	110.67
4	B	2520	AS1	C2-C1-N2	27.39	159.17	110.67
4	C	3520	AS1	C2-C1-N2	27.36	159.12	110.67
4	A	520	AS1	C1-N2-C	7.18	138.34	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2520	AS1	C1-N2-C	6.45	136.68	121.86
4	C	3520	AS1	C1-N2-C	6.37	136.49	121.86
4	D	4520	AS1	C1-N2-C	6.36	136.46	121.86
4	A	520	AS1	CA-CB-CD	5.12	127.13	112.75
4	C	3520	AS1	N1-C-N2	5.07	137.27	125.00
4	B	2520	AS1	N1-C-N2	5.06	137.25	125.00
4	C	3520	AS1	CA-CB-CD	5.02	126.87	112.75
4	D	4520	AS1	CA-CB-CD	4.97	126.72	112.75
4	D	4520	AS1	N1-C-N2	4.91	136.88	125.00
4	B	2520	AS1	CA-CB-CD	4.88	126.48	112.75
4	A	520	AS1	N1-C-N2	4.70	136.39	125.00
3	C	3510	AMP	C4-C5-N7	4.70	114.31	109.34
4	B	2520	AS1	N3-C-N2	-4.57	106.92	123.23
4	D	4520	AS1	OG1-CG-OG2	-4.52	113.83	124.08
4	C	3520	AS1	N3-C-N2	-4.46	107.32	123.23
4	C	3520	AS1	OG1-CG-OG2	-4.43	114.04	124.08
4	D	4520	AS1	N3-C-N2	-4.37	107.64	123.23
3	B	2510	AMP	C4-C5-N7	4.35	113.93	109.34
4	B	2520	AS1	OG1-CG-OG2	-4.30	114.32	124.08
4	A	520	AS1	OG1-CG-OG2	-4.26	114.42	124.08
4	A	520	AS1	N3-C-N2	-4.25	108.08	123.23
4	C	3520	AS1	CB-CA-N1	4.21	118.66	110.64
3	A	510	AMP	C4-C5-N7	4.12	113.69	109.34
3	D	4510	AMP	C4-C5-N7	4.08	113.65	109.34
3	D	4510	AMP	O2P-P-O5'	4.06	117.25	106.67
4	B	2520	AS1	CG-CA-N1	4.06	119.98	110.57
3	B	2510	AMP	O2P-P-O5'	3.98	117.06	106.67
3	A	510	AMP	O3P-P-O5'	3.96	116.98	106.67
4	D	4520	AS1	CB-CA-N1	3.92	118.11	110.64
3	C	3510	AMP	N3-C2-N1	-3.90	123.38	128.67
4	A	520	AS1	CB-CA-N1	3.87	118.03	110.64
4	A	520	AS1	CB-CA-CG	3.81	118.41	110.79
4	C	3520	AS1	CG-CA-N1	3.78	119.34	110.57
4	D	4520	AS1	CG-CA-N1	3.73	119.22	110.57
3	B	2510	AMP	O3P-P-O5'	3.69	116.29	106.67
3	A	510	AMP	O2P-P-O5'	3.69	116.29	106.67
3	D	4510	AMP	N3-C2-N1	-3.66	123.71	128.67
3	A	510	AMP	N3-C2-N1	-3.63	123.74	128.67
4	A	520	AS1	CG-CA-N1	3.63	119.00	110.57
3	C	3510	AMP	O2P-P-O5'	3.61	116.08	106.67
4	B	2520	AS1	CB-CA-N1	3.58	117.47	110.64
3	C	3510	AMP	N6-C6-N1	3.51	125.83	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3520	AS1	CB-CA-CG	3.50	117.79	110.79
3	C	3510	AMP	O3P-P-O5'	3.46	115.69	106.67
3	B	2510	AMP	N3-C2-N1	-3.44	124.01	128.67
4	D	4520	AS1	CB-CA-CG	3.39	117.56	110.79
4	B	2520	AS1	CB-CA-CG	3.39	117.56	110.79
3	D	4510	AMP	O3P-P-O5'	3.28	115.21	106.67
4	A	520	AS1	C3-C4-N4	3.18	118.40	110.12
3	B	2510	AMP	N6-C6-N1	3.15	125.06	118.33
4	C	3520	AS1	C3-C4-N4	3.13	118.28	110.12
4	D	4520	AS1	C3-C4-N4	3.04	118.03	110.12
4	C	3520	AS1	N3-C-N1	-3.01	113.09	118.86
3	B	2510	AMP	O5'-C5'-C4'	3.00	119.21	108.99
3	A	510	AMP	N6-C6-N1	2.97	124.68	118.33
3	D	4510	AMP	O4'-C1'-N9	2.97	112.68	108.75
4	B	2520	AS1	C3-C4-N4	2.95	117.80	110.12
3	B	2510	AMP	O3'-C3'-C4'	-2.91	102.72	111.08
3	D	4510	AMP	O3'-C3'-C4'	-2.87	102.83	111.08
3	C	3510	AMP	O4'-C1'-N9	2.85	112.52	108.75
3	B	2510	AMP	O4'-C4'-C5'	-2.83	100.25	109.33
3	D	4510	AMP	N6-C6-N1	2.83	124.38	118.33
3	C	3510	AMP	O3'-C3'-C4'	-2.79	103.07	111.08
4	B	2520	AS1	N3-C-N1	-2.73	113.63	118.86
3	C	3510	AMP	O2P-P-O1P	-2.68	100.39	110.83
3	B	2510	AMP	O2P-P-O1P	-2.62	100.64	110.83
3	A	510	AMP	O2P-P-O1P	-2.61	100.66	110.83
4	D	4520	AS1	N3-C-N1	-2.53	114.01	118.86
3	D	4510	AMP	O2P-P-O1P	-2.53	100.98	110.83
3	C	3510	AMP	O5'-C5'-C4'	2.47	117.39	108.99
3	A	510	AMP	O4'-C1'-N9	2.43	111.97	108.75
4	A	520	AS1	N3-C-N1	-2.42	114.23	118.86
3	A	510	AMP	O3'-C3'-C4'	-2.40	104.19	111.08
3	D	4510	AMP	C2'-C3'-C4'	-2.24	98.28	102.61
4	D	4520	AS1	OD2-CD-CB	-2.10	116.41	122.84
4	B	2520	AS1	OD1-CD-CB	2.09	120.49	114.00
3	C	3510	AMP	O3'-C3'-C2'	2.06	118.44	111.82
3	D	4510	AMP	O5'-C5'-C4'	2.04	115.94	108.99
4	B	2520	AS1	OD2-CD-CB	-2.03	116.60	122.84
4	D	4520	AS1	OD1-CD-CB	2.02	120.28	114.00

