



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:49 AM UTC

PDB ID : 1KOR / pdb_00001kor
Title : Crystal Structure of Thermus thermophilus HB8 Argininosuccinate Synthetase in complex with inhibitors
Authors : Goto, M.; Nakajima, Y.; Hirotsu, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2001-12-22
Resolution : 1.95 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

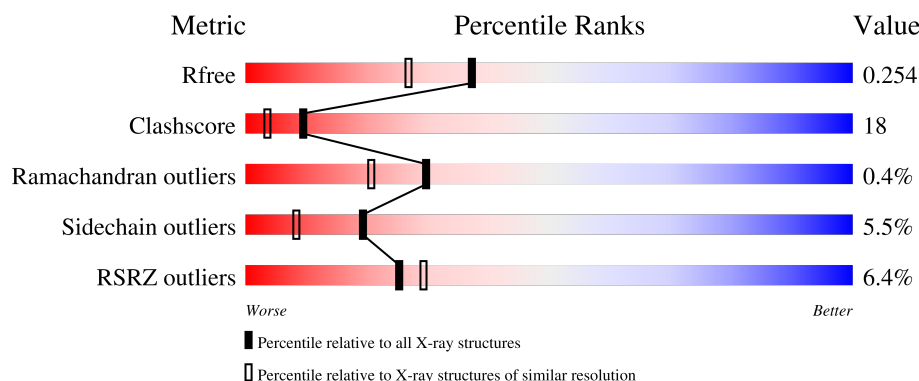
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	4% 68% 23% 5%
1	B	400	4% 70% 24%
1	C	400	11% 64% 28%
1	D	400	6% 62% 31%

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	SIN	A	530	-	X	-	-
4	SIN	C	2530	-	X	-	-
4	SIN	D	3530	-	X	-	-

2 Entry composition [i](#)

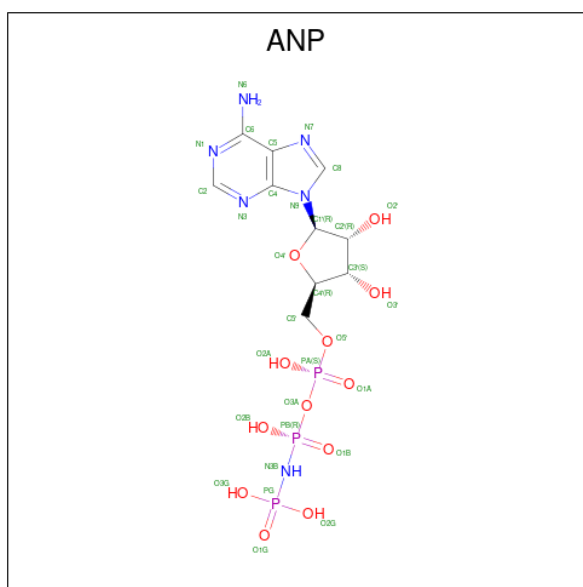
There are 5 unique types of molecules in this entry. The entry contains 13218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



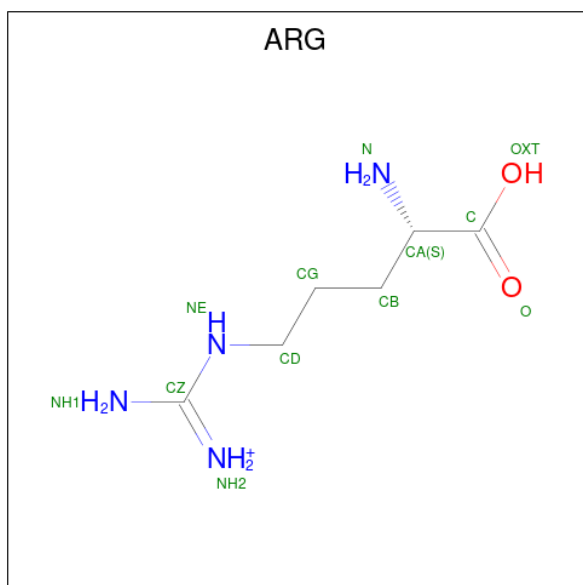
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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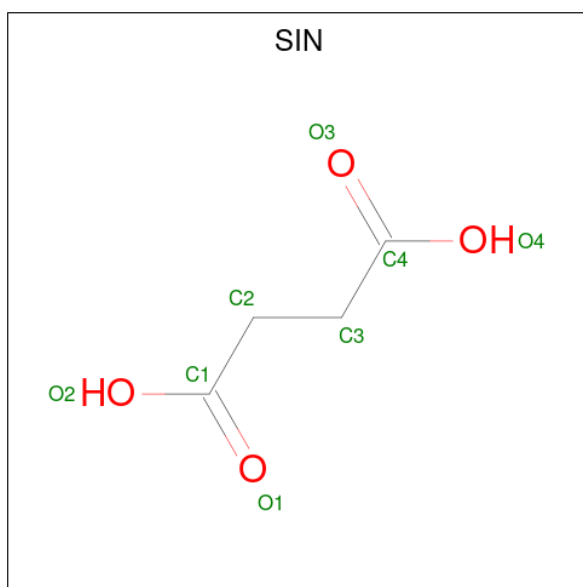
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		
4	B	1	Total	C	O	0	0
			8	4	4		
4	C	1	Total	C	O	0	0
			8	4	4		
4	D	1	Total	C	O	0	0
			8	4	4		

