



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:07 AM UTC

PDB ID : 1KH3 / pdb_00001kh3
Title : Crystal Structure of Thermus thermophilus HB8 Argininosuccinate Synthetase in complex with inhibitor
Authors : goto, m.; Hirotsu, k.; miyahara, i.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2001-11-29
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

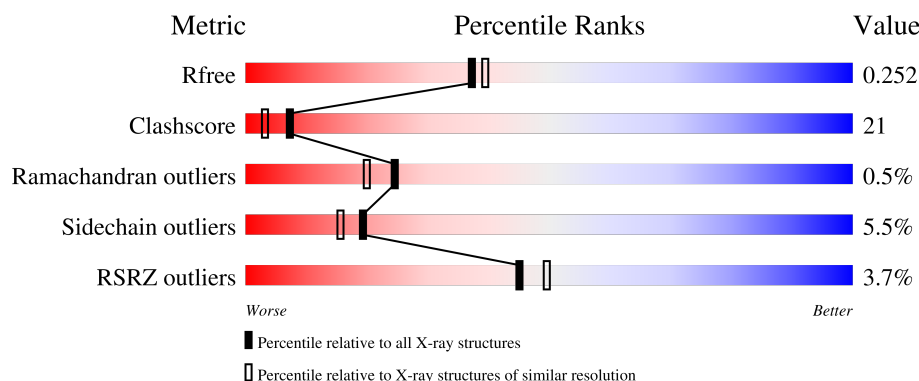
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	3% 64% 26% 5%
1	B	400	4% 65% 28% .
1	C	400	5% 63% 28% 6% .
1	D	400	2% 58% 34% .

2 Entry composition [i](#)

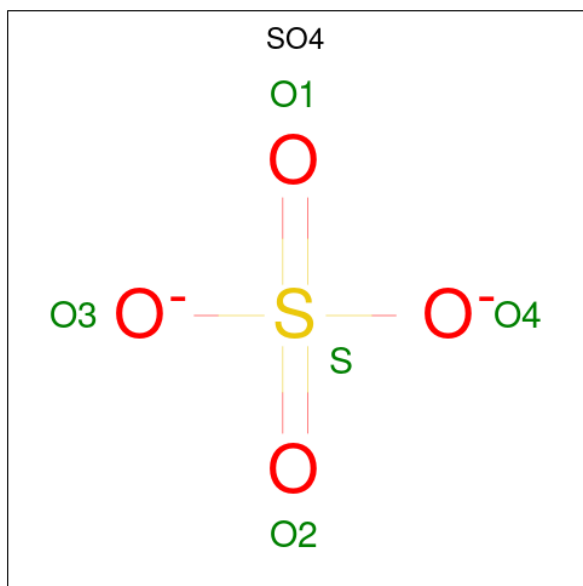
There are 7 unique types of molecules in this entry. The entry contains 13014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	380	Total	C	N	O	S	0	0	0
			3017	1931	526	551	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 (CCD ID: 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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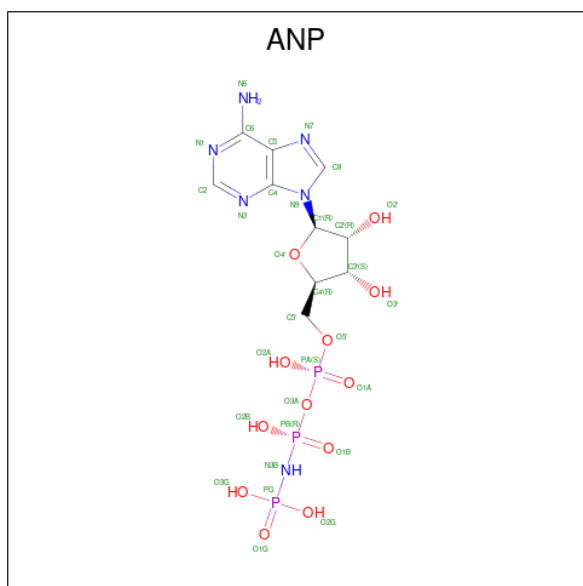
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



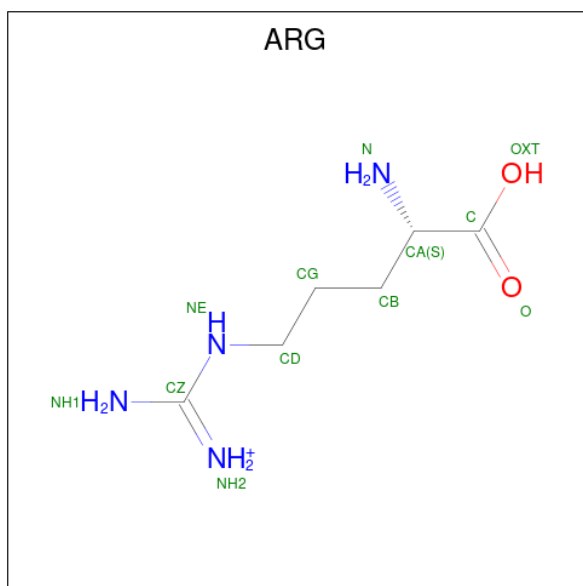
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	C	1	Total 31	C 10	N 6	O 12	P 3	0	0

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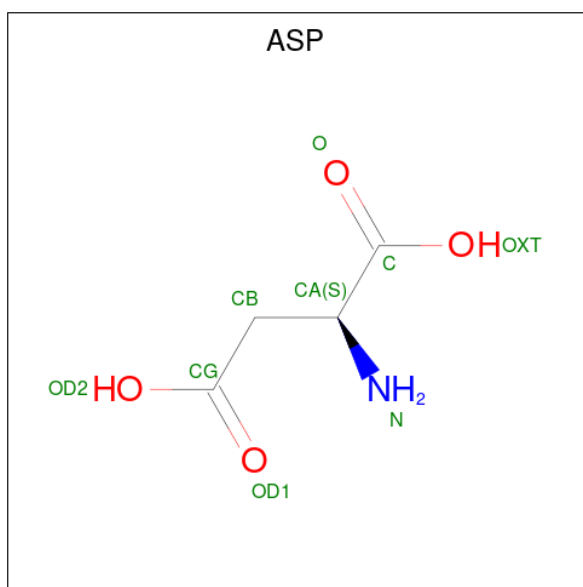
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O		0	0
			12	6	4	2			
5	A	1	Total	C	N	O		0	0
			12	6	4	2			
5	A	1	Total	C	N	O		0	0
			12	6	4	2			
5	A	1	Total	C	N	O		0	0
			12	6	4	2			

- Molecule 6 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			9	4	1	4		
6	A	1	Total	C	N	O	0	0
			9	4	1	4		
6	A	1	Total	C	N	O	0	0
			9	4	1	4		
6	A	1	Total	C	N	O	0	0
			9	4	1	4		

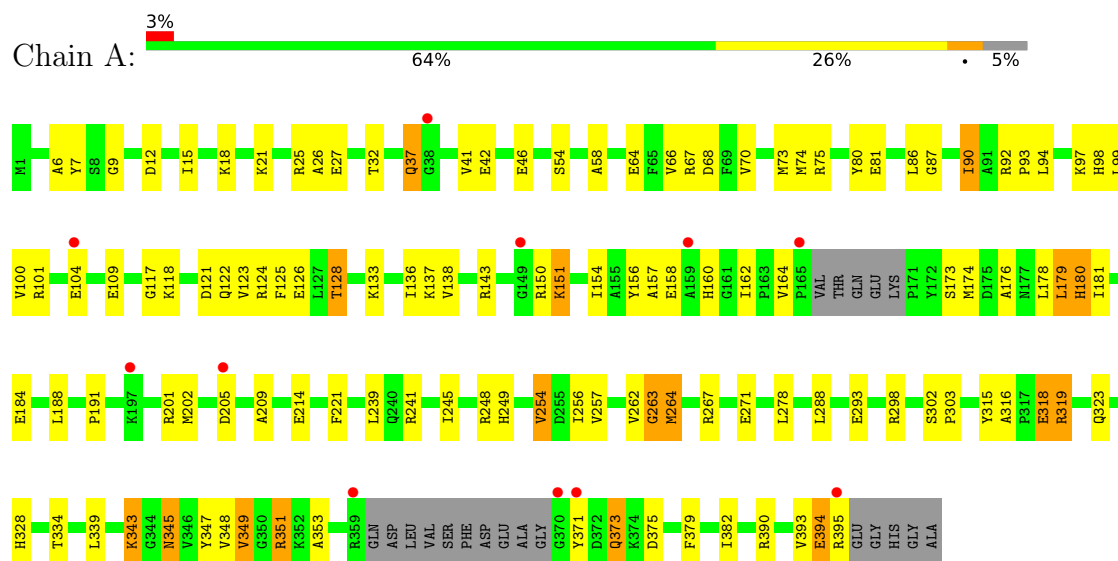
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	160	Total	O	0	0
			160	160		
7	B	161	Total	O	0	0
			161	161		
7	C	125	Total	O	0	0
			125	125		
7	D	121	Total	O	0	0
			121	121		