All (4) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
4	A	520	AS1	C4
4	B	2520	AS1	C4
4	C	3520	AS1	C4
4	D	4520	AS1	C4

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	520	AS1	N2-C1-C2-C3
4	A	520	AS1	C2-C1-N2-C
4	A	520	AS1	N2-C-N1-CA
4	A	520	AS1	N3-C-N1-CA
4	A	520	AS1	CB-CA-N1-C
4	A	520	AS1	CG-CA-CB-CD
4	B	2520	AS1	C2-C1-N2-C
4	B	2520	AS1	N2-C-N1-CA
4	B	2520	AS1	N3-C-N1-CA
4	B	2520	AS1	CB-CA-N1-C
4	B	2520	AS1	CG-CA-CB-CD
4	C	3520	AS1	C2-C1-N2-C
4	C	3520	AS1	N2-C-N1-CA
4	C	3520	AS1	N3-C-N1-CA
4	C	3520	AS1	CB-CA-N1-C
4	C	3520	AS1	CG-CA-CB-CD
4	D	4520	AS1	C2-C3-C4-N4
4	D	4520	AS1	C2-C1-N2-C
4	D	4520	AS1	N2-C-N1-CA
4	D	4520	AS1	N3-C-N1-CA
4	D	4520	AS1	CB-CA-N1-C
4	D	4520	AS1	CG-CA-CB-CD
4	B	2520	AS1	N2-C1-C2-C3
4	C	3520	AS1	N2-C1-C2-C3
4	B	2520	AS1	N1-CA-CB-CD
4	D	4520	AS1	C1-C2-C3-C4
4	A	520	AS1	C3-C4-C5-O52
4	C	3520	AS1	C3-C4-C5-O52
4	D	4520	AS1	C3-C4-C5-O52
4	B	2520	AS1	C2-C3-C4-N4
4	C	3520	AS1	C2-C3-C4-N4
4	B	2520	AS1	C3-C4-C5-O52
3	B	2510	AMP	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
4	B	2520	AS1	C3-C4-C5-O51
4	C	3520	AS1	C3-C4-C5-O51
4	D	4520	AS1	C3-C4-C5-O51
4	A	520	AS1	C3-C4-C5-O51
4	C	3520	AS1	N4-C4-C5-O52
3	C	3510	AMP	C4'-C5'-O5'-P
4	A	520	AS1	N1-CA-CG-OG2
4	A	520	AS1	C2-C3-C4-N4

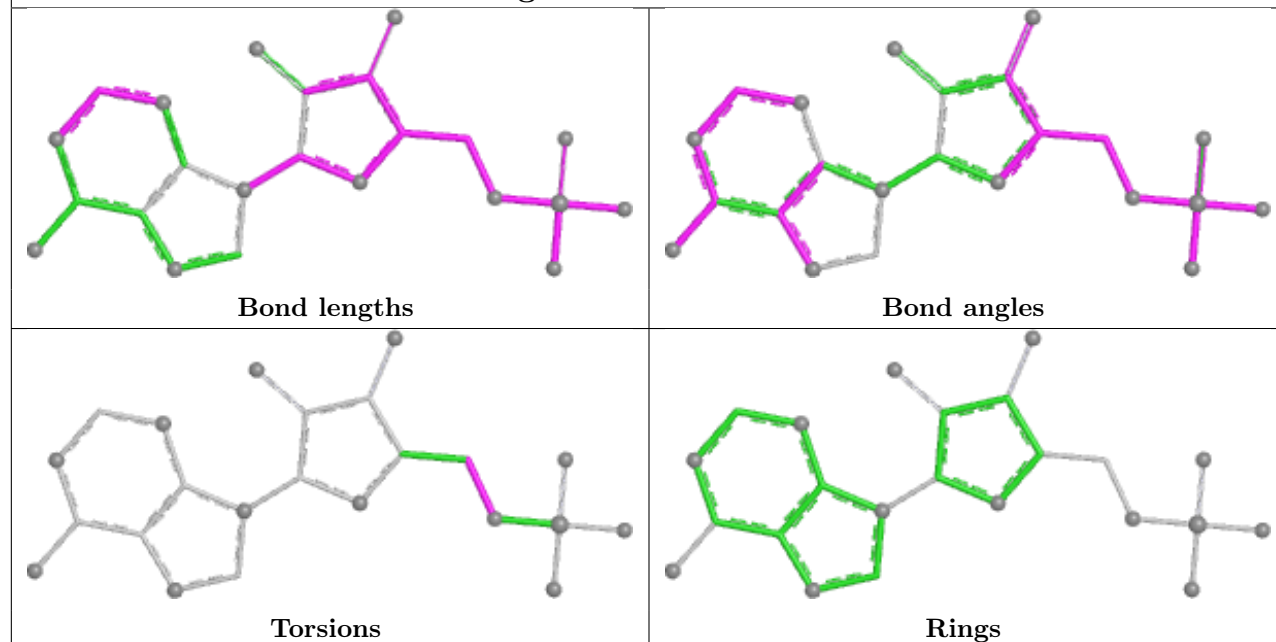
There are no ring outliers.

8 monomers are involved in 38 short contacts:

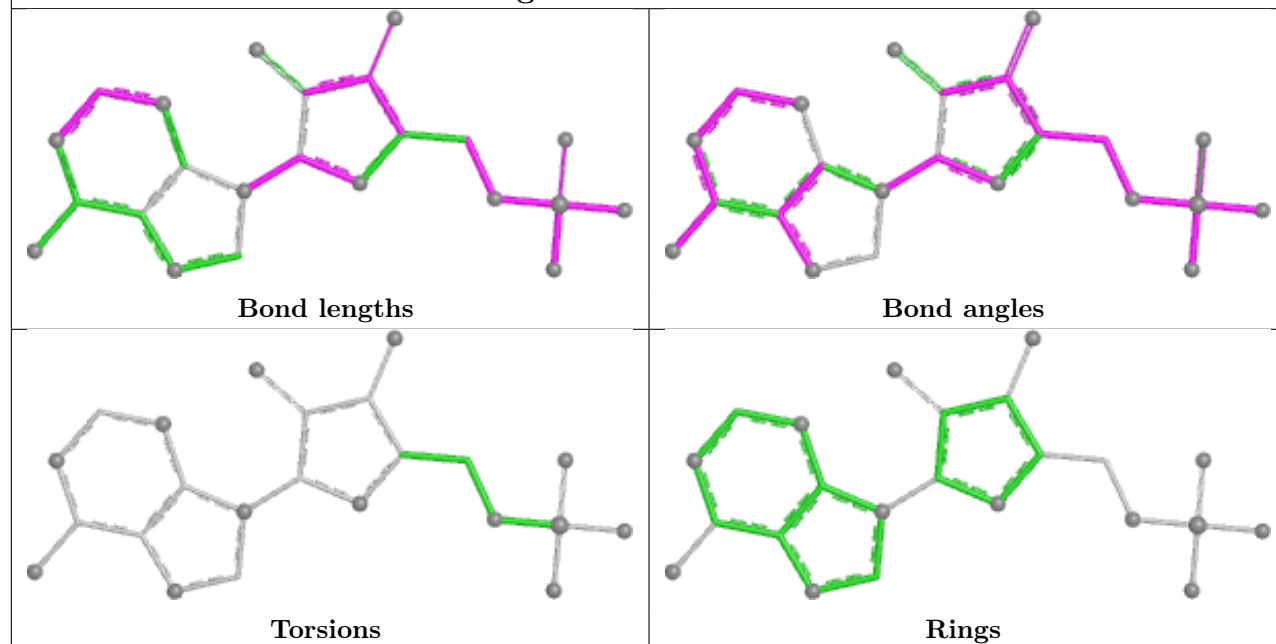
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2510	AMP	3	0
3	D	4510	AMP	2	0
3	A	510	AMP	2	0
4	B	2520	AS1	6	0
4	C	3520	AS1	9	0
4	A	520	AS1	8	0
3	C	3510	AMP	1	0
4	D	4520	AS1	8	0