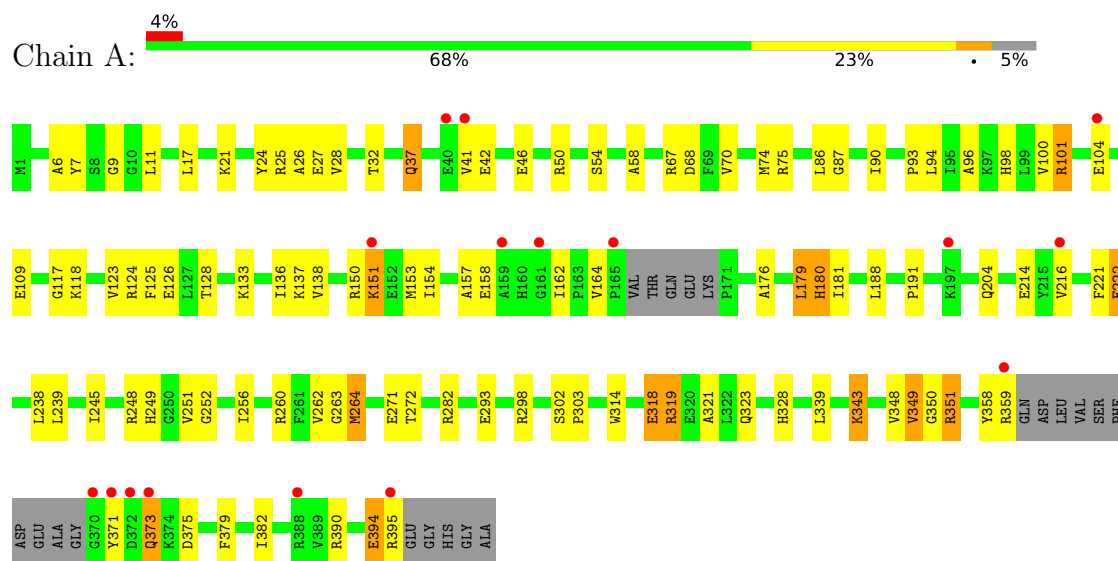
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	211	Total	O	0	0
			211	211		
5	B	230	Total	O	0	0
			230	230		
5	C	176	Total	O	0	0
			176	176		
5	D	182	Total	O	0	0
			182	182		