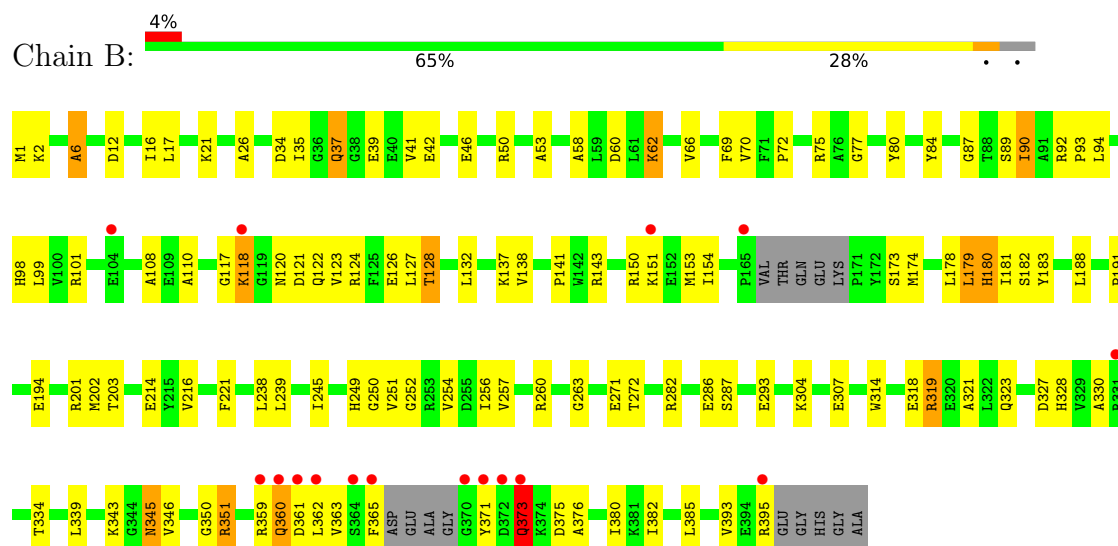
3 Residue-property plots

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

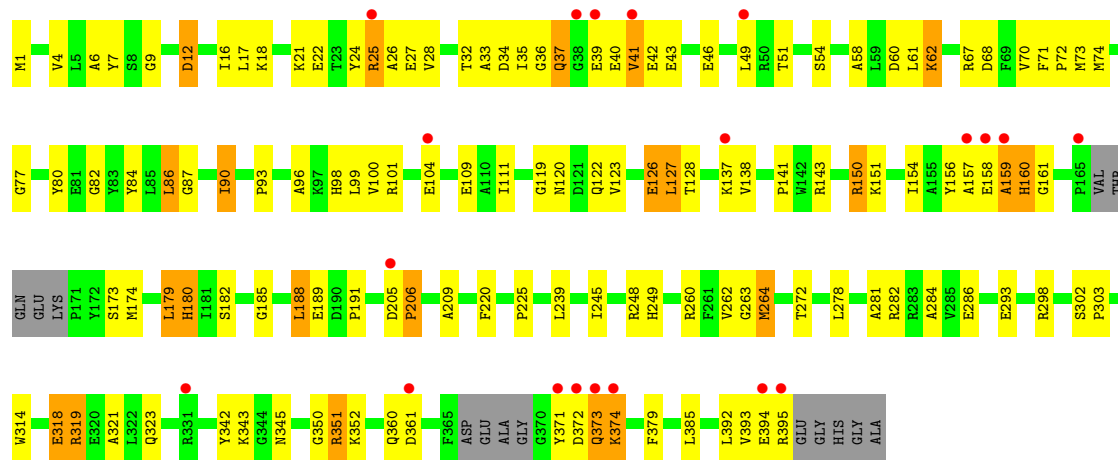


• Molecule 1: Argininosuccinate Synthetase

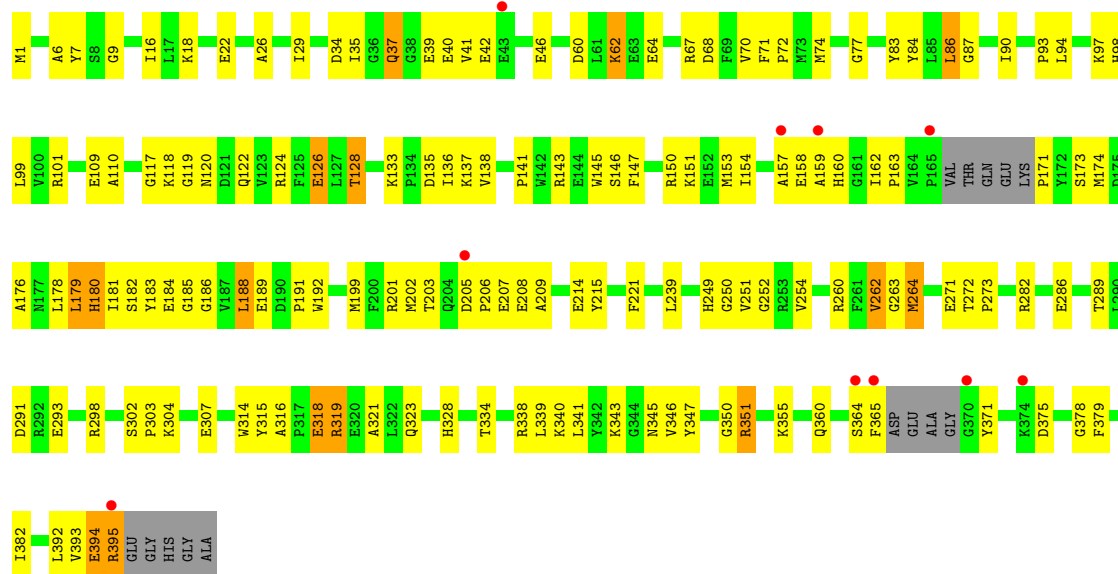


• Molecule 1: Argininosuccinate Synthetase





• 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	229.10Å 229.10Å 160.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.15 10.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.15) 98.6 (10.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.256 0.223 , 0.252	Depositor DCC
R_{free} test set	16829 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 52.1	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	0.94	EDS
Total number of atoms	13014	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.44	0/3085	0.93	7/4169 (0.2%)
1	B	0.45	0/3135	0.92	6/4237 (0.1%)
1	C	0.44	0/3135	0.95	11/4237 (0.3%)
1	D	0.45	0/3135	0.92	7/4237 (0.2%)
All	All	0.45	0/12490	0.93	31/16880 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	GLY	N-CA-C	11.31	127.02	113.79
1	C	263	GLY	N-CA-C	9.20	125.96	114.37
1	B	263	GLY	N-CA-C	8.40	124.95	114.37
1	D	263	GLY	N-CA-C	7.98	123.97	114.48
1	C	394	GLU	N-CA-C	-7.29	104.26	113.01
1	B	360	GLN	N-CA-C	-6.84	105.05	113.19
1	C	28	VAL	N-CA-C	6.71	117.52	107.51
1	D	145	TRP	N-CA-C	6.31	119.06	110.35
1	D	119	GLY	N-CA-C	6.26	121.44	112.81
1	A	348	VAL	N-CA-C	-5.99	101.85	109.58
1	C	119	GLY	N-CA-C	5.83	120.86	112.81
1	C	43	GLU	N-CA-C	-5.77	104.90	111.14
1	C	82	GLY	N-CA-C	5.56	122.48	115.42
1	B	6	ALA	N-CA-C	-5.52	99.79	108.63
1	C	86	LEU	N-CA-C	5.51	119.30	112.24
1	C	49	LEU	N-CA-C	-5.48	105.47	111.82
1	A	86	LEU	N-CA-C	5.40	119.03	111.74
1	A	353	ALA	CA-C-N	5.37	125.01	119.05
1	A	353	ALA	C-N-CA	5.37	125.01	119.05
1	A	394	GLU	N-CA-C	-5.34	105.86	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	GLU	N-CA-C	5.32	117.16	111.36
1	C	12	ASP	N-CA-C	5.28	117.44	111.11
1	C	126	GLU	N-CA-C	5.27	117.11	111.36
1	D	86	LEU	N-CA-C	5.26	118.84	111.74
1	A	345	ASN	N-CA-C	5.20	118.22	109.95
1	D	110	ALA	N-CA-C	5.19	117.57	109.52
1	B	345	ASN	N-CA-C	5.19	118.19	110.14
1	B	89	SER	N-CA-C	5.19	117.33	111.11
1	B	257	VAL	N-CA-C	-5.16	99.73	107.37
1	C	127	LEU	N-CA-C	-5.02	105.81	111.28
1	D	289	THR	N-CA-C	5.00	119.65	113.50

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	3017	0	3006	131	0
1	B	3066	0	3052	129	0
1	C	3066	0	3052	152	0
1	D	3066	0	3052	148	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	13	1	0
4	B	31	0	13	1	0
4	C	31	0	13	0	0
4	D	31	0	13	2	0
5	A	48	0	48	15	0
6	A	36	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	160	0	0	7	0
7	B	161	0	0	12	0
7	C	125	0	0	7	0
7	D	121	0	0	4	0
All	All	13014	0	12274	509	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 21.