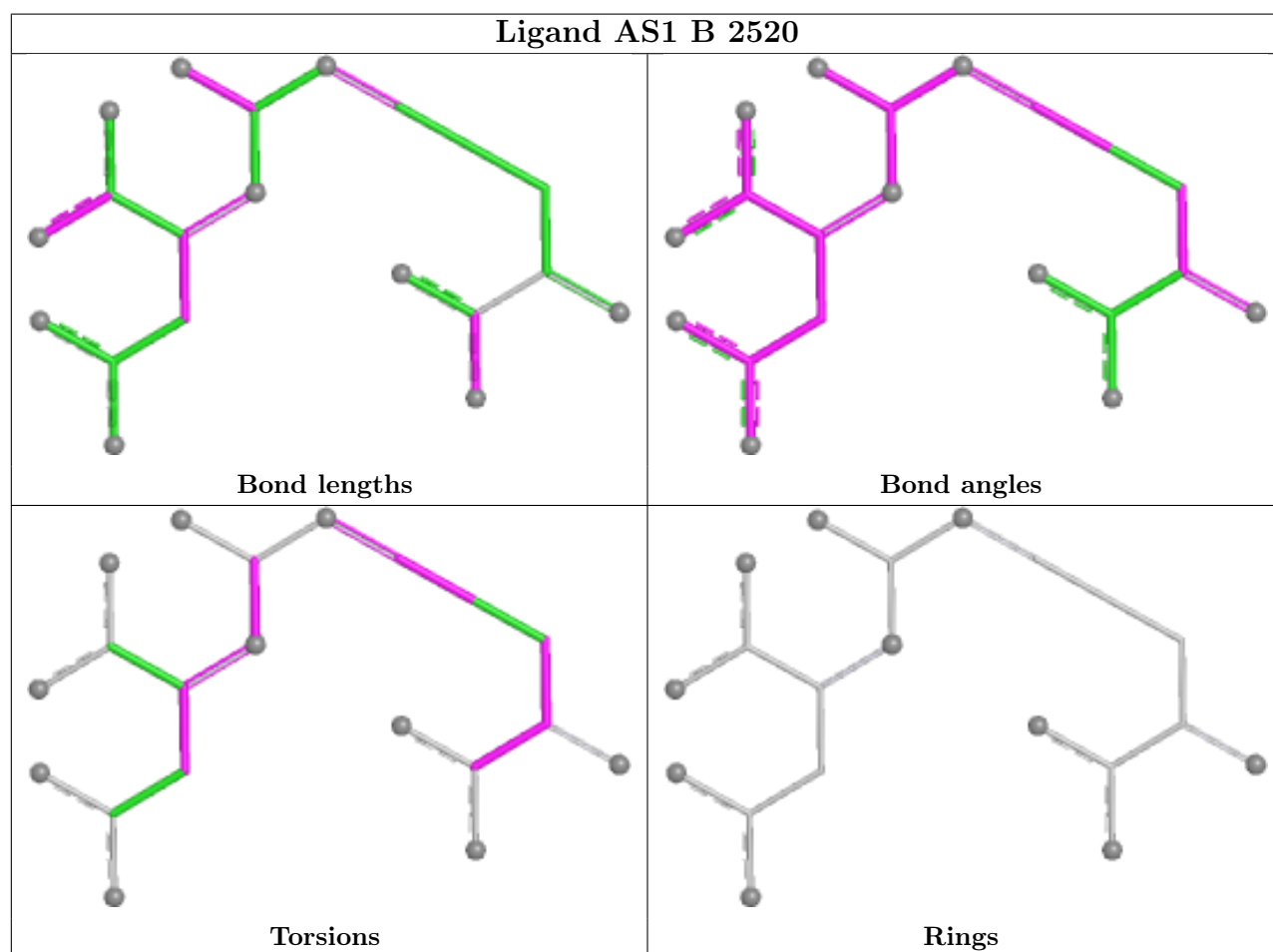
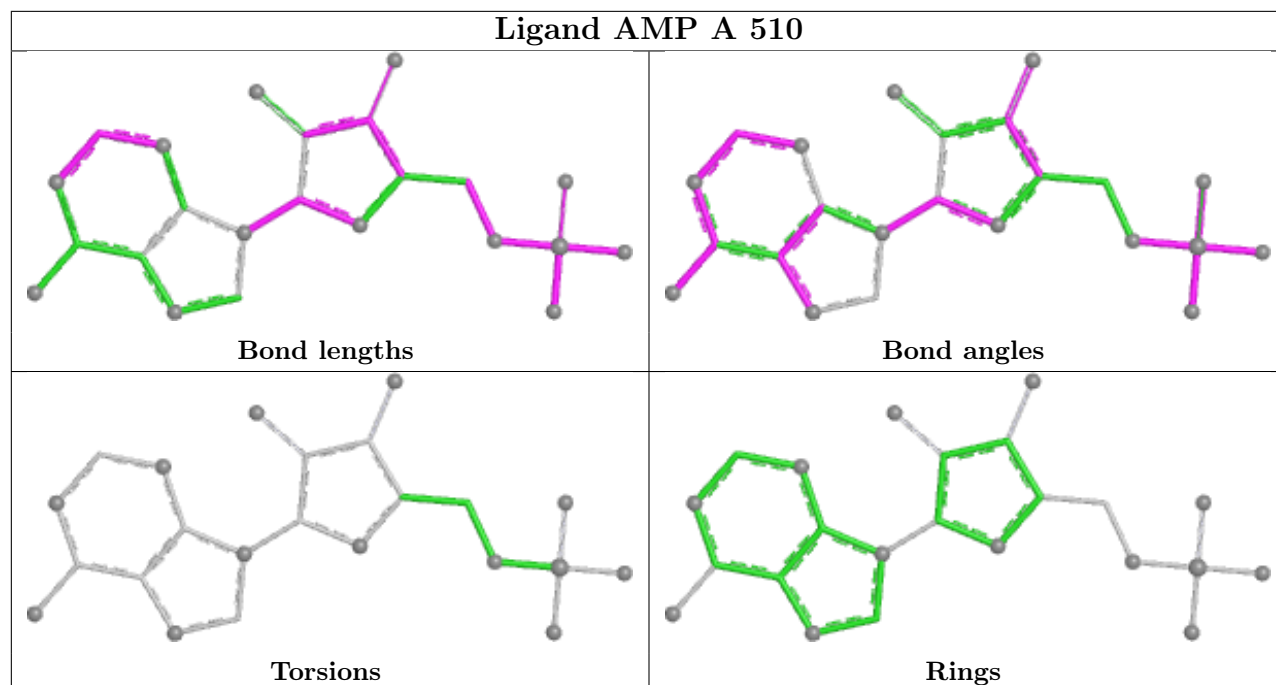
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