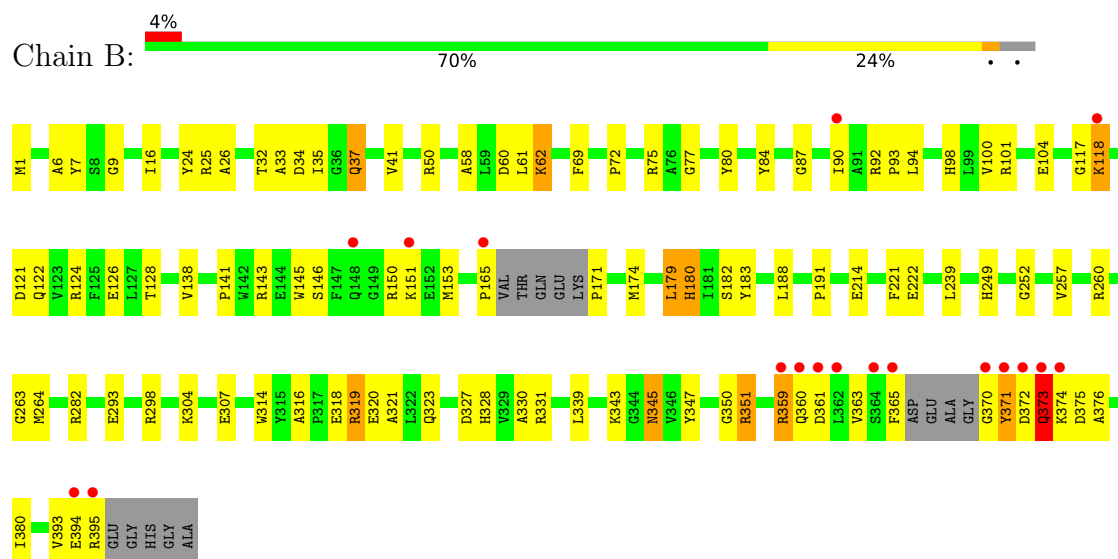
3 Residue-property plots [i](#)

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

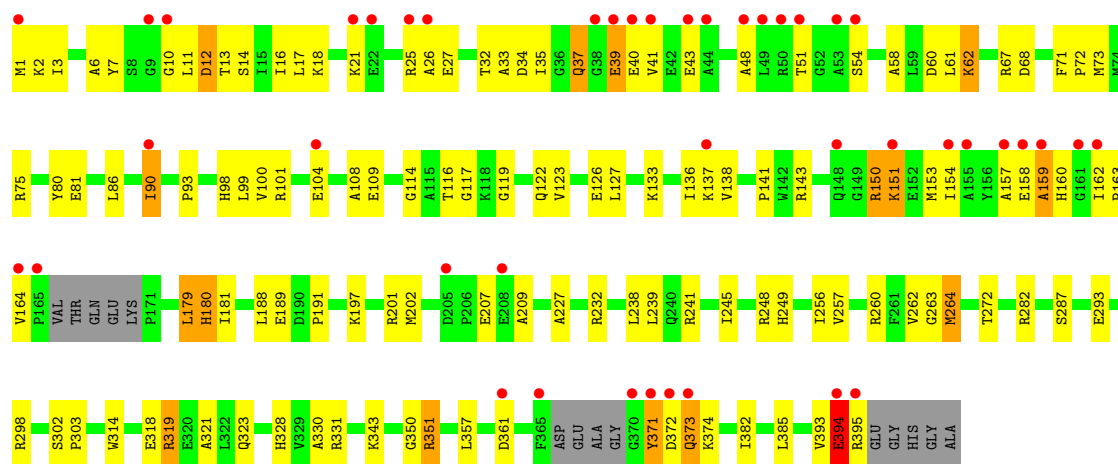
• Molecule 1: Argininosuccinate Synthetase



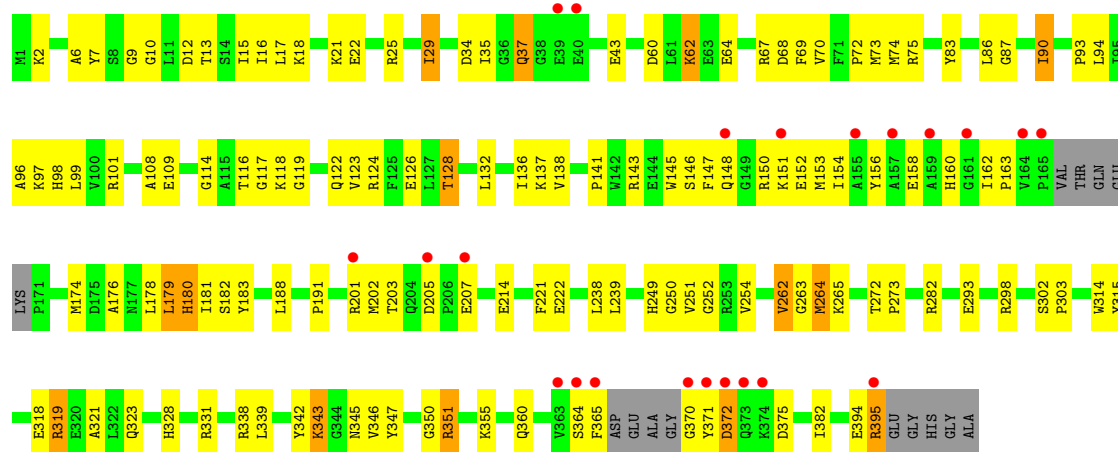
• Molecule 1: Argininosuccinate Synthetase