All (509) 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:A:262:VAL:HG23	1:A:264:MET:HE1	1.18	1.13
1:D:151:LYS:H	1:D:151:LYS:HD2	1.01	1.10
1:A:151:LYS:H	1:A:151:LYS:HD2	1.11	1.10
1:B:151:LYS:H	1:B:151:LYS:HD2	1.14	1.06
1:B:35:ILE:H	1:B:37:GLN:NE2	1.53	1.06
1:A:123:VAL:HG22	1:B:380:ILE:HD11	1.41	1.02
1:A:124:ARG:O	1:A:128:THR:HG22	1.62	0.99
1:D:35:ILE:H	1:D:37:GLN:NE2	1.60	0.99
1:C:151:LYS:H	1:C:151:LYS:HD2	1.24	0.98
1:A:262:VAL:HG23	1:A:264:MET:CE	1.93	0.97
1:D:124:ARG:O	1:D:128:THR:HG22	1.67	0.94
1:C:109:GLU:O	1:C:137:LYS:HE2	1.71	0.90
1:A:373:GLN:H	1:A:373:GLN:NE2	1.68	0.89
1:A:151:LYS:HD2	1:A:151:LYS:N	1.88	0.89
1:D:151:LYS:HD2	1:D:151:LYS:N	1.86	0.89
1:B:41:VAL:HG12	1:B:58:ALA:HB1	1.55	0.88
1:D:35:ILE:H	1:D:37:GLN:HE22	1.21	0.88
1:A:264:MET:HE3	1:A:264:MET:H	1.39	0.87
1:B:118:LYS:H	1:B:118:LYS:HD2	1.39	0.85
5:A:3520:ARG:HH22	1:D:173:SER:C	1.85	0.85
1:D:351:ARG:HD2	1:D:351:ARG:N	1.92	0.85
1:A:293:GLU:CB	1:C:318:GLU:HG2	2.07	0.84
1:B:124:ARG:O	1:B:128:THR:HG23	1.77	0.83
1:C:37:GLN:H	1:C:37:GLN:NE2	1.76	0.83
1:A:67:ARG:HG2	1:A:67:ARG:HH11	1.44	0.83
1:A:173:SER:C	5:A:520:ARG:HH22	1.87	0.83
1:D:118:LYS:O	1:D:264:MET:HE1	1.79	0.82
1:D:151:LYS:H	1:D:151:LYS:CD	1.80	0.81
1:B:151:LYS:H	1:B:151:LYS:CD	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:4520:ARG:HH22	1:B:173:SER:C	1.89	0.81
5:A:2520:ARG:HH22	1:C:173:SER:C	1.88	0.80
1:C:122:GLN:HE21	1:C:143:ARG:HH11	1.29	0.80
1:C:35:ILE:H	1:C:37:GLN:NE2	1.77	0.80
1:B:35:ILE:N	1:B:37:GLN:NE2	2.29	0.80
1:C:1:MET:O	1:C:26:ALA:HB1	1.82	0.80
1:C:122:GLN:NE2	1:C:143:ARG:HH11	1.82	0.78
1:A:293:GLU:HB2	1:C:318:GLU:CG	2.13	0.77
1:B:359:ARG:HH21	1:B:362:LEU:HD21	1.48	0.77
1:C:351:ARG:HD2	1:C:351:ARG:N	2.00	0.77
1:B:293:GLU:CB	1:D:318:GLU:HG2	2.15	0.76
1:A:100:VAL:O	1:A:104:GLU:HG3	1.83	0.76
1:B:151:LYS:HD2	1:B:151:LYS:N	1.98	0.76
1:B:314:TRP:O	1:B:319:ARG:HD3	1.86	0.75
1:A:293:GLU:HB2	1:C:318:GLU:HG2	1.68	0.75
1:D:83:TYR:HB3	1:D:254:VAL:HG21	1.69	0.74
1:D:18:LYS:HG3	1:D:162:ILE:HD11	1.70	0.74
1:D:319:ARG:HH21	1:D:323:GLN:HE21	1.34	0.73
1:C:37:GLN:H	1:C:37:GLN:HE21	1.36	0.73
1:B:351:ARG:HD2	1:B:351:ARG:N	2.04	0.72
1:A:293:GLU:HB3	1:C:318:GLU:HG2	1.71	0.72
1:B:293:GLU:HB3	1:D:318:GLU:HG2	1.70	0.71
1:B:41:VAL:CG1	1:B:58:ALA:HB1	2.19	0.71
1:C:319:ARG:HH21	1:C:323:GLN:NE2	1.88	0.71
1:A:349:VAL:HG22	1:B:194:GLU:HG3	1.73	0.70
1:A:318:GLU:HG2	1:C:293:GLU:CB	2.22	0.69
1:B:318:GLU:HG3	1:D:293:GLU:HB2	1.74	0.69
1:C:262:VAL:O	1:C:262:VAL:HG12	1.90	0.69
1:B:87:GLY:HA3	1:B:180:HIS:CD2	2.27	0.69
1:D:109:GLU:O	1:D:137:LYS:HE2	1.91	0.69
1:D:174:MET:HE1	1:D:201:ARG:CD	2.22	0.69
1:C:21:LYS:O	1:C:25:ARG:HA	1.93	0.69
1:D:393:VAL:O	1:D:395:ARG:HG3	1.92	0.69
1:B:118:LYS:HD2	1:B:118:LYS:N	2.09	0.68
1:C:245:ILE:O	1:C:248:ARG:HG2	1.93	0.68
1:C:86:LEU:O	1:C:90:ILE:HG13	1.94	0.68
5:A:4520:ARG:NH2	1:B:173:SER:O	2.25	0.68
1:B:293:GLU:HB2	1:D:318:GLU:CG	2.24	0.68
1:A:109:GLU:O	1:A:137:LYS:HE2	1.94	0.68
1:C:17:LEU:HD13	1:C:51:THR:HB	1.76	0.67
1:A:93:PRO:HG3	7:A:1201:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:HD2	1:A:351:ARG:N	2.09	0.67
1:D:124:ARG:O	1:D:128:THR:CG2	2.42	0.67
1:A:390:ARG:O	1:A:394:GLU:HG2	1.94	0.67
1:C:319:ARG:HH21	1:C:323:GLN:HE21	1.42	0.67
1:A:37:GLN:HG2	7:A:1494:HOH:O	1.95	0.67
1:A:371:TYR:HD1	1:A:375:ASP:HB2	1.60	0.67
1:C:374:LYS:HE2	7:C:1162:HOH:O	1.95	0.66
1:A:319:ARG:HH21	1:A:323:GLN:NE2	1.93	0.66
1:A:318:GLU:HG2	1:C:293:GLU:HB3	1.78	0.66
1:A:319:ARG:HH21	1:A:323:GLN:HE21	1.43	0.66
1:C:156:TYR:O	1:C:159:ALA:HB3	1.96	0.66
1:C:109:GLU:HG3	1:C:137:LYS:HE3	1.77	0.66
1:C:343:LYS:HD2	1:D:343:LYS:HD2	1.78	0.66
1:C:41:VAL:HG12	1:C:58:ALA:HB1	1.78	0.66
1:D:62:LYS:H	1:D:62:LYS:HD3	1.62	0.65
1:B:318:GLU:CG	1:D:293:GLU:HB2	2.26	0.65
1:A:67:ARG:HH12	1:A:68:ASP:CG	2.03	0.65
1:B:37:GLN:HG2	7:B:1237:HOH:O	1.95	0.64
1:A:42:GLU:O	1:A:46:GLU:HG3	1.96	0.64
1:A:318:GLU:CG	1:C:293:GLU:HB2	2.27	0.64
1:A:373:GLN:H	1:A:373:GLN:HE21	1.46	0.64
1:C:151:LYS:H	1:C:151:LYS:CD	1.99	0.64
7:A:1551:HOH:O	1:B:345:ASN:HB2	1.98	0.64
1:A:151:LYS:H	1:A:151:LYS:CD	1.89	0.64
1:B:75:ARG:HG2	1:B:330:ALA:CB	2.28	0.63
1:B:216:VAL:HG22	7:B:1549:HOH:O	1.97	0.63
1:D:37:GLN:NE2	1:D:37:GLN:H	1.96	0.63
1:C:60:ASP:OD1	1:C:62:LYS:HE3	1.99	0.63
1:D:83:TYR:CB	1:D:254:VAL:HG21	2.28	0.63
1:A:262:VAL:CG2	1:A:264:MET:HE1	2.12	0.62
1:C:122:GLN:HE21	1:C:143:ARG:NH1	1.95	0.62
1:C:371:TYR:HA	7:C:1158:HOH:O	1.99	0.62
1:B:360:GLN:HA	1:B:363:VAL:HG22	1.79	0.62
1:C:159:ALA:O	1:C:161:GLY:N	2.32	0.62
1:B:35:ILE:H	1:B:37:GLN:HE22	1.42	0.62
1:D:214:GLU:OE1	1:D:249:HIS:HE1	1.82	0.62
1:B:122:GLN:HE21	1:B:143:ARG:HH11	1.48	0.61
1:D:395:ARG:HG3	1:D:395:ARG:HH11	1.66	0.61
1:B:314:TRP:CE3	1:B:319:ARG:HD2	2.36	0.61
1:A:67:ARG:HH11	1:A:67:ARG:CG	2.14	0.61
1:B:42:GLU:O	1:B:46:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH1	1:A:68:ASP:OD1	2.33	0.60
1:C:98:HIS:HD2	1:C:101:ARG:NH1	2.00	0.60
1:A:41:VAL:HG12	1:A:58:ALA:HB1	1.84	0.60
1:B:293:GLU:HB2	1:D:318:GLU:HG2	1.81	0.60
7:C:1251:HOH:O	1:D:191:PRO:HG2	2.01	0.60
1:B:117:GLY:HA2	1:B:122:GLN:NE2	2.16	0.60
1:B:282:ARG:O	1:B:286:GLU:HG3	2.01	0.60
1:C:343:LYS:HD2	1:D:343:LYS:CD	2.32	0.60
1:B:50:ARG:NH1	7:B:1386:HOH:O	2.34	0.60
1:C:18:LYS:NZ	1:C:160:HIS:O	2.34	0.60
1:C:262:VAL:HG11	1:D:371:TYR:OH	2.02	0.60
1:C:21:LYS:O	1:C:25:ARG:CA	2.50	0.60
1:A:123:VAL:HG22	1:B:380:ILE:CD1	2.25	0.60
1:C:248:ARG:HG3	1:C:249:HIS:CD2	2.37	0.60
1:B:117:GLY:HA2	1:B:122:GLN:HE22	1.67	0.59
1:C:93:PRO:HG3	7:C:1365:HOH:O	2.02	0.59
1:C:150:ARG:O	1:C:154:ILE:HG13	2.00	0.59
1:C:395:ARG:HG3	1:C:395:ARG:HH11	1.67	0.59
1:D:395:ARG:HB2	1:D:395:ARG:CZ	2.32	0.59
1:B:1:MET:O	1:B:26:ALA:HB1	2.03	0.59
1:A:245:ILE:O	1:A:248:ARG:HG2	2.03	0.59
1:B:318:GLU:HG2	1:D:293:GLU:HB3	1.85	0.59
1:C:73:MET:HE1	1:C:90:ILE:HG12	1.84	0.59
1:D:67:ARG:HD2	1:D:68:ASP:OD1	2.02	0.59
1:A:173:SER:O	5:A:520:ARG:NH2	2.36	0.59
1:D:7:TYR:CE2	1:D:9:GLY:HA2	2.38	0.59
1:C:41:VAL:CG1	1:C:58:ALA:HB1	2.33	0.58
1:D:6:ALA:HB2	1:D:99:LEU:HD11	1.83	0.58
1:A:27:GLU:HG3	1:A:54:SER:HB3	1.85	0.58
1:C:109:GLU:CG	1:C:137:LYS:HE3	2.33	0.58
1:D:93:PRO:HG3	7:D:1516:HOH:O	2.02	0.58
1:D:22:GLU:CD	1:D:160:HIS:HE2	2.11	0.58
1:B:126:GLU:HG2	1:B:138:VAL:HG11	1.84	0.58
1:B:93:PRO:HA	1:B:128:THR:HG21	1.85	0.58
1:A:6:ALA:HB2	1:A:99:LEU:HD11	1.86	0.58
1:A:104:GLU:HG2	1:A:133:LYS:HZ2	1.69	0.58
1:D:282:ARG:O	1:D:286:GLU:HG3	2.03	0.57
1:B:93:PRO:HG3	7:B:1266:HOH:O	2.04	0.57
1:A:302:SER:HB2	1:A:303:PRO:HD3	1.86	0.57
1:A:104:GLU:OE2	1:A:133:LYS:NZ	2.33	0.57
1:B:35:ILE:N	1:B:37:GLN:HE22	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:HG2	1:C:293:GLU:HB2	1.87	0.57
1:A:382:ILE:HD12	1:C:262:VAL:HG13	1.86	0.57
1:B:371:TYR:HD1	1:B:375:ASP:HB2	1.70	0.57
1:D:150:ARG:HA	1:D:153:MET:HE3	1.87	0.57
1:A:345:ASN:HB3	1:A:347:TYR:CE1	2.40	0.57
1:A:98:HIS:HD2	1:A:101:ARG:NH1	2.03	0.56
1:B:180:HIS:ND1	1:B:180:HIS:C	2.62	0.56
1:C:17:LEU:O	1:C:17:LEU:HD23	2.04	0.56
1:C:18:LYS:HD2	1:C:160:HIS:HB3	1.85	0.56
1:D:360:GLN:HG2	1:D:364:SER:OG	2.05	0.56
1:C:209:ALA:O	1:C:343:LYS:NZ	2.39	0.56
1:C:18:LYS:NZ	1:C:160:HIS:HB3	2.20	0.56
5:A:3520:ARG:HH21	1:D:184:GLU:HG2	1.71	0.56
1:B:37:GLN:NE2	1:B:37:GLN:H	2.04	0.56
1:B:318:GLU:CG	1:D:293:GLU:CB	2.84	0.56
1:A:373:GLN:NE2	1:A:373:GLN:N	2.48	0.55
1:D:35:ILE:N	1:D:37:GLN:HE22	1.97	0.55
1:B:34:ASP:HB2	1:B:41:VAL:HG21	1.87	0.55
1:C:126:GLU:HG2	1:C:138:VAL:HG11	1.88	0.55
1:A:104:GLU:HG2	1:A:133:LYS:NZ	2.20	0.55
1:A:125:PHE:O	1:A:128:THR:HG23	2.07	0.55
1:A:150:ARG:HG3	1:A:154:ILE:HD13	1.89	0.55
1:D:350:GLY:C	1:D:351:ARG:HD2	2.31	0.55
1:D:126:GLU:HG2	1:D:138:VAL:HG11	1.87	0.55
1:B:318:GLU:HG2	1:D:293:GLU:CB	2.37	0.55
1:D:351:ARG:N	1:D:351:ARG:CD	2.69	0.55
1:D:176:ALA:CB	1:D:181:ILE:HG12	2.36	0.55
1:B:359:ARG:NH2	1:B:362:LEU:HD21	2.20	0.55
1:C:350:GLY:C	1:C:351:ARG:HD2	2.32	0.55
1:A:87:GLY:HA2	1:A:179:LEU:HD13	1.87	0.54
1:A:382:ILE:HD12	1:C:262:VAL:CG1	2.38	0.54
1:B:6:ALA:HB2	1:B:99:LEU:HD11	1.89	0.54
1:C:21:LYS:O	1:C:25:ARG:N	2.41	0.54
1:C:220:PHE:CE2	1:C:225:PRO:HG3	2.42	0.54
1:D:87:GLY:HA2	1:D:179:LEU:HD13	1.89	0.54
1:A:75:ARG:NH2	7:A:1451:HOH:O	2.41	0.54
1:A:180:HIS:C	1:A:180:HIS:ND1	2.65	0.54
1:A:351:ARG:HD3	1:B:191:PRO:HB2	1.89	0.54
1:C:98:HIS:CD2	1:C:101:ARG:NH1	2.76	0.54
1:C:393:VAL:O	1:C:395:ARG:NH1	2.40	0.54
1:C:373:GLN:HG2	1:C:374:LYS:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:C	1:A:298:ARG:HD2	2.33	0.54
1:B:350:GLY:C	1:B:351:ARG:HD2	2.32	0.54
1:A:90:ILE:HD11	1:A:179:LEU:HD12	1.90	0.54
1:B:216:VAL:HG21	1:B:245:ILE:HG21	1.90	0.54
1:C:37:GLN:HB2	1:C:39:GLU:HG2	1.90	0.54
1:C:109:GLU:O	1:C:137:LYS:CE	2.51	0.54
1:D:1:MET:O	1:D:26:ALA:HB1	2.08	0.54
1:B:382:ILE:HG13	1:C:379:PHE:HB2	1.90	0.54
1:D:29:ILE:HD12	1:D:29:ILE:N	2.23	0.54
1:D:42:GLU:O	1:D:46:GLU:HG3	2.08	0.54
1:A:214:GLU:OE1	1:A:249:HIS:HE1	1.91	0.54
1:B:359:ARG:C	1:B:361:ASP:H	2.16	0.54
1:C:24:TYR:O	1:C:25:ARG:C	2.50	0.53
1:B:118:LYS:N	1:B:118:LYS:CD	2.70	0.53
1:D:371:TYR:HB2	1:D:375:ASP:OD1	2.08	0.53
1:B:249:HIS:HD2	7:B:1070:HOH:O	1.90	0.53
1:D:122:GLN:HE21	1:D:143:ARG:HH11	1.57	0.53
1:D:221:PHE:O	1:D:334:THR:OG1	2.20	0.53
1:D:338:ARG:HD3	7:D:1261:HOH:O	2.09	0.53
1:D:345:ASN:HB3	1:D:347:TYR:CE1	2.44	0.53
5:A:2520:ARG:NH2	1:C:173:SER:O	2.42	0.53
5:A:3520:ARG:NH2	1:D:173:SER:O	2.42	0.53
1:A:264:MET:HE3	1:A:264:MET:N	2.18	0.53
1:B:98:HIS:HD2	1:B:101:ARG:NH1	2.07	0.53
1:D:120:ASN:HD21	1:D:260:ARG:HG2	1.74	0.53
1:A:98:HIS:CD2	1:A:101:ARG:NH1	2.76	0.53
1:A:395:ARG:HH22	1:D:355:LYS:HE3	1.72	0.53
1:C:360:GLN:OE1	1:D:189:GLU:OE2	2.27	0.53
1:D:314:TRP:O	1:D:319:ARG:HD3	2.09	0.53
1:C:374:LYS:HE3	1:D:143:ARG:O	2.08	0.53
1:D:205:ASP:OD1	1:D:207:GLU:OE2	2.27	0.53
1:A:41:VAL:CG1	1:A:58:ALA:HB1	2.40	0.52
1:C:73:MET:SD	1:C:90:ILE:HG21	2.49	0.52
1:A:221:PHE:O	1:A:334:THR:OG1	2.17	0.52
1:A:21:LYS:HD2	1:A:26:ALA:O	2.10	0.52
1:B:75:ARG:NH2	7:B:1271:HOH:O	2.42	0.52
1:B:124:ARG:O	1:B:128:THR:CG2	2.55	0.52
1:A:126:GLU:HG2	1:A:138:VAL:HG11	1.91	0.52
1:B:395:ARG:HH11	1:B:395:ARG:HG3	1.73	0.52
1:D:117:GLY:HA2	1:D:122:GLN:NE2	2.24	0.52
1:C:35:ILE:N	1:C:37:GLN:NE2	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HG2	1:A:136:ILE:HB	1.91	0.52
1:C:150:ARG:HH11	1:C:150:ARG:HB2	1.75	0.52
1:A:70:VAL:O	1:A:74:MET:HG3	2.10	0.52
1:C:373:GLN:HG2	1:C:374:LYS:H	1.75	0.52
1:A:67:ARG:NH1	1:A:68:ASP:CG	2.67	0.52
1:B:87:GLY:HA2	1:B:179:LEU:HD13	1.92	0.52
1:D:40:GLU:OE1	1:D:42:GLU:HB2	2.09	0.52
1:D:98:HIS:HD2	1:D:101:ARG:NH1	2.08	0.52
1:D:314:TRP:CE3	1:D:319:ARG:HD2	2.44	0.52
1:A:7:TYR:CE2	1:A:9:GLY:HA2	2.45	0.51
1:B:110:ALA:HB2	1:B:137:LYS:HB3	1.92	0.51
1:B:221:PHE:O	1:B:334:THR:OG1	2.15	0.51
1:B:150:ARG:HA	1:B:153:MET:HE3	1.93	0.51
1:C:25:ARG:HB3	1:C:25:ARG:NH1	2.26	0.51
1:D:137:LYS:HD3	1:D:137:LYS:N	2.26	0.51
1:A:137:LYS:N	1:A:137:LYS:HD3	2.26	0.51
1:A:249:HIS:HD2	7:A:1275:HOH:O	1.91	0.51
1:A:264:MET:CE	1:A:264:MET:H	2.18	0.51
1:C:343:LYS:CD	1:D:343:LYS:HD2	2.38	0.51
1:C:282:ARG:O	1:C:286:GLU:HG3	2.11	0.51
1:A:379:PHE:HB2	1:D:382:ILE:HG13	1.93	0.51
1:D:70:VAL:O	1:D:74:MET:HG3	2.10	0.51
1:D:319:ARG:HH21	1:D:323:GLN:NE2	2.04	0.51
1:B:34:ASP:HA	1:B:37:GLN:HE22	1.75	0.51
1:C:158:GLU:O	1:C:159:ALA:O	2.29	0.51
1:C:342:TYR:OH	1:D:207:GLU:HA	2.11	0.51
1:D:133:LYS:O	1:D:136:ILE:HG22	2.11	0.51
1:D:117:GLY:HA2	1:D:122:GLN:HE22	1.76	0.51