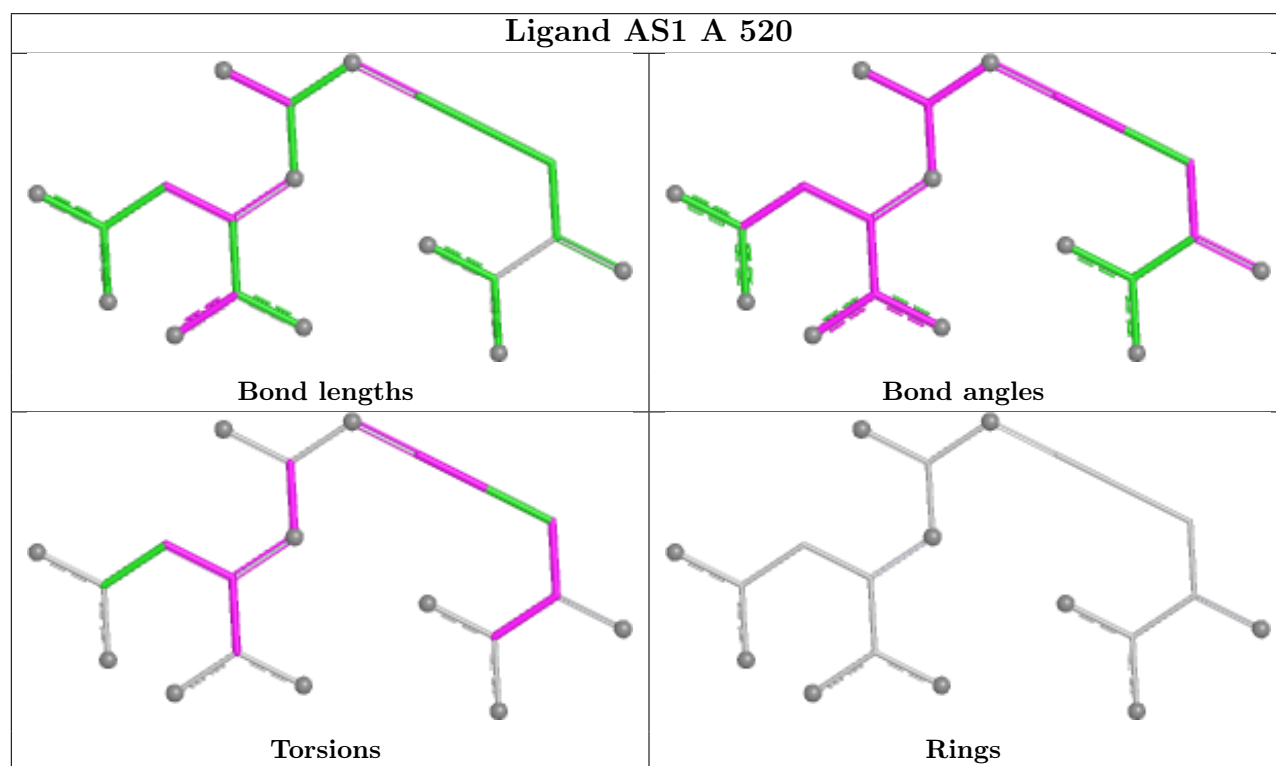
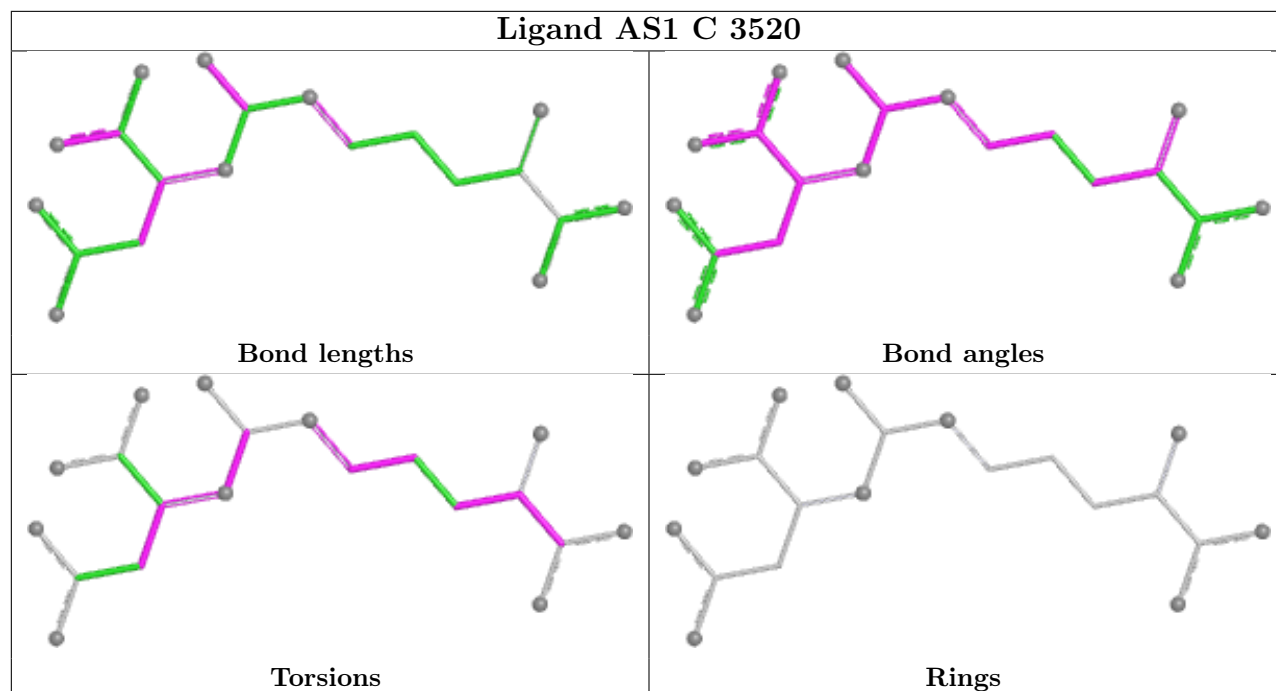
Ligand AMP B 2510