• 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	229.43Å 229.43Å 160.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.95 10.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.95) 97.9 (10.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.250 0.233 , 0.254	Depositor DCC
R_{free} test set	22549 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.002 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13218	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 2.72% 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: SIN, ANP

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	0.43	0/3085	0.98	10/4169 (0.2%)
1	B	0.42	0/3135	0.96	10/4237 (0.2%)
1	C	0.42	0/3135	0.94	9/4237 (0.2%)
1	D	0.43	0/3135	0.98	8/4237 (0.2%)
All	All	0.43	0/12490	0.96	37/16880 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	PHE	CB-CA-C	-20.66	81.89	111.23
1	A	221	PHE	CB-CA-C	-20.33	82.37	111.23
1	B	222	GLU	N-CA-C	13.41	129.41	112.24
1	B	221	PHE	CB-CA-C	-12.25	90.54	110.14
1	A	263	GLY	N-CA-C	11.24	126.94	113.79
1	C	263	GLY	N-CA-C	9.66	125.09	113.79
1	D	263	GLY	N-CA-C	8.75	122.94	113.58
1	B	221	PHE	N-CA-C	-8.54	94.34	108.34
1	D	222	GLU	N-CA-CB	7.54	126.30	113.10
1	D	145	TRP	N-CA-C	7.30	119.95	110.53
1	D	119	GLY	N-CA-C	7.26	122.83	112.81
1	A	394	GLU	N-CA-C	-7.11	103.86	112.54
1	C	371	TYR	N-CA-C	7.06	119.92	108.41
1	C	86	LEU	N-CA-C	6.63	120.73	112.24
1	A	86	LEU	N-CA-C	6.51	120.57	112.24
1	A	222	GLU	N-CA-CB	6.46	124.41	113.10
1	D	86	LEU	N-CA-C	6.41	120.45	112.24
1	C	394	GLU	N-CA-C	-6.33	105.65	113.19
1	B	263	GLY	N-CA-C	6.33	123.50	114.64
1	C	12	ASP	N-CA-C	6.17	118.01	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	VAL	N-CA-C	-6.11	101.66	109.30
1	D	43	GLU	N-CA-C	-5.87	104.80	111.14
1	C	119	GLY	N-CA-C	5.83	120.86	112.81
1	C	14	SER	N-CA-C	-5.73	105.12	111.36
1	B	252	GLY	N-CA-C	5.64	123.67	115.32
1	B	145	TRP	N-CA-C	5.55	117.24	110.41
1	A	28	VAL	N-CA-C	5.38	115.59	107.80
1	B	345	ASN	N-CA-C	5.31	118.37	110.14
1	A	164	VAL	N-CA-C	5.23	113.69	107.73
1	A	256	ILE	N-CA-C	5.18	117.50	108.90
1	C	256	ILE	N-CA-C	5.17	117.48	108.90
1	A	222	GLU	N-CA-C	5.08	120.87	113.40
1	D	12	ASP	N-CA-C	5.07	116.89	111.36
1	B	394	GLU	N-CA-C	-5.05	106.38	112.54
1	C	257	VAL	N-CA-C	-5.03	99.93	107.37
1	B	6	ALA	N-CA-C	-5.02	99.59	108.23
1	B	257	VAL	N-CA-C	-5.01	99.96	107.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	3006	112	0
1	B	3066	0	3052	108	0
1	C	3066	0	3052	144	0
1	D	3066	0	3052	126	0
2	A	31	0	13	2	0
2	B	31	0	13	2	0
2	C	31	0	13	5	0
2	D	31	0	13	6	0
3	A	12	0	12	1	0
3	B	12	0	12	3	0
3	C	12	0	12	0	0
3	D	12	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	4	0	0
4	B	8	0	4	0	0
4	C	8	0	4	1	0
4	D	8	0	4	1	0
5	A	211	0	0	14	0
5	B	230	0	0	11	0
5	C	176	0	0	7	0
5	D	182	0	0	6	0
All	All	13218	0	12278	443	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 18.