1:B:371:TYR:HB2	1:B:375:ASP:OD1	2.11	0.50
5:A:3520:ARG:NH2	1:D:184:GLU:HG2	2.25	0.50
1:C:74:MET:HE1	1:C:278:LEU:HD12	1.93	0.50
1:B:120:ASN:HD21	1:B:260:ARG:HG2	1.76	0.50
1:B:77:GLY:HA2	7:B:1168:HOH:O	2.10	0.50
1:B:328:HIS:CD2	1:D:321:ALA:HA	2.46	0.50
1:C:262:VAL:O	1:C:262:VAL:CG1	2.60	0.50
1:C:185:GLY:O	1:C:188:LEU:HB2	2.11	0.50
1:C:302:SER:HB2	1:C:303:PRO:HD3	1.93	0.50
1:D:304:LYS:O	1:D:307:GLU:HG2	2.12	0.50
1:B:181:ILE:HD12	1:B:202:MET:HB2	1.93	0.50
1:B:359:ARG:C	1:B:361:ASP:N	2.69	0.50
1:C:351:ARG:N	1:C:351:ARG:CD	2.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:LEU:N	1:D:339:LEU:HD12	2.26	0.50
1:C:25:ARG:NH1	1:C:25:ARG:CB	2.74	0.50
1:D:97:LYS:HD2	1:D:315:TYR:OH	2.12	0.50
1:B:319:ARG:HH21	1:B:323:GLN:HE21	1.60	0.49
1:C:32:THR:CG2	1:C:41:VAL:HG13	2.42	0.49
1:D:16:ILE:HG23	1:D:141:PRO:HG2	1.94	0.49
1:B:393:VAL:C	1:B:395:ARG:H	2.20	0.49
1:C:34:ASP:HA	1:C:37:GLN:HE22	1.77	0.49
1:D:150:ARG:O	1:D:154:ILE:HD13	2.11	0.49
1:C:393:VAL:C	1:C:395:ARG:N	2.67	0.49
1:C:298:ARG:HD2	1:C:298:ARG:C	2.37	0.49
1:B:12:ASP:OD1	1:B:150:ARG:NH2	2.39	0.49
1:D:316:ALA:HB1	1:D:318:GLU:OE2	2.12	0.49
1:C:96:ALA:HB3	1:C:128:THR:HG21	1.92	0.49
1:A:293:GLU:HB2	1:C:318:GLU:HG3	1.92	0.49
1:B:2:LYS:HB2	1:B:108:ALA:HA	1.95	0.49
1:B:150:ARG:O	1:B:154:ILE:HD13	2.11	0.49
1:C:262:VAL:HB	1:C:264:MET:HE1	1.95	0.49
1:B:90:ILE:HD11	1:B:179:LEU:HD12	1.94	0.49
1:C:6:ALA:HB2	1:C:99:LEU:HD11	1.95	0.49
1:A:32:THR:CG2	1:A:41:VAL:HG13	2.44	0.48
1:A:191:PRO:HG2	7:B:1561:HOH:O	2.13	0.48
1:C:180:HIS:ND1	1:C:180:HIS:C	2.71	0.48
1:B:214:GLU:OE1	1:B:249:HIS:HE1	1.96	0.48
1:C:27:GLU:HG3	1:C:54:SER:CB	2.42	0.48
1:B:373:GLN:O	1:B:376:ALA:HB3	2.12	0.48
1:A:27:GLU:HG3	1:A:54:SER:CB	2.43	0.48
1:D:209:ALA:O	1:D:343:LYS:NZ	2.47	0.48
1:D:365:PHE:N	7:D:1390:HOH:O	2.47	0.48
5:A:3520:ARG:NH2	1:D:173:SER:C	2.64	0.48
1:A:371:TYR:OH	1:B:118:LYS:HA	2.13	0.48
1:B:351:ARG:N	1:B:351:ARG:CD	2.75	0.48
1:D:37:GLN:H	1:D:37:GLN:HE21	1.62	0.48
1:C:70:VAL:O	1:C:74:MET:HG3	2.14	0.48
1:D:298:ARG:O	1:D:298:ARG:HD2	2.14	0.47
1:C:73:MET:SD	1:C:90:ILE:CG2	3.02	0.47
1:C:122:GLN:HE22	1:C:143:ARG:HD3	1.79	0.47
1:D:251:VAL:HG11	1:D:346:VAL:CG2	2.44	0.47
1:B:69:PHE:CE1	1:B:94:LEU:HD23	2.48	0.47
1:C:262:VAL:HB	1:C:264:MET:CE	2.44	0.47
1:D:171:PRO:O	1:D:186:GLY:HA3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:THR:HB	1:D:250:GLY:HA2	1.96	0.47
1:A:98:HIS:HD2	1:A:101:ARG:HH12	1.62	0.47
1:C:21:LYS:HD2	1:C:26:ALA:O	2.15	0.47
1:D:215:TYR:CZ	1:D:340:LYS:HD3	2.49	0.47
1:A:92:ARG:HE	1:A:121:ASP:CG	2.22	0.47
1:C:17:LEU:HD23	1:C:17:LEU:C	2.38	0.47
1:C:205:ASP:O	1:C:206:PRO:C	2.58	0.47
1:D:41:VAL:HG23	1:D:42:GLU:N	2.29	0.47
1:B:339:LEU:N	1:B:339:LEU:HD12	2.29	0.47
1:D:64:GLU:OE1	1:D:98:HIS:HE1	1.97	0.47
1:D:251:VAL:CG1	1:D:252:GLY:N	2.78	0.47
1:A:174:MET:HE1	1:A:201:ARG:CD	2.44	0.47
1:C:32:THR:O	1:C:58:ALA:HA	2.14	0.47
1:C:40:GLU:O	1:C:40:GLU:HG3	2.15	0.47
1:D:18:LYS:CG	1:D:162:ILE:HD11	2.42	0.47
1:D:34:ASP:HB2	1:D:41:VAL:HG11	1.95	0.47
1:A:67:ARG:HG2	1:A:67:ARG:NH1	2.22	0.47
1:A:97:LYS:HD2	1:A:315:TYR:OH	2.15	0.47
1:A:117:GLY:C	1:A:122:GLN:HE22	2.22	0.47
1:A:393:VAL:C	1:A:395:ARG:N	2.73	0.47
1:B:34:ASP:HB3	1:B:60:ASP:HA	1.97	0.47
1:B:393:VAL:C	1:B:395:ARG:N	2.69	0.47
1:C:120:ASN:HD21	1:C:260:ARG:HG2	1.80	0.47
1:C:33:ALA:HB1	1:C:61:LEU:HD12	1.97	0.47
1:B:101:ARG:HD3	7:B:1166:HOH:O	2.14	0.47
1:B:251:VAL:HG11	1:B:346:VAL:CG2	2.45	0.47
1:C:392:LEU:O	1:C:395:ARG:HA	2.15	0.47
1:A:21:LYS:O	1:A:25:ARG:HA	2.15	0.46
1:A:118:LYS:HD3	1:B:365:PHE:CE2	2.51	0.46
1:B:16:ILE:HG23	1:B:141:PRO:HG2	1.97	0.46
1:C:100:VAL:O	1:C:104:GLU:HG3	2.15	0.46
1:A:154:ILE:HG13	1:A:164:VAL:HG11	1.97	0.46
1:A:343:LYS:HD2	1:B:343:LYS:HD3	1.98	0.46
7:A:1195:HOH:O	1:B:191:PRO:HG2	2.14	0.46
1:C:314:TRP:O	1:C:319:ARG:HD3	2.15	0.46
1:A:371:TYR:CE1	1:D:382:ILE:HD11	2.50	0.46
1:B:254:VAL:CG1	1:B:256:ILE:HG23	2.46	0.46
1:C:18:LYS:CD	1:C:160:HIS:HB3	2.45	0.46
1:C:37:GLN:HE21	1:C:37:GLN:N	2.09	0.46
1:D:262:VAL:O	1:D:262:VAL:HG13	2.13	0.46
1:C:16:ILE:HG23	1:C:141:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LYS:HD2	1:C:160:HIS:CB	2.45	0.46
1:A:257:VAL:HB	1:B:287:SER:HB2	1.97	0.46
1:B:321:ALA:HA	1:D:328:HIS:CD2	2.51	0.46
1:C:101:ARG:NH2	7:C:1285:HOH:O	2.41	0.46
1:C:360:GLN:HG3	1:D:189:GLU:HB3	1.96	0.46
1:C:393:VAL:C	1:C:395:ARG:H	2.21	0.46
1:C:36:GLY:N	1:C:37:GLN:HE21	2.14	0.46
1:C:189:GLU:O	1:C:191:PRO:HD3	2.16	0.46
1:D:394:GLU:O	1:D:395:ARG:C	2.58	0.46
1:A:181:ILE:HD12	1:A:202:MET:HB2	1.97	0.46
1:B:80:TYR:HB3	1:B:84:TYR:HB3	1.98	0.46
1:A:67:ARG:CG	1:A:67:ARG:NH1	2.76	0.46
1:D:98:HIS:HD2	1:D:101:ARG:HH11	1.64	0.46
1:D:319:ARG:NH2	1:D:323:GLN:HE21	2.07	0.46
1:B:182:SER:HB2	7:B:1105:HOH:O	2.16	0.45
1:C:67:ARG:HG2	1:C:68:ASP:OD1	2.17	0.45
1:D:252:GLY:O	1:D:271:GLU:HA	2.16	0.45
1:B:385:LEU:HD22	1:C:371:TYR:HD1	1.80	0.45
1:D:22:GLU:OE2	1:D:160:HIS:NE2	2.40	0.45
1:D:60:ASP:OD2	1:D:62:LYS:HE2	2.16	0.45
1:D:341:LEU:HD22	1:D:346:VAL:HG22	1.98	0.45
1:B:122:GLN:NE2	1:B:143:ARG:HH11	2.10	0.45
1:C:157:ALA:O	1:C:158:GLU:C	2.59	0.45
1:B:92:ARG:HE	1:B:121:ASP:CG	2.25	0.45
1:C:40:GLU:O	1:C:42:GLU:N	2.50	0.45
1:C:179:LEU:O	1:C:272:THR:HG23	2.16	0.45
1:C:373:GLN:HE21	1:C:373:GLN:HB3	1.52	0.45
1:A:349:VAL:HG13	7:B:1076:HOH:O	2.16	0.45
4:A:510:ANP:HNB1	5:A:520:ARG:HH12	1.64	0.45
1:D:146:SER:O	1:D:147:PHE:C	2.59	0.45
1:A:15:ILE:HG23	1:A:156:TYR:CD2	2.52	0.45
1:D:176:ALA:HB1	1:D:181:ILE:HG12	1.97	0.45
1:A:157:ALA:HB1	1:A:162:ILE:HB	1.98	0.45
1:B:203:THR:HB	1:B:250:GLY:HA2	1.99	0.45
1:C:27:GLU:CG	1:C:54:SER:OG	2.65	0.45
1:D:84:TYR:CE2	1:D:86:LEU:HA	2.52	0.45
1:B:293:GLU:HB2	1:D:318:GLU:HG3	1.98	0.45
1:A:154:ILE:O	1:A:158:GLU:HG3	2.17	0.44
1:C:27:GLU:HG3	1:C:54:SER:OG	2.16	0.44
1:A:74:MET:HE1	1:A:278:LEU:HD12	1.97	0.44
1:A:371:TYR:CD1	1:D:382:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ARG:HH21	1:B:362:LEU:CD2	2.24	0.44
1:C:60:ASP:OD1	1:C:62:LYS:CE	2.65	0.44
1:C:260:ARG:HD2	1:C:264:MET:SD	2.58	0.44
1:D:185:GLY:O	1:D:188:LEU:HB2	2.18	0.44
1:C:80:TYR:HB3	1:C:84:TYR:HB3	1.99	0.44
1:D:158:GLU:O	1:D:159:ALA:C	2.60	0.44
1:A:349:VAL:HG22	1:B:194:GLU:CG	2.44	0.44
5:A:4520:ARG:HH12	4:B:4510:ANP:HNB1	1.66	0.44
1:C:25:ARG:CB	1:C:25:ARG:HH11	2.31	0.44
1:A:254:VAL:CG1	1:A:256:ILE:HG23	2.48	0.44
1:B:21:LYS:HD3	7:B:1417:HOH:O	2.18	0.44
1:B:34:ASP:OD1	1:B:62:LYS:HD2	2.18	0.44
1:B:179:LEU:O	1:B:272:THR:HG23	2.18	0.44
1:C:74:MET:HB3	1:C:282:ARG:NH1	2.33	0.44
1:D:392:LEU:O	1:D:395:ARG:HG2	2.18	0.44
1:B:17:LEU:HD11	1:B:53:ALA:HB2	2.00	0.44
1:C:77:GLY:HA2	7:C:1193:HOH:O	2.17	0.44
1:C:87:GLY:HA3	1:C:180:HIS:CD2	2.53	0.44
1:C:395:ARG:HG3	1:C:395:ARG:NH1	2.31	0.44
1:D:181:ILE:HD12	1:D:202:MET:HB2	2.00	0.44
1:B:181:ILE:CD1	1:B:202:MET:HB2	2.48	0.43
1:C:90:ILE:HD11	1:C:179:LEU:HD12	2.01	0.43
1:B:174:MET:HG2	1:B:183:TYR:CD2	2.53	0.43
1:D:174:MET:HE1	1:D:201:ARG:HD3	2.00	0.43
1:D:6:ALA:HB3	4:D:3510:ANP:O2'	2.18	0.43
1:D:60:ASP:OD1	1:D:62:LYS:HD3	2.17	0.43
1:D:206:PRO:C	1:D:208:GLU:H	2.27	0.43
1:C:71:PHE:HB2	1:C:72:PRO:HD3	2.00	0.43
1:C:123:VAL:HG12	1:C:127:LEU:CD1	2.48	0.43
1:D:151:LYS:N	1:D:151:LYS:CD	2.60	0.43
1:A:12:ASP:OD1	1:A:150:ARG:NH2	2.47	0.43
1:A:191:PRO:HB2	1:B:351:ARG:HD3	2.01	0.43
5:A:2520:ARG:HG2	1:C:182:SER:OG	2.19	0.43
1:B:98:HIS:CD2	1:B:101:ARG:NH1	2.86	0.43
1:A:150:ARG:O	1:A:151:LYS:C	2.62	0.43
1:A:241:ARG:O	1:A:245:ILE:HG13	2.19	0.43
1:C:18:LYS:HZ3	1:C:160:HIS:HB3	1.84	0.43
1:A:205:ASP:OD2	1:A:205:ASP:C	2.61	0.42
1:A:209:ALA:HB3	1:A:343:LYS:HG2	2.01	0.42
1:B:75:ARG:HD2	1:B:327:ASP:OD2	2.19	0.42
1:D:181:ILE:HG22	1:D:183:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:NH2	7:C:1320:HOH:O	2.52	0.42
1:D:378:GLY:O	1:D:382:ILE:HG12	2.19	0.42
1:A:64:GLU:OE1	1:A:98:HIS:HE1	2.01	0.42
1:D:199:MET:O	1:D:201:ARG:NH1	2.52	0.42
1:C:372:ASP:C	1:C:372:ASP:OD2	2.61	0.42
1:C:98:HIS:CD2	1:C:101:ARG:HH11	2.36	0.42
1:C:151:LYS:HD2	1:C:151:LYS:N	2.09	0.42
1:A:87:GLY:HA3	1:A:180:HIS:CD2	2.55	0.42
1:C:39:GLU:O	1:C:41:VAL:N	2.51	0.42
1:C:352:LYS:HE3	1:D:192:TRP:CH2	2.54	0.42
1:D:157:ALA:HB1	1:D:162:ILE:HB	2.01	0.42
1:D:393:VAL:C	1:D:395:ARG:N	2.78	0.42
1:A:176:ALA:HB1	1:A:181:ILE:HG12	2.02	0.42
1:A:288:LEU:HD11	1:A:351:ARG:HG2	2.01	0.42
1:A:379:PHE:HA	1:D:379:PHE:HA	2.01	0.42
1:B:304:LYS:O	1:B:307:GLU:HG2	2.18	0.42
1:D:302:SER:HB2	1:D:303:PRO:HD3	2.01	0.42
1:B:395:ARG:HG3	1:B:395:ARG:NH1	2.34	0.42
1:B:94:LEU:HD13	1:B:94:LEU:C	2.45	0.42
1:C:4:VAL:O	1:C:111:ILE:HA	2.20	0.42
1:C:12:ASP:OD1	1:C:150:ARG:NH2	2.51	0.42
1:D:40:GLU:OE2	1:D:40:GLU:HA	2.19	0.42
1:D:74:MET:HB3	1:D:282:ARG:CZ	2.49	0.42
1:A:339:LEU:HD12	1:A:339:LEU:N	2.35	0.41
1:B:69:PHE:C	1:B:72:PRO:HD2	2.45	0.41
1:C:12:ASP:O	1:C:16:ILE:HG13	2.19	0.41
1:D:179:LEU:O	1:D:272:THR:HG23	2.20	0.41
1:A:267:ARG:HD3	1:A:267:ARG:C	2.45	0.41
1:B:123:VAL:HG12	1:B:127:LEU:HD12	2.01	0.41
1:A:263:GLY:HA3	1:C:385:LEU:HD23	2.03	0.41
1:D:174:MET:HA	1:D:182:SER:O	2.20	0.41
1:A:73:MET:HE3	7:A:1484:HOH:O	2.20	0.41
1:B:251:VAL:CG1	1:B:252:GLY:N	2.82	0.41
1:B:319:ARG:HH21	1:B:323:GLN:NE2	2.18	0.41
1:A:18:LYS:HE3	1:A:160:HIS:HB3	2.03	0.41
1:B:128:THR:O	1:B:132:LEU:HG	2.20	0.41
1:D:136:ILE:C	1:D:137:LYS:HD3	2.46	0.41
1:A:180:HIS:HB2	1:A:271:GLU:O	2.21	0.41
1:A:328:HIS:CD2	1:C:321:ALA:HA	2.56	0.41
1:D:84:TYR:CZ	1:D:86:LEU:HA	2.55	0.41
1:D:395:ARG:HG3	1:D:395:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HA	1:A:70:VAL:HB	2.01	0.41
1:A:184:GLU:OE2	5:A:520:ARG:HG3	2.21	0.41
1:A:316:ALA:HB1	1:A:318:GLU:OE2	2.20	0.41
1:A:150:ARG:HG3	1:A:154:ILE:CD1	2.49	0.41
1:A:318:GLU:HG3	1:C:293:GLU:HB2	2.03	0.41
6:A:3530:ASP:N	4:D:3510:ANP:O2B	2.54	0.41
1:B:180:HIS:HB2	1:B:271:GLU:O	2.20	0.41
1:C:174:MET:HA	1:C:182:SER:O	2.21	0.41
1:D:71:PHE:HB2	1:D:72:PRO:HD3	2.03	0.41
1:D:77:GLY:HA2	7:D:1450:HOH:O	2.21	0.41
1:D:135:ASP:OD2	1:D:135:ASP:N	2.51	0.41
1:D:394:GLU:O	1:D:395:ARG:O	2.38	0.41
1:C:7:TYR:CE2	1:C:9:GLY:HA2	2.56	0.41
1:C:154:ILE:O	1:C:158:GLU:HG3	2.21	0.41
1:A:254:VAL:HG13	1:A:256:ILE:HG23	2.02	0.40
1:D:180:HIS:ND1	1:D:180:HIS:C	2.79	0.40
1:A:176:ALA:CB	1:A:181:ILE:HG12	2.51	0.40
1:A:245:ILE:O	1:A:248:ARG:CG	2.69	0.40
1:B:174:MET:HE1	1:B:201:ARG:NE	2.35	0.40
1:B:238:LEU:HD23	1:B:238:LEU:C	2.45	0.40
1:B:66:VAL:HA	1:B:70:VAL:HB	2.02	0.40
1:D:39:GLU:HA	1:D:39:GLU:OE1	2.22	0.40
1:A:80:TYR:CD2	1:A:81:GLU:HG3	2.56	0.40
1:A:191:PRO:O	1:B:350:GLY:HA2	2.21	0.40
1:D:395:ARG:NH1	1:D:395:ARG:CG	2.82	0.40
1:A:143:ARG:HD2	1:B:373:GLN:O	2.22	0.40
1:C:281:ALA:O	1:C:284:ALA:HB3	2.22	0.40
1:D:162:ILE:O	1:D:163:PRO:C	2.64	0.40
1:D:206:PRO:C	1:D:208:GLU:N	2.78	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	374/400 (94%)	362 (97%)	11 (3%)	1 (0%)	36	34
1	B	380/400 (95%)	366 (96%)	13 (3%)	1 (0%)	36	34
1	C	380/400 (95%)	356 (94%)	20 (5%)	4 (1%)	11	7
1	D	380/400 (95%)	367 (97%)	12 (3%)	1 (0%)	36	34
All	All	1514/1600 (95%)	1451 (96%)	56 (4%)	7 (0%)	24	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	159	ALA
1	C	160	HIS
1	C	22	GLU
1	C	41	VAL
1	A	343	LYS
1	B	373	GLN
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	304/319 (95%)	287 (94%)	17 (6%)	19	15
1	B	310/319 (97%)	296 (96%)	14 (4%)	24	22
1	C	310/319 (97%)	291 (94%)	19 (6%)	17	12
1	D	310/319 (97%)	292 (94%)	18 (6%)	18	14
All	All	1234/1276 (97%)	1166 (94%)	68 (6%)	19	15