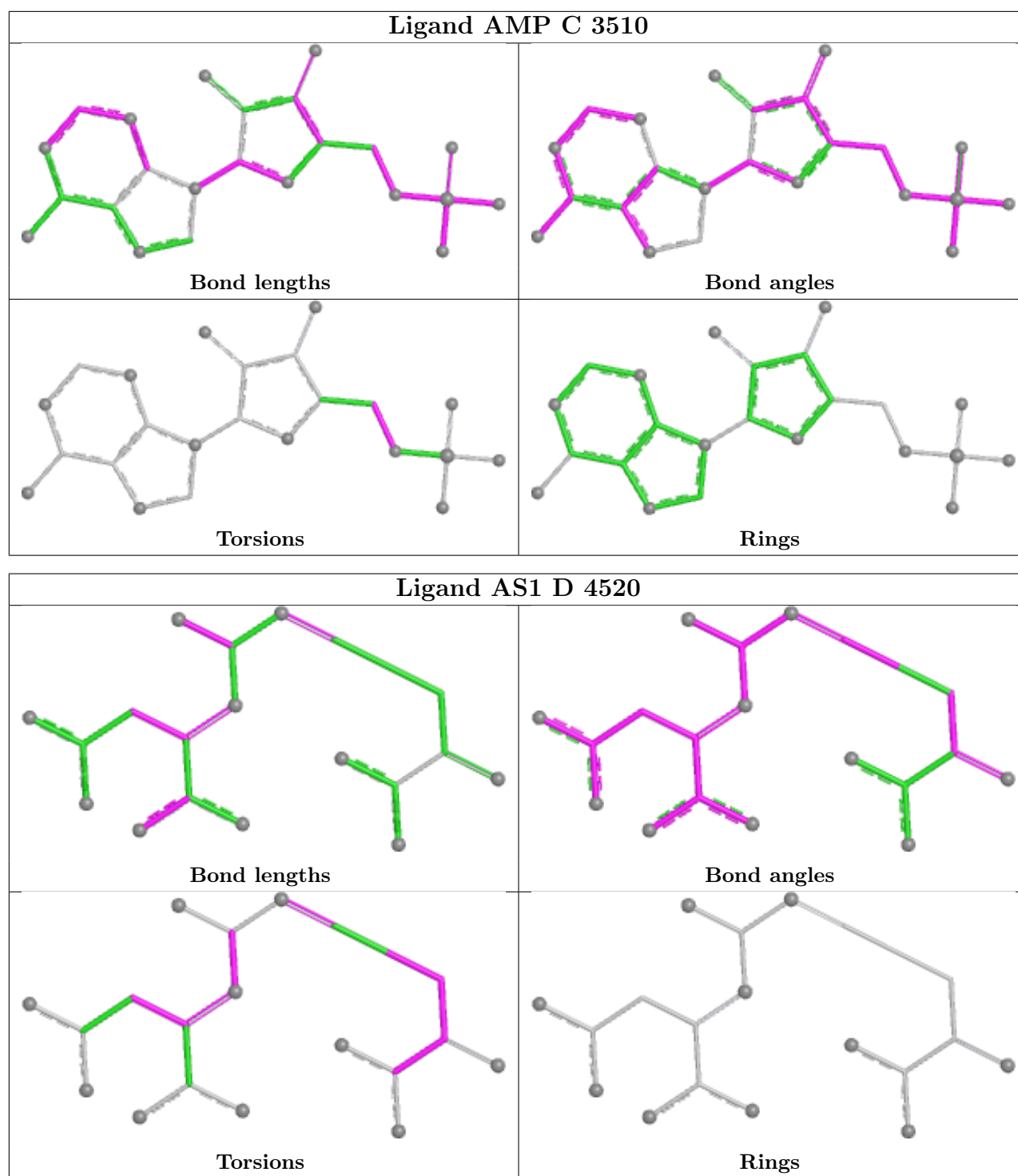


Ligand AMP D 4510









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(Å ²)	Q<0.9
1	A	386/400 (96%)	-0.36	6 (1%) 70 69	20, 27, 49, 78	0
1	B	386/400 (96%)	-0.41	7 (1%) 67 66	20, 27, 47, 65	0
1	C	386/400 (96%)	-0.08	19 (4%) 36 34	21, 29, 55, 72	0
1	D	386/400 (96%)	-0.23	10 (2%) 57 55	21, 30, 52, 72	0
All	All	1544/1600 (96%)	-0.27	42 (2%) 56 54	20, 29, 51, 78	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	ARG	5.0
1	C	395	ARG	5.0
1	D	395	ARG	4.6
1	B	395	ARG	4.2
1	C	165	PRO	3.9
1	A	361	ASP	3.7
1	A	165	PRO	3.6
1	C	157	ALA	3.4
1	A	365	PHE	3.3
1	B	365	PHE	3.2
1	A	370	GLY	3.0
1	B	361	ASP	3.0
1	B	370	GLY	3.0
1	C	373	GLN	3.0
1	C	43	GLU	2.8
1	C	25	ARG	2.7
1	C	49	LEU	2.6
1	D	161	GLY	2.5
1	D	372	ASP	2.5
1	D	155	ALA	2.5
1	C	137	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	165	PRO	2.4
1	C	372	ASP	2.4
1	C	104	GLU	2.4
1	C	394	GLU	2.4
1	D	201	ARG	2.4
1	D	205	ASP	2.4
1	C	39	GLU	2.3
1	C	151	LYS	2.3
1	D	371	TYR	2.3
1	D	151	LYS	2.2
1	A	364	SER	2.2
1	C	26	ALA	2.1
1	C	205	ASP	2.1
1	C	364	SER	2.1
1	C	21	LYS	2.1
1	B	364	SER	2.1
1	C	159	ALA	2.0
1	C	370	GLY	2.0
1	B	201	ARG	2.0
1	D	365	PHE	2.0
1	B	10	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