All (443) 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:264:MET:HE3	1:A:264:MET:H	1.05	1.16
1:D:151:LYS:H	1:D:151:LYS:HD2	1.06	1.14
1:A:151:LYS:H	1:A:151:LYS:HD2	1.12	1.11
1:B:151:LYS:H	1:B:151:LYS:HD2	1.18	1.07
1:A:123:VAL:HG22	1:B:380:ILE:HD11	1.38	1.05
1:C:151:LYS:H	1:C:151:LYS:HD2	1.17	1.03
1:A:262:VAL:HG23	1:A:264:MET:CE	1.94	0.97
1:D:35:ILE:H	1:D:37:GLN:NE2	1.63	0.97
1:A:264:MET:H	1:A:264:MET:CE	1.85	0.89
1:A:124:ARG:O	1:A:128:THR:HG22	1.71	0.89
1:B:35:ILE:H	1:B:37:GLN:NE2	1.72	0.89
1:A:151:LYS:H	1:A:151:LYS:CD	1.87	0.88
1:D:124:ARG:O	1:D:128:THR:HG23	1.74	0.87
1:A:262:VAL:HG23	1:A:264:MET:HE1	1.57	0.86
1:A:264:MET:HE3	1:A:264:MET:N	1.88	0.86
1:A:151:LYS:HD2	1:A:151:LYS:N	1.89	0.86
1:C:109:GLU:HG2	1:C:137:LYS:HE3	1.58	0.86
1:C:35:ILE:H	1:C:37:GLN:NE2	1.72	0.86
1:C:151:LYS:HD2	1:C:151:LYS:N	1.91	0.85
1:B:41:VAL:HG12	1:B:58:ALA:HB1	1.58	0.85
1:D:351:ARG:HD2	1:D:351:ARG:N	1.91	0.85
1:A:104:GLU:HG2	1:A:133:LYS:HZ2	1.42	0.85
1:A:319:ARG:HH21	1:A:323:GLN:HE21	1.22	0.84
1:A:373:GLN:H	1:A:373:GLN:NE2	1.74	0.84
1:B:351:ARG:HD2	1:B:351:ARG:N	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLU:O	1:C:137:LYS:HE2	1.79	0.82
1:D:83:TYR:HB3	1:D:254:VAL:HG21	1.60	0.82
1:B:370:GLY:O	1:B:371:TYR:HB3	1.80	0.81
1:B:118:LYS:H	1:B:118:LYS:HD2	1.46	0.81
1:A:262:VAL:HG23	1:A:264:MET:HE2	1.61	0.81
1:B:314:TRP:O	1:B:319:ARG:HD3	1.80	0.80
1:D:151:LYS:HD2	1:D:151:LYS:N	1.92	0.78
1:A:351:ARG:HD2	1:A:351:ARG:N	1.99	0.78
1:A:293:GLU:HB2	1:C:318:GLU:CG	2.14	0.77
1:C:351:ARG:HD2	1:C:351:ARG:N	1.99	0.77
1:C:21:LYS:O	1:C:25:ARG:HA	1.86	0.76
1:D:118:LYS:O	1:D:264:MET:HE1	1.86	0.75
1:C:37:GLN:NE2	1:C:37:GLN:H	1.85	0.75
1:B:150:ARG:HA	1:B:153:MET:HE3	1.68	0.75
1:D:151:LYS:H	1:D:151:LYS:CD	1.85	0.75
1:C:40:GLU:HG2	1:C:43:GLU:HG3	1.68	0.74
1:B:293:GLU:HB3	1:D:318:GLU:HG2	1.67	0.73
1:A:318:GLU:HG2	1:C:293:GLU:CB	2.18	0.73
1:D:35:ILE:H	1:D:37:GLN:HE22	1.36	0.73
1:C:37:GLN:HB2	1:C:39:GLU:HG2	1.69	0.73
1:A:109:GLU:O	1:A:137:LYS:HE2	1.88	0.72
1:C:37:GLN:H	1:C:37:GLN:HE21	1.37	0.72
1:B:319:ARG:HH21	1:B:323:GLN:HE21	1.36	0.72
1:A:318:GLU:CG	1:C:293:GLU:HB2	2.20	0.71
1:B:293:GLU:CB	1:D:318:GLU:HG2	2.20	0.71
1:A:126:GLU:HG2	1:A:138:VAL:HG11	1.72	0.71