All (68) 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	128	THR

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Mol	Chain	Res	Type
1	A	151	LYS
1	A	178	LEU
1	A	179	LEU
1	A	180	HIS
1	A	188	LEU
1	A	239	LEU
1	A	254	VAL
1	A	264	MET
1	A	318	GLU
1	A	319	ARG
1	A	349	VAL
1	A	351	ARG
1	A	373	GLN
1	B	37	GLN
1	B	39	GLU
1	B	62	LYS
1	B	90	ILE
1	B	118	LYS
1	B	128	THR
1	B	178	LEU
1	B	179	LEU
1	B	180	HIS
1	B	188	LEU
1	B	239	LEU
1	B	319	ARG
1	B	351	ARG
1	B	373	GLN
1	C	25	ARG
1	C	37	GLN
1	C	46	GLU
1	C	62	LYS
1	C	90	ILE
1	C	150	ARG
1	C	179	LEU
1	C	180	HIS
1	C	188	LEU
1	C	206	PRO
1	C	239	LEU
1	C	264	MET
1	C	318	GLU
1	C	319	ARG
1	C	345	ASN

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Mol	Chain	Res	Type
1	C	351	ARG
1	C	361	ASP
1	C	373	GLN
1	C	374	LYS
1	D	37	GLN
1	D	62	LYS
1	D	90	ILE
1	D	94	LEU
1	D	128	THR
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	291	ASP
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	249	HIS
1	A	323	GLN
1	A	373	GLN
1	B	37	GLN
1	B	98	HIS
1	B	122	GLN
1	B	148	GLN
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	160	HIS

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Mol	Chain	Res	Type
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	249	HIS
1	D	323	GLN
1	D	360	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ANP	C	2510	3	33,33,33	2.20	9 (27%)	45,52,52	2.42	14 (31%)
5	ARG	A	520	-	10,11,11	1.05	1 (10%)	9,13,13	1.29	1 (11%)
5	ARG	A	4520	-	10,11,11	1.08	1 (10%)	9,13,13	1.52	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ARG	A	3520	-	10,11,11	0.83	0	9,13,13	1.16	1 (11%)
4	ANP	B	4510	3	33,33,33	2.13	10 (30%)	45,52,52	2.35	14 (31%)
4	ANP	D	3510	3	33,33,33	2.29	9 (27%)	45,52,52	2.46	14 (31%)
5	ARG	A	2520	-	10,11,11	1.10	1 (10%)	9,13,13	1.28	2 (22%)
6	ASP	A	2530	-	7,8,8	1.20	0	6,10,10	0.79	0
2	SO4	D	3540	-	4,4,4	1.86	2 (50%)	6,6,6	0.84	0
2	SO4	B	4540	-	4,4,4	1.84	2 (50%)	6,6,6	0.86	0
6	ASP	A	4530	-	7,8,8	1.12	0	6,10,10	0.83	0
6	ASP	A	3530	-	7,8,8	1.17	0	6,10,10	0.78	0
2	SO4	C	2540	-	4,4,4	1.83	2 (50%)	6,6,6	0.85	0
6	ASP	A	530	-	7,8,8	1.13	0	6,10,10	0.75	0
2	SO4	A	540	-	4,4,4	1.82	1 (25%)	6,6,6	0.85	0
4	ANP	A	510	3	33,33,33	2.32	9 (27%)	45,52,52	2.42	14 (31%)