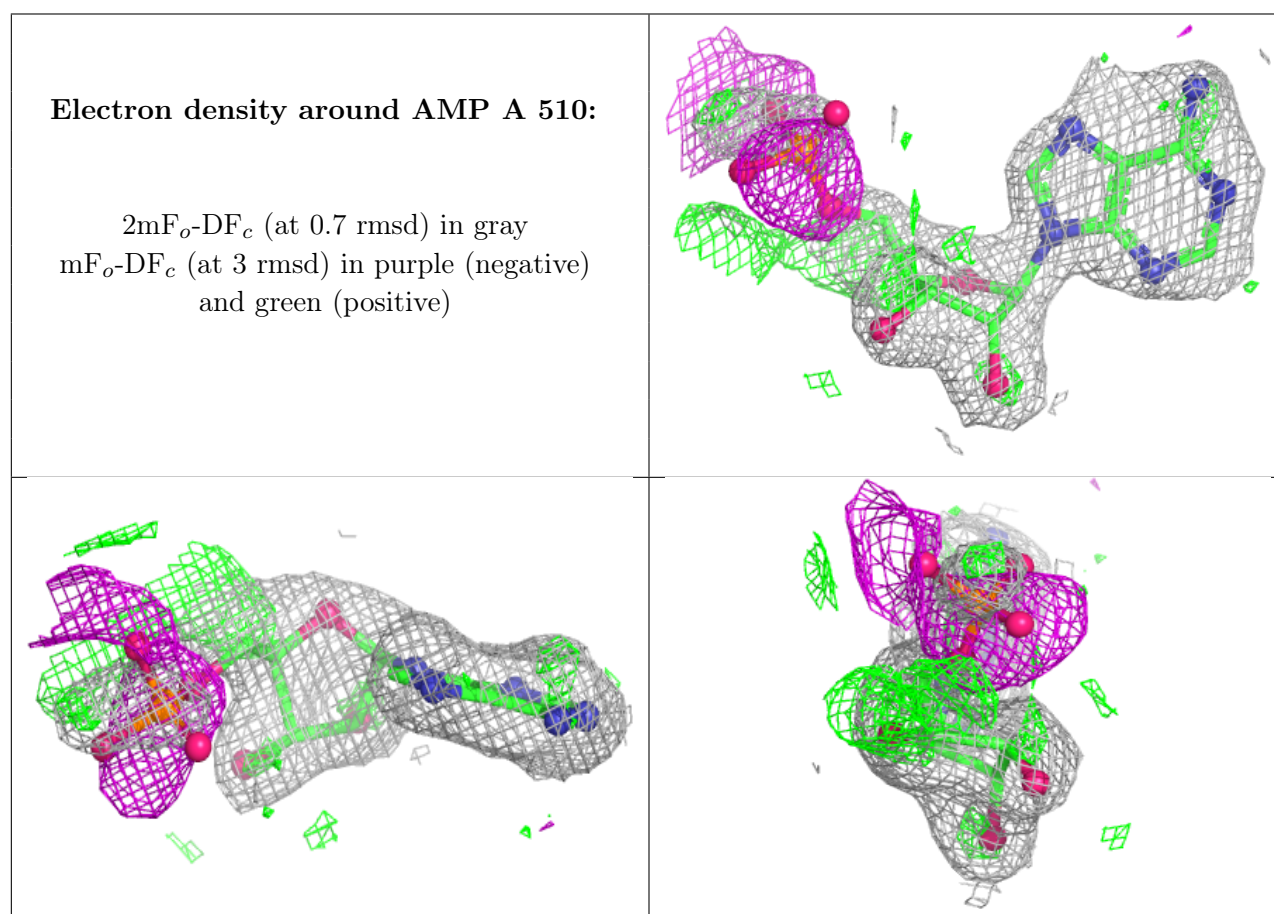
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AMP	A	510	23/23	0.70	0.20	36,45,68,68	23
3	AMP	C	3510	23/23	0.70	0.18	41,47,69,70	23

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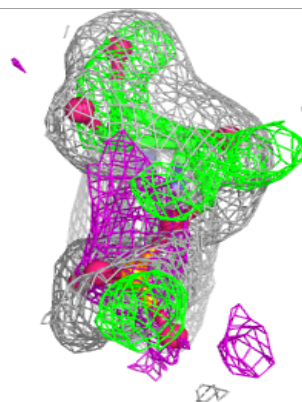
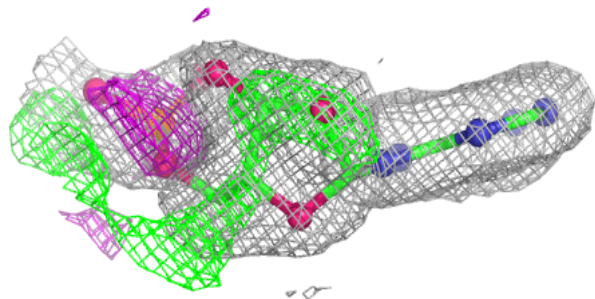
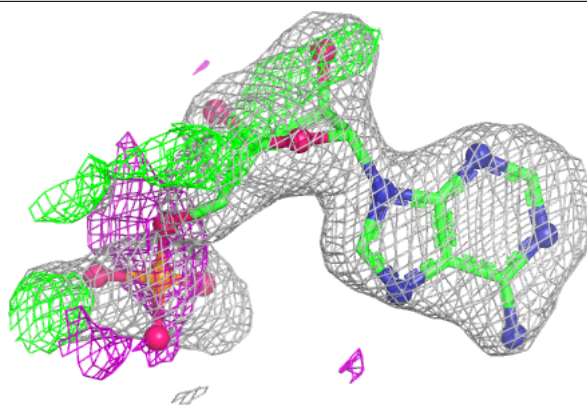
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AMP	B	2510	23/23	0.71	0.18	31,41,60,63	23
3	AMP	D	4510	23/23	0.71	0.20	40,47,69,70	23
4	AS1	C	3520	20/20	0.72	0.22	23,35,54,54	0
4	AS1	A	520	20/20	0.73	0.21	24,36,53,54	0
4	AS1	D	4520	20/20	0.74	0.22	23,39,56,58	0
4	AS1	B	2520	20/20	0.75	0.22	22,36,59,61	0
2	SO4	B	2540	5/5	0.92	0.10	37,40,41,42	0
2	SO4	A	540	5/5	0.95	0.08	41,43,44,44	0
2	SO4	C	3540	5/5	0.95	0.09	43,44,45,45	0
2	SO4	D	4540	5/5	0.96	0.07	44,45,46,47	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.