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
4	ANP	C	2510	3	-	3/18/38/38	0/3/3/3
5	ARG	A	520	-	-	0/11/11/11	-
5	ARG	A	4520	-	-	0/11/11/11	-
5	ARG	A	3520	-	-	0/11/11/11	-
4	ANP	B	4510	3	-	3/18/38/38	0/3/3/3
4	ANP	D	3510	3	-	3/18/38/38	0/3/3/3
5	ARG	A	2520	-	-	0/11/11/11	-
6	ASP	A	2530	-	-	0/8/8/8	-
6	ASP	A	4530	-	-	0/8/8/8	-
6	ASP	A	3530	-	-	0/8/8/8	-
6	ASP	A	530	-	-	0/8/8/8	-
4	ANP	A	510	3	-	3/18/38/38	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	ANP	PB-O3A	7.41	1.68	1.59
4	C	2510	ANP	PB-O3A	7.09	1.67	1.59
4	D	3510	ANP	PB-O3A	6.82	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4510	ANP	PB-O3A	5.49	1.65	1.59
4	D	3510	ANP	PG-N3B	4.73	1.75	1.63
4	A	510	ANP	PB-O2B	-4.48	1.44	1.56
4	D	3510	ANP	PB-O1B	4.22	1.52	1.46
4	B	4510	ANP	PG-O1G	4.17	1.52	1.46
4	C	2510	ANP	PB-O2B	-4.16	1.45	1.56
4	B	4510	ANP	PG-N3B	4.12	1.74	1.63
4	B	4510	ANP	PB-O2B	-4.10	1.45	1.56
4	A	510	ANP	PB-O1B	4.06	1.52	1.46
4	D	3510	ANP	PG-O1G	3.96	1.52	1.46
4	C	2510	ANP	PG-N3B	3.92	1.73	1.63
4	A	510	ANP	PG-N3B	3.91	1.73	1.63
4	D	3510	ANP	PB-O2B	-3.59	1.47	1.56
4	A	510	ANP	PG-O1G	3.49	1.51	1.46
4	C	2510	ANP	PG-O1G	3.46	1.51	1.46
4	B	4510	ANP	PB-O1B	3.27	1.51	1.46
2	D	3540	SO4	O1-S	3.08	1.63	1.44
2	B	4540	SO4	O1-S	3.03	1.62	1.44
4	C	2510	ANP	PB-O1B	3.01	1.50	1.46
2	A	540	SO4	O1-S	3.00	1.62	1.44
2	C	2540	SO4	O1-S	3.00	1.62	1.44
4	D	3510	ANP	C1'-N9	2.71	1.53	1.46
4	A	510	ANP	C5-N7	-2.67	1.34	1.39
4	C	2510	ANP	C5-N7	-2.65	1.34	1.39
4	B	4510	ANP	C5-N7	-2.63	1.34	1.39
4	D	3510	ANP	C2-N1	2.60	1.38	1.33
4	A	510	ANP	C2-N1	2.59	1.38	1.33
4	B	4510	ANP	C1'-N9	2.59	1.53	1.46
5	A	2520	ARG	CZ-NE	-2.46	1.28	1.33
4	A	510	ANP	C1'-N9	2.44	1.53	1.46
4	C	2510	ANP	C1'-N9	2.40	1.53	1.46
4	C	2510	ANP	PG-O3G	-2.36	1.50	1.56
4	B	4510	ANP	PG-O2G	-2.35	1.50	1.56
4	C	2510	ANP	C2-N1	2.35	1.38	1.33
5	A	4520	ARG	CZ-NE	-2.33	1.28	1.33
4	D	3510	ANP	C5-N7	-2.28	1.34	1.39
5	A	520	ARG	CZ-NE	-2.26	1.29	1.33
4	B	4510	ANP	C2-N1	2.26	1.37	1.33
4	B	4510	ANP	PG-O3G	-2.26	1.50	1.56
4	D	3510	ANP	PG-O3G	-2.19	1.51	1.56
4	A	510	ANP	PG-O3G	-2.12	1.51	1.56
2	D	3540	SO4	O3-S	-2.05	1.31	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2540	SO4	O3-S	-2.05	1.31	1.48
2	B	4540	SO4	O3-S	-2.04	1.31	1.48

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4510	ANP	C5-C4-N3	-7.09	116.95	126.72
4	D	3510	ANP	C5-C4-N3	-7.08	116.97	126.72
4	A	510	ANP	C5-C4-N3	-7.06	116.99	126.72
4	C	2510	ANP	C5-C4-N3	-6.93	117.18	126.72
4	A	510	ANP	N3-C4-N9	6.32	137.91	127.17
4	B	4510	ANP	N3-C4-N9	6.18	137.68	127.17
4	D	3510	ANP	N3-C4-N9	6.14	137.61	127.17
4	C	2510	ANP	N3-C4-N9	6.13	137.60	127.17
4	A	510	ANP	O1B-PB-N3B	-5.44	103.76	111.77
4	D	3510	ANP	O1B-PB-N3B	-5.37	103.86	111.77
4	C	2510	ANP	O1B-PB-N3B	-5.35	103.90	111.77
4	D	3510	ANP	O1G-PG-N3B	-5.00	104.40	111.77
4	B	4510	ANP	O1B-PB-N3B	-4.83	104.65	111.77
4	C	2510	ANP	O1G-PG-N3B	-4.75	104.77	111.77
4	B	4510	ANP	C2-N3-C4	4.18	122.03	111.83
4	D	3510	ANP	C2-N3-C4	4.18	122.03	111.83
4	C	2510	ANP	C2-N3-C4	4.07	121.78	111.83
4	A	510	ANP	C2-N3-C4	4.05	121.72	111.83
4	A	510	ANP	O1G-PG-N3B	-3.97	105.92	111.77
4	C	2510	ANP	C4'-O4'-C1'	3.71	117.65	109.47
4	B	4510	ANP	C4'-O4'-C1'	3.67	117.56	109.47
4	D	3510	ANP	C4'-O4'-C1'	3.66	117.54	109.47
4	A	510	ANP	O4'-C1'-N9	3.58	114.96	108.09
4	C	2510	ANP	O4'-C1'-N9	3.55	114.90	108.09
4	B	4510	ANP	O4'-C1'-N9	3.52	114.85	108.09
4	B	4510	ANP	O1G-PG-N3B	-3.51	106.60	111.77
4	D	3510	ANP	O4'-C1'-N9	3.50	114.81	108.09
4	A	510	ANP	C4'-O4'-C1'	3.40	116.96	109.47
4	D	3510	ANP	O3A-PB-N3B	3.32	115.80	106.59
4	C	2510	ANP	N3-C2-N1	-3.29	123.60	128.58
4	A	510	ANP	N3-C2-N1	-3.21	123.72	128.58
4	A	510	ANP	O3A-PB-N3B	3.21	115.50	106.59
5	A	4520	ARG	CG-CD-NE	-3.20	103.21	112.20
4	D	3510	ANP	N3-C2-N1	-3.18	123.77	128.58
4	B	4510	ANP	O3A-PB-N3B	3.14	115.29	106.59
4	B	4510	ANP	N3-C2-N1	-3.10	123.89	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	510	ANP	O5'-C5'-C4'	-3.05	98.59	108.99
4	D	3510	ANP	O4'-C1'-C2'	-3.05	100.09	106.62
4	B	4510	ANP	O4'-C1'-C2'	-2.99	100.22	106.62
4	C	2510	ANP	O3A-PB-N3B	2.97	114.82	106.59
4	A	510	ANP	C6-C5-C4	2.92	121.17	117.18
4	D	3510	ANP	O4'-C4'-C3'	-2.90	99.41	105.15
4	C	2510	ANP	O4'-C1'-C2'	-2.89	100.42	106.62
4	D	3510	ANP	O5'-C5'-C4'	-2.84	99.31	108.99
4	A	510	ANP	O4'-C1'-C2'	-2.81	100.60	106.62
4	B	4510	ANP	O5'-C5'-C4'	-2.81	99.43	108.99
4	D	3510	ANP	C6-C5-C4	2.79	120.98	117.18
4	C	2510	ANP	C6-C5-C4	2.72	120.89	117.18
4	B	4510	ANP	C6-C5-C4	2.68	120.84	117.18
5	A	520	ARG	CG-CD-NE	-2.62	104.86	112.20
4	A	510	ANP	O4'-C4'-C3'	-2.55	100.10	105.15
4	C	2510	ANP	O4'-C4'-C3'	-2.51	100.17	105.15
4	C	2510	ANP	O5'-C5'-C4'	-2.50	100.49	108.99
5	A	2520	ARG	CG-CD-NE	-2.49	105.21	112.20
4	B	4510	ANP	O4'-C4'-C3'	-2.47	100.25	105.15
4	C	2510	ANP	C3'-C2'-C1'	2.46	106.11	101.46
5	A	3520	ARG	CG-CD-NE	-2.39	105.48	112.20
5	A	4520	ARG	NE-CZ-NH2	-2.33	116.68	120.67
4	B	4510	ANP	C3'-C2'-C1'	2.31	105.84	101.46
4	A	510	ANP	C3'-C2'-C1'	2.31	105.83	101.46
4	D	3510	ANP	C3'-C2'-C1'	2.29	105.80	101.46
5	A	2520	ARG	NE-CZ-NH2	-2.14	117.00	120.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	510	ANP	PB-N3B-PG-O1G
4	B	4510	ANP	PB-N3B-PG-O1G
4	C	2510	ANP	PB-N3B-PG-O1G
4	D	3510	ANP	PB-N3B-PG-O1G
4	A	510	ANP	PB-O3A-PA-O2A
4	B	4510	ANP	PB-O3A-PA-O2A
4	C	2510	ANP	PB-O3A-PA-O2A
4	D	3510	ANP	PB-O3A-PA-O2A
4	A	510	ANP	PB-O3A-PA-O1A
4	B	4510	ANP	PB-O3A-PA-O1A
4	C	2510	ANP	PB-O3A-PA-O1A

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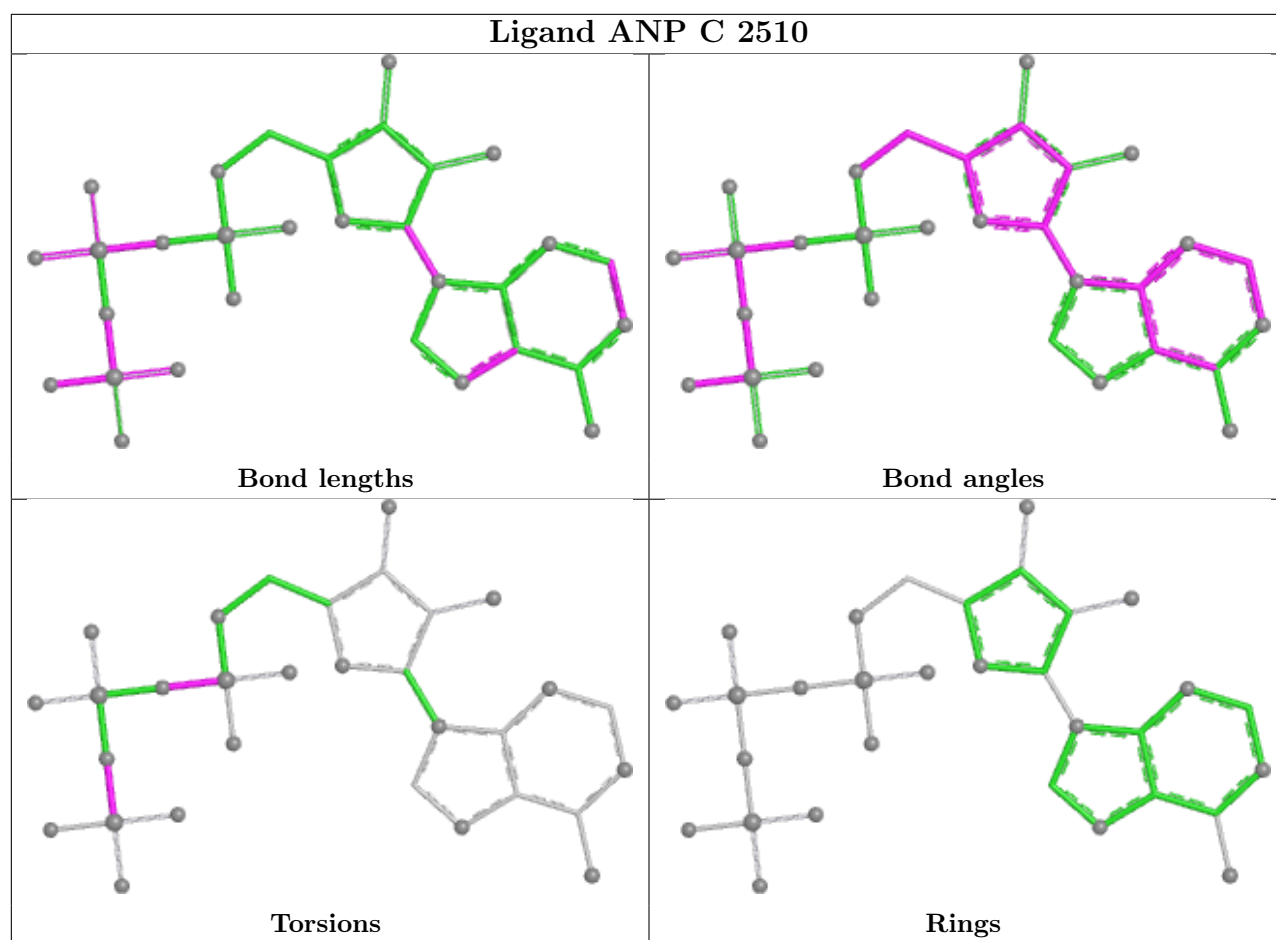
Mol	Chain	Res	Type	Atoms
4	D	3510	ANP	PB-O3A-PA-O1A

There are no ring outliers.

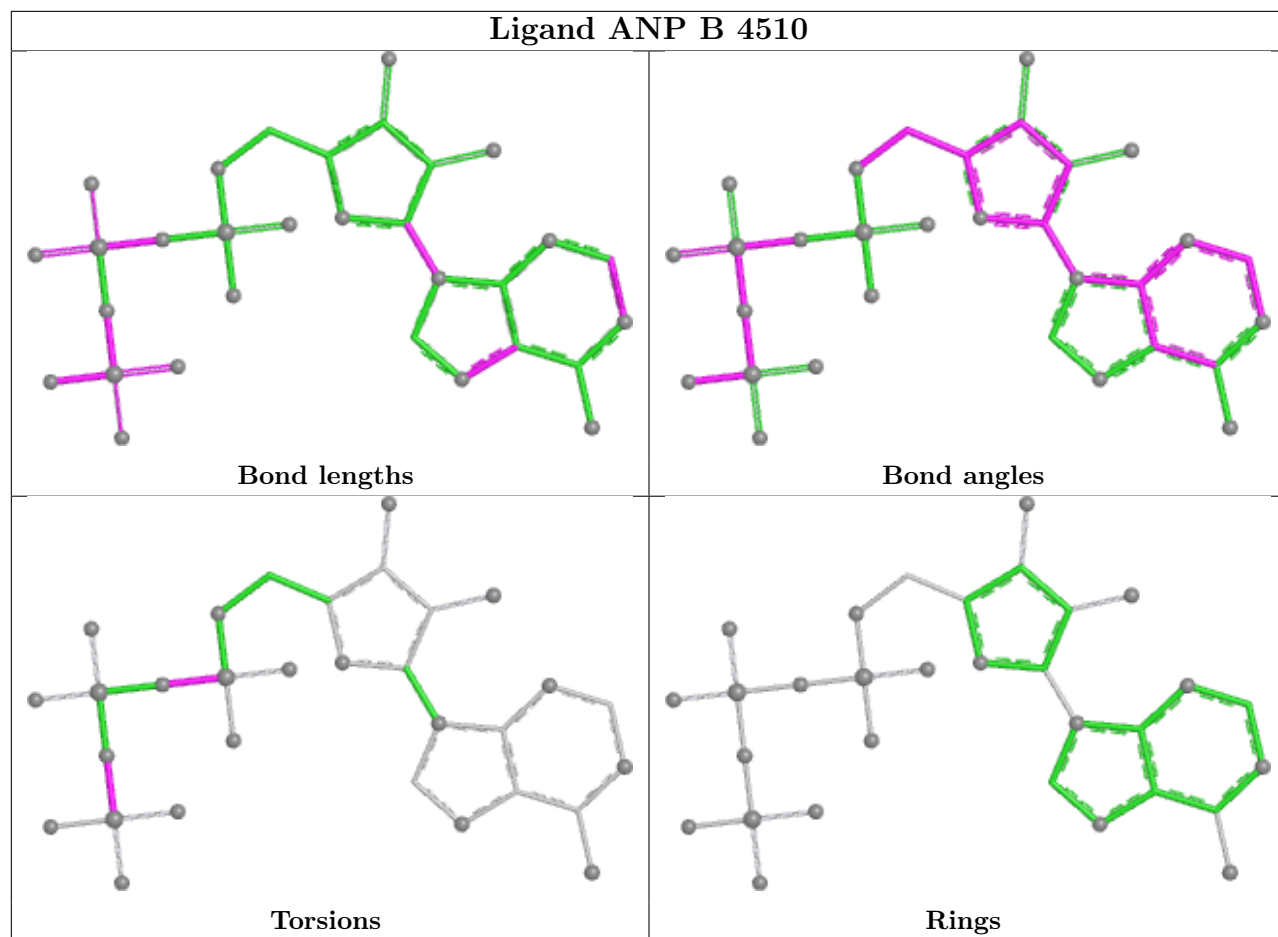
8 monomers are involved in 17 short contacts:

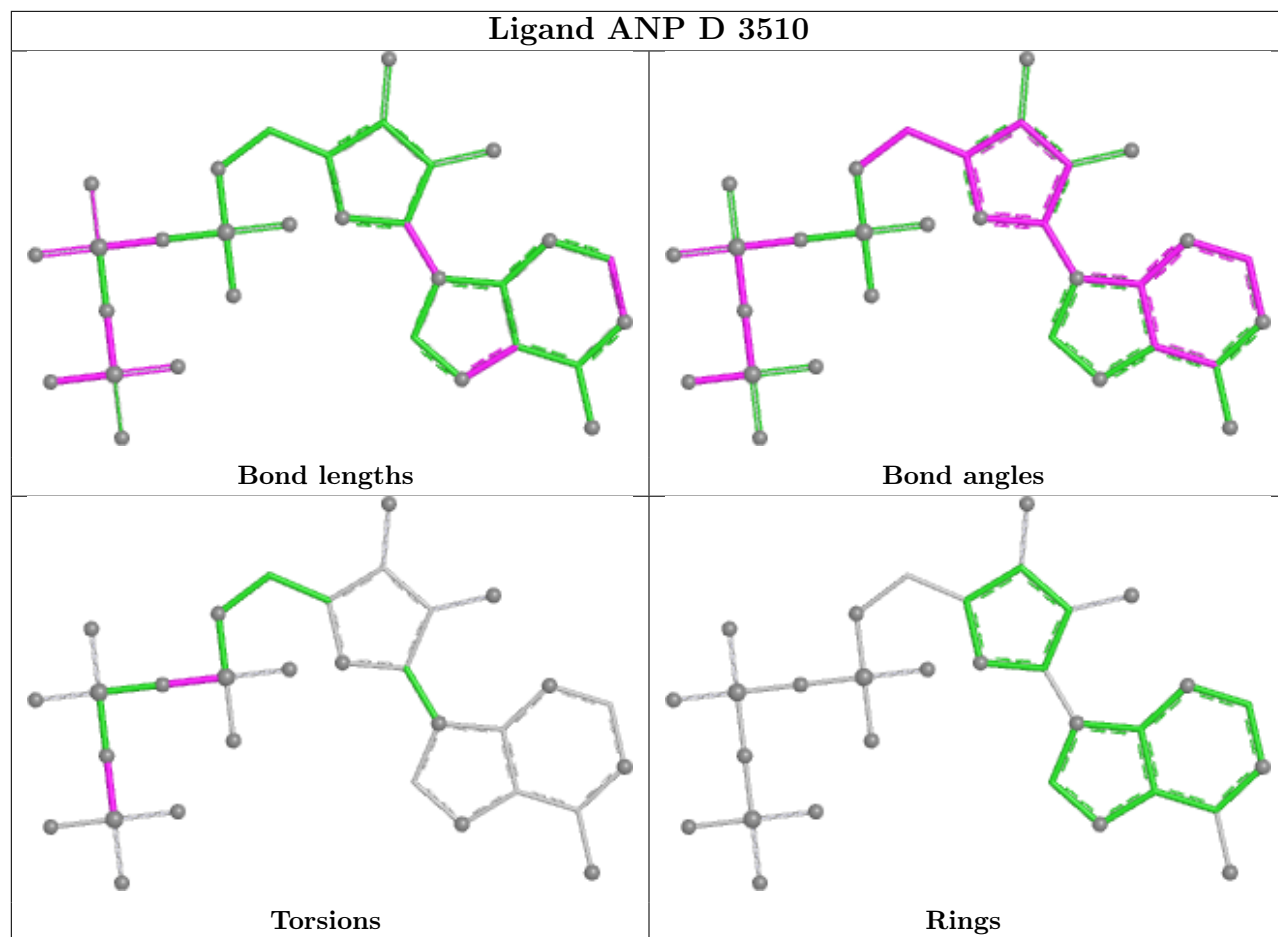
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	520	ARG	4	0
5	A	4520	ARG	3	0
5	A	3520	ARG	5	0
4	B	4510	ANP	1	0
4	D	3510	ANP	2	0
5	A	2520	ARG	3	0
6	A	3530	ASP	1	0
4	A	510	ANP	1	0

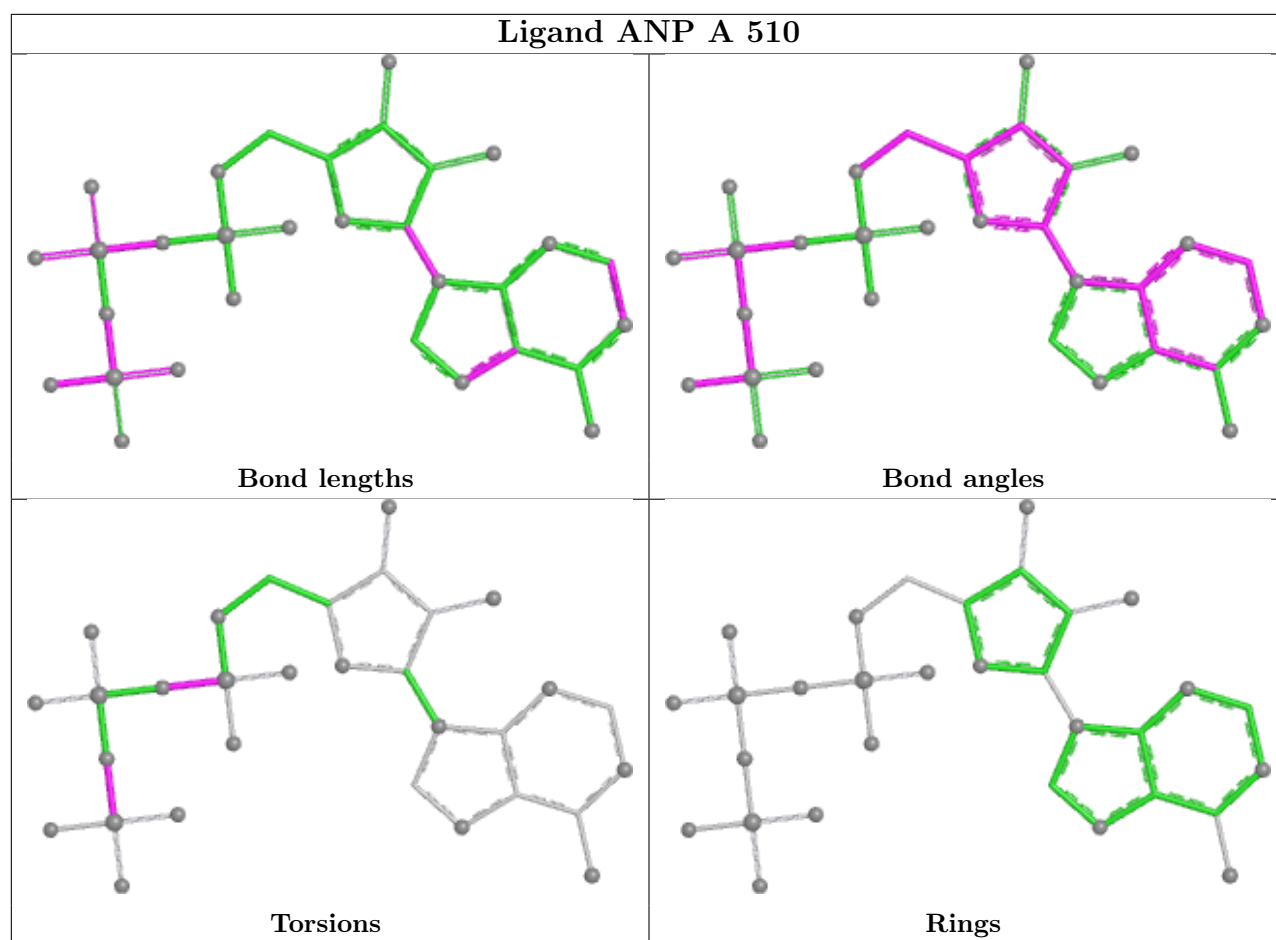
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand ANP B 4510