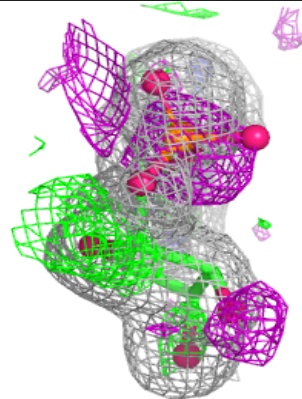
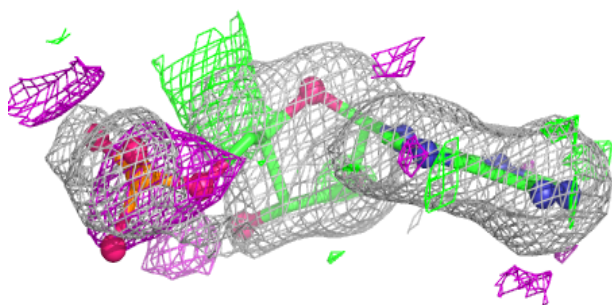
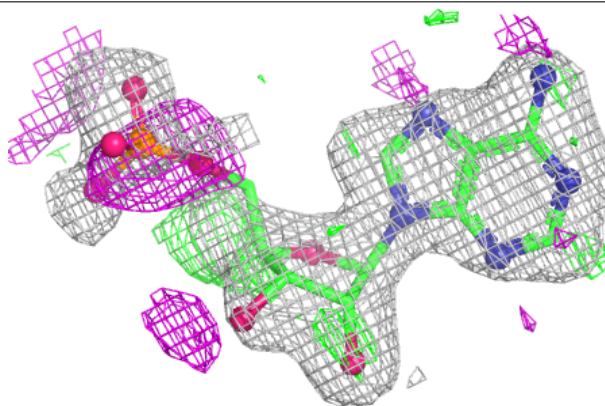


Electron density around AMP C 3510:

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

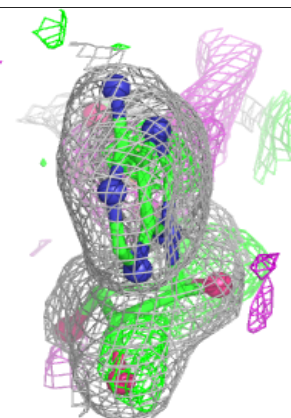
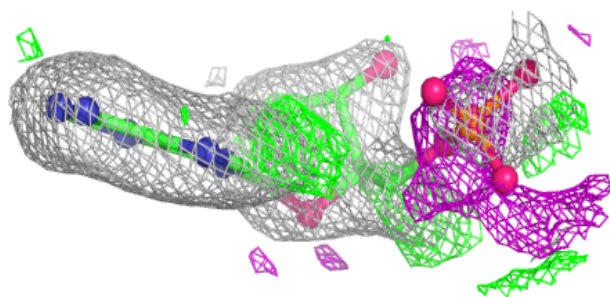
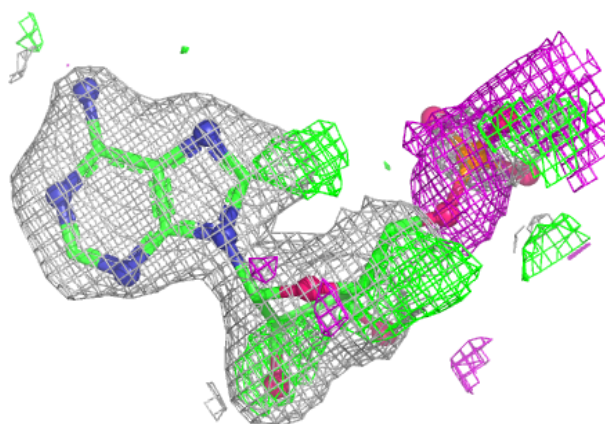
**Electron density around AMP B 2510:**

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



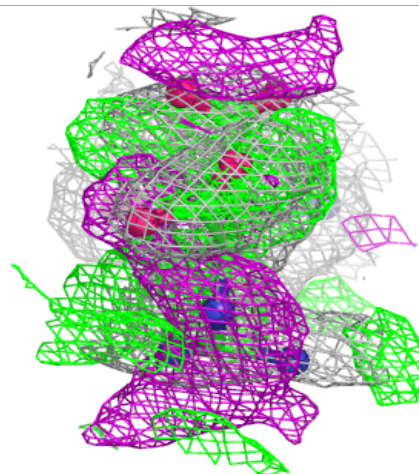
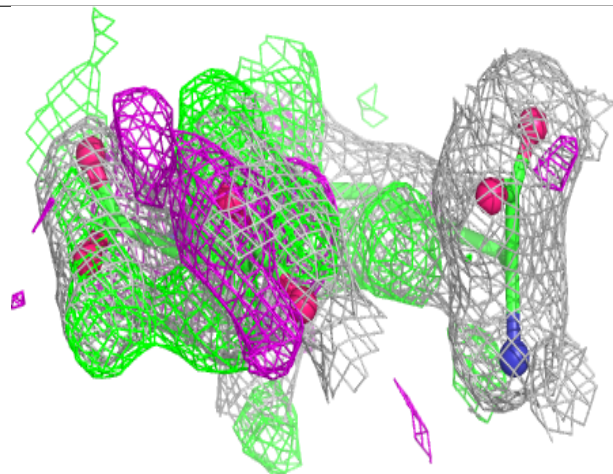
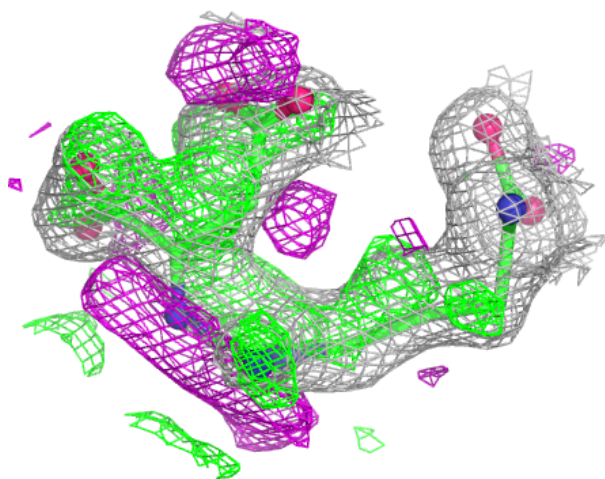
Electron density around AMP D 4510:

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



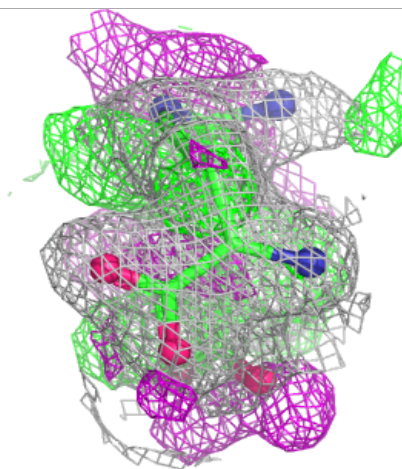
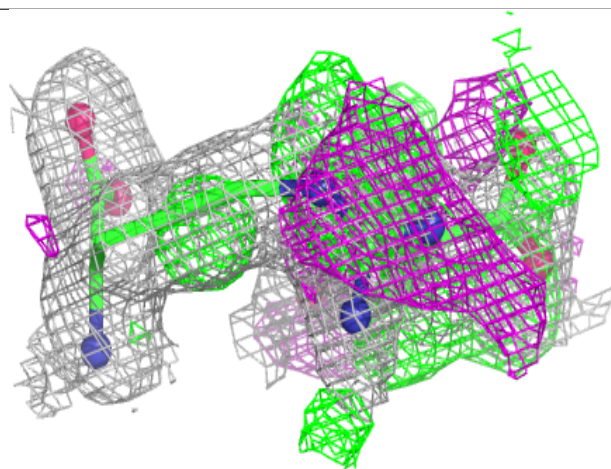
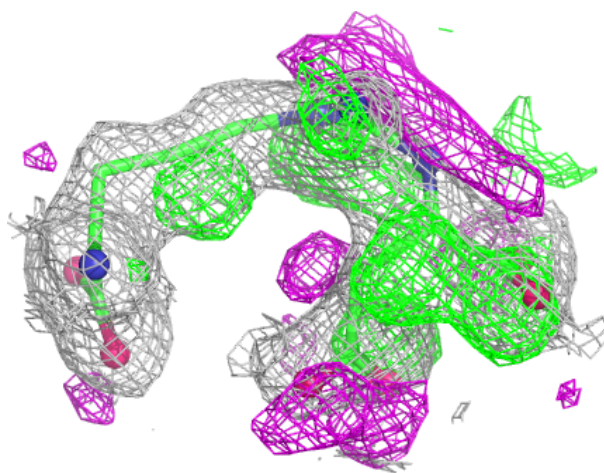
Electron density around AS1 C 3520:

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



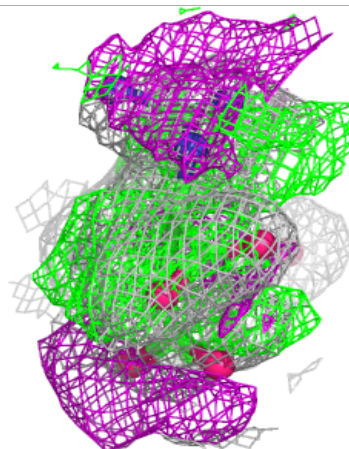
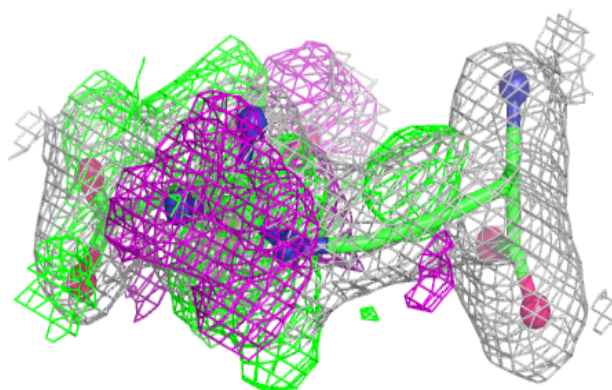
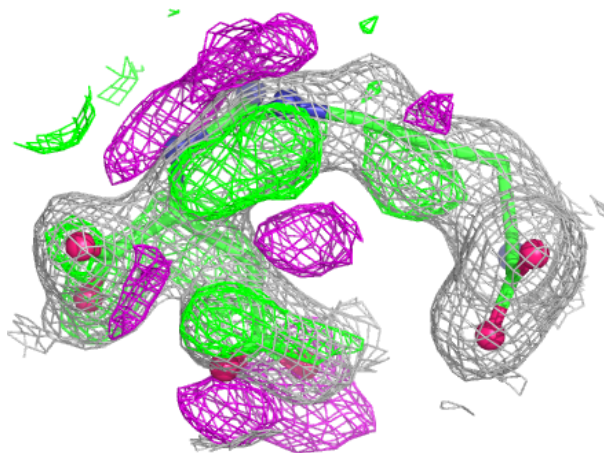
Electron density around AS1 A 520:

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



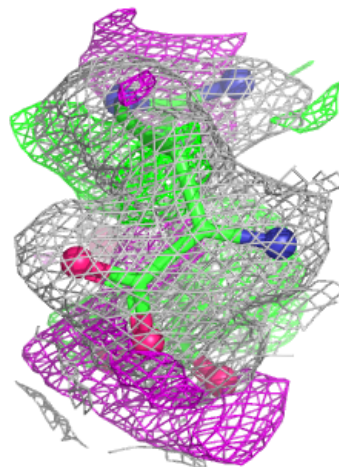
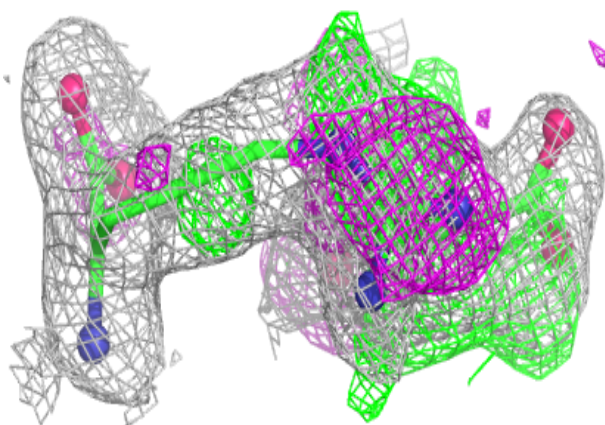
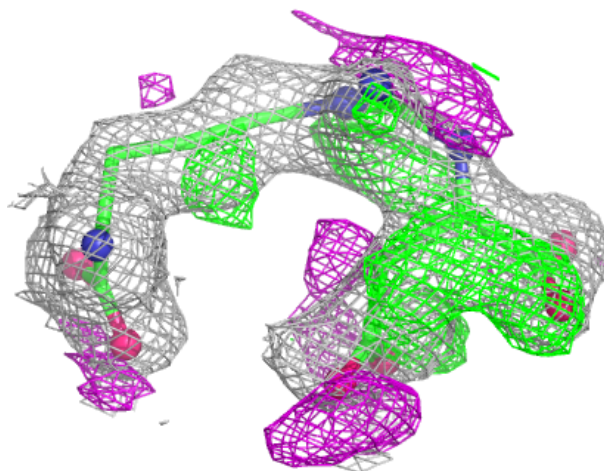
Electron density around AS1 D 4520:

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



Electron density around AS1 B 2520:

$2mF_o-DF_c$ (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.