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	380/400 (95%)	-0.17	11 (2%) 53 57	20, 28, 52, 76	0
1	B	386/400 (96%)	-0.26	16 (4%) 41 46	19, 28, 49, 67	0
1	C	386/400 (96%)	0.16	20 (5%) 33 36	21, 33, 60, 84	0
1	D	386/400 (96%)	0.10	10 (2%) 57 61	22, 33, 55, 77	0
All	All	1538/1600 (96%)	-0.04	57 (3%) 45 49	19, 30, 55, 84	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	TYR	6.7
1	C	165	PRO	6.3
1	C	39	GLU	5.4
1	C	395	ARG	4.6
1	A	370	GLY	4.4
1	A	395	ARG	4.3
1	B	371	TYR	4.0
1	C	158	GLU	3.9
1	D	370	GLY	3.8
1	A	165	PRO	3.7
1	B	395	ARG	3.6
1	C	373	GLN	3.6
1	C	361	ASP	3.6
1	B	365	PHE	3.6
1	B	118	LYS	3.5
1	C	25	ARG	3.5
1	D	395	ARG	3.3
1	D	364	SER	3.3
1	A	359	ARG	3.2
1	D	365	PHE	3.2
1	C	159	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	394	GLU	3.0
1	D	159	ALA	3.0
1	B	151	LYS	3.0
1	B	165	PRO	2.9
1	B	373	GLN	2.9
1	C	137	LYS	2.9
1	D	205	ASP	2.9
1	B	361	ASP	2.8
1	B	364	SER	2.8
1	C	41	VAL	2.8
1	A	38	GLY	2.7
1	C	104	GLU	2.7
1	A	104	GLU	2.7
1	D	165	PRO	2.6
1	C	205	ASP	2.6
1	A	149	GLY	2.6
1	D	374	LYS	2.4
1	C	372	ASP	2.4
1	B	104	GLU	2.3
1	C	331	ARG	2.3
1	B	331	ARG	2.3
1	C	374	LYS	2.3
1	A	197	LYS	2.3
1	B	359	ARG	2.2
1	D	43	GLU	2.2
1	C	157	ALA	2.1
1	D	157	ALA	2.1
1	C	38	GLY	2.1
1	C	49	LEU	2.1
1	B	372	ASP	2.1
1	B	362	LEU	2.0
1	A	205	ASP	2.0
1	C	371	TYR	2.0
1	A	159	ALA	2.0
1	B	360	GLN	2.0
1	B	370	GLY	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

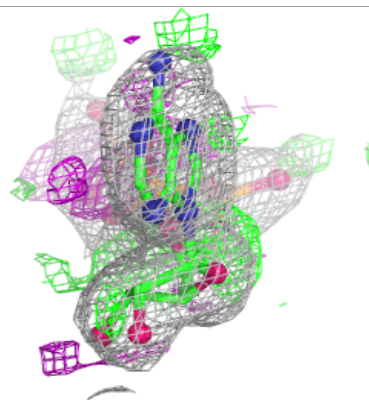
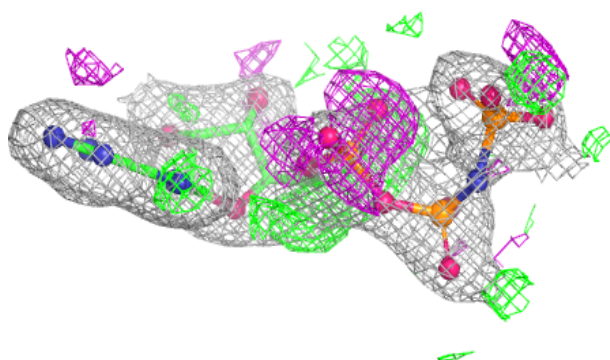
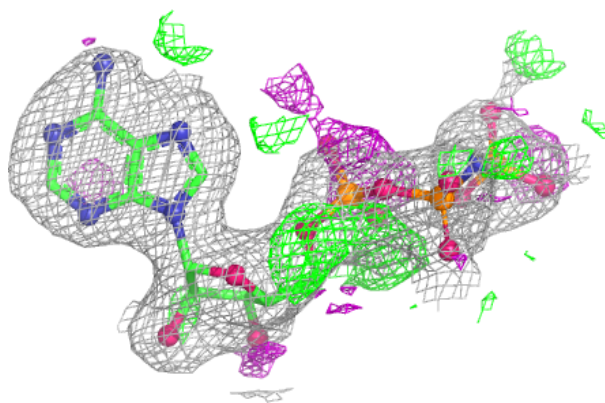
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	2540	5/5	0.63	0.38	75,81,85,86	5
3	MG	C	2550	1/1	0.68	0.13	43,43,43,43	0
2	SO4	D	3540	5/5	0.72	0.24	61,74,78,81	0
3	MG	A	550	1/1	0.74	0.14	42,42,42,42	0
2	SO4	A	540	5/5	0.82	0.21	48,61,63,64	5
5	ARG	A	2520	12/12	0.84	0.19	24,38,55,56	0
5	ARG	A	520	12/12	0.85	0.16	19,28,49,52	0
3	MG	D	3550	1/1	0.86	0.07	55,55,55,55	0
5	ARG	A	3520	12/12	0.86	0.17	28,33,53,58	0
5	ARG	A	4520	12/12	0.87	0.15	20,29,45,49	0
4	ANP	C	2510	31/31	0.90	0.10	25,35,47,55	0
4	ANP	D	3510	31/31	0.90	0.11	33,41,60,62	0
3	MG	B	4550	1/1	0.91	0.14	38,38,38,38	0
2	SO4	B	4540	5/5	0.92	0.13	32,51,58,60	0
4	ANP	A	510	31/31	0.92	0.09	25,32,41,44	0
6	ASP	A	2530	9/9	0.93	0.09	20,25,30,30	0
6	ASP	A	3530	9/9	0.93	0.08	26,28,32,34	0
4	ANP	B	4510	31/31	0.94	0.08	20,31,40,41	0
6	ASP	A	530	9/9	0.94	0.07	24,29,30,38	0
6	ASP	A	4530	9/9	0.95	0.06	25,27,29,29	0

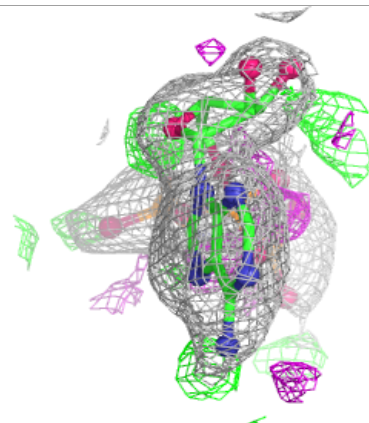
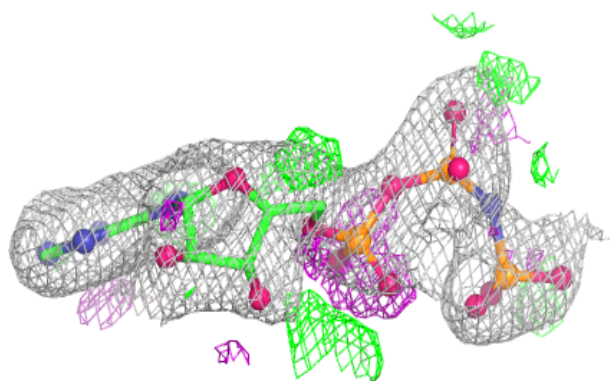
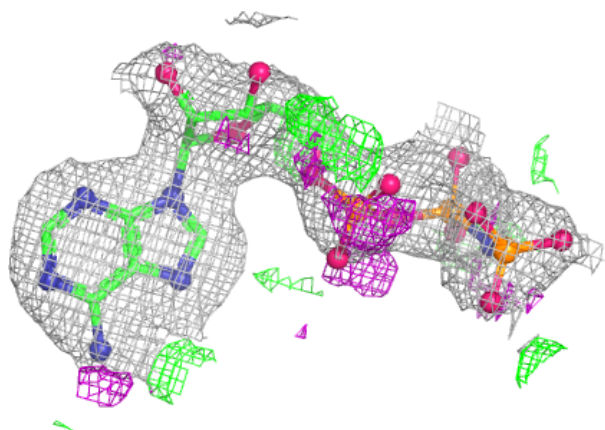
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP C 2510:

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

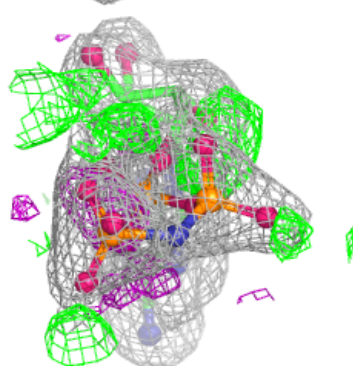
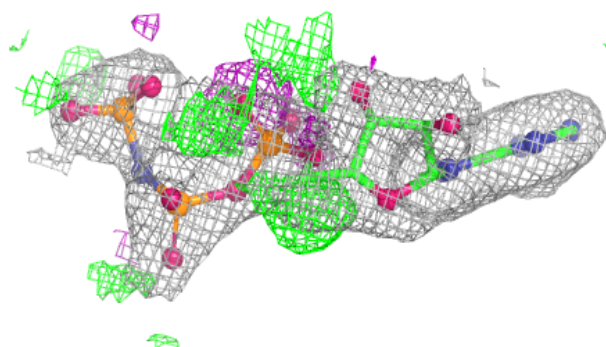
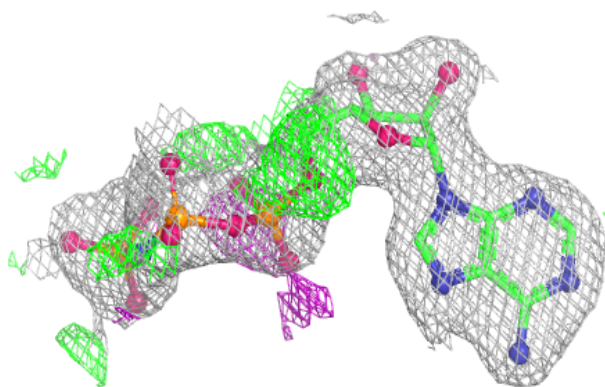
**Electron density around ANP D 3510:**

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

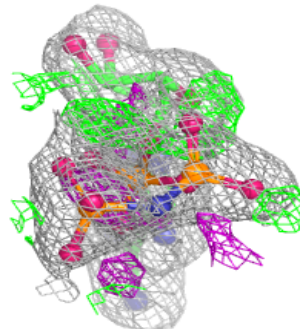
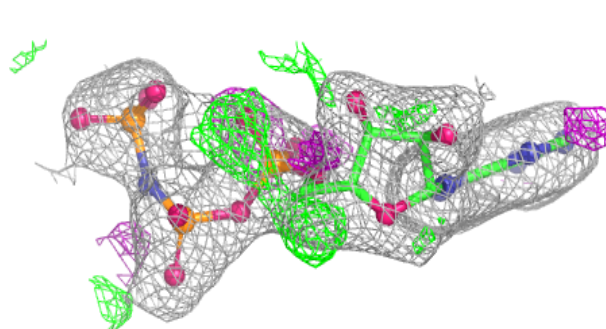
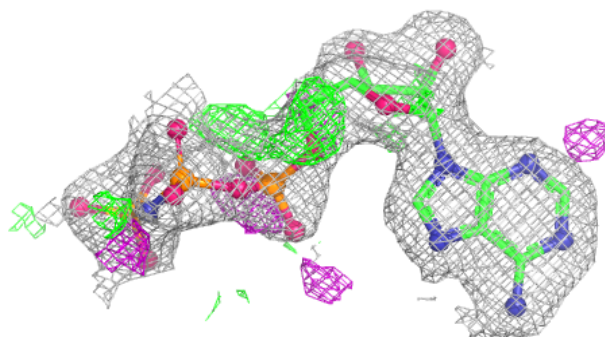


Electron density around ANP A 510:

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

**Electron density around ANP B 4510:**

$2mF_o-DF_c$ (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.