1:C:151:LYS:H	1:C:151:LYS:CD	1.89	0.71
1:B:100:VAL:O	1:B:104:GLU:HG3	1.90	0.71
1:A:118:LYS:HD3	1:B:365:PHE:CE2	2.25	0.71
1:A:100:VAL:O	1:A:104:GLU:HG3	1.91	0.70
1:B:37:GLN:NE2	1:B:37:GLN:H	1.90	0.70
1:A:21:LYS:HD2	1:A:26:ALA:O	1.92	0.69
1:A:75:ARG:NH2	5:A:4292:HOH:O	2.25	0.69
1:D:109:GLU:O	1:D:137:LYS:HE2	1.92	0.69
1:D:360:GLN:HG2	1:D:364:SER:OG	1.93	0.69
5:A:4591:HOH:O	1:B:345:ASN:HB2	1.93	0.69
1:D:395:ARG:HG3	1:D:395:ARG:HH11	1.57	0.69
1:B:318:GLU:CG	1:D:293:GLU:HB2	2.23	0.69
1:B:128:THR:HG22	5:B:4136:HOH:O	1.92	0.69
1:B:151:LYS:HD2	1:B:151:LYS:N	2.00	0.69
1:C:227:ALA:HB2	1:C:232:ARG:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:HD2	1:B:118:LYS:N	2.06	0.69
1:A:293:GLU:CB	1:C:318:GLU:HG2	2.22	0.68
1:C:314:TRP:O	1:C:319:ARG:HD3	1.92	0.68
1:A:104:GLU:HG2	1:A:133:LYS:NZ	2.09	0.68
1:C:18:LYS:HG3	1:C:162:ILE:HD11	1.75	0.68
1:C:27:GLU:HG3	1:C:54:SER:OG	1.93	0.68
1:D:126:GLU:HG2	1:D:138:VAL:HG11	1.75	0.68
1:B:318:GLU:HG3	1:D:293:GLU:HB2	1.76	0.67
1:C:18:LYS:NZ	1:C:160:HIS:HB3	2.11	0.66
1:B:87:GLY:HA2	1:B:179:LEU:HD13	1.77	0.66
1:B:293:GLU:HB2	1:D:318:GLU:CG	2.26	0.66
1:D:37:GLN:NE2	1:D:37:GLN:H	1.94	0.66
1:A:67:ARG:NH1	1:A:68:ASP:OD1	2.29	0.66
1:D:29:ILE:HD12	1:D:29:ILE:N	2.11	0.66
1:A:318:GLU:HG2	1:C:293:GLU:HB2	1.78	0.66
1:C:122:GLN:NE2	1:C:143:ARG:HH11	1.93	0.65
1:C:319:ARG:HH21	1:C:323:GLN:HE21	1.43	0.65
1:B:151:LYS:H	1:B:151:LYS:CD	1.94	0.65
1:B:93:PRO:HA	1:B:128:THR:HG21	1.78	0.65
1:D:214:GLU:OE1	1:D:249:HIS:HE1	1.80	0.65
1:B:93:PRO:HG3	5:B:4180:HOH:O	1.97	0.65
1:A:318:GLU:HG2	1:C:293:GLU:HB3	1.79	0.64
1:A:373:GLN:H	1:A:373:GLN:HE21	1.44	0.64
1:A:150:ARG:HD2	1:A:153:MET:HE3	1.80	0.64
1:C:245:ILE:O	1:C:248:ARG:HG2	1.98	0.64
1:C:122:GLN:HE21	1:C:143:ARG:HH11	1.45	0.64
1:A:349:VAL:HG13	5:A:4240:HOH:O	1.96	0.64
1:C:373:GLN:H	1:C:373:GLN:NE2	1.96	0.64
1:A:293:GLU:HB2	1:C:318:GLU:HG3	1.79	0.64
1:A:104:GLU:OE2	1:A:133:LYS:NZ	2.28	0.64
1:C:33:ALA:HB1	1:C:61:LEU:HD12	1.80	0.64
1:C:262:VAL:O	1:C:262:VAL:HG12	1.96	0.64
1:B:318:GLU:HG2	1:D:293:GLU:HB3	1.81	0.63
1:B:75:ARG:HD2	1:B:327:ASP:OD2	1.99	0.63
1:B:371:TYR:HB2	1:B:375:ASP:OD1	1.98	0.63
1:B:41:VAL:CG1	1:B:58:ALA:HB1	2.26	0.63
5:C:4616:HOH:O	1:D:191:PRO:HG2	1.99	0.62
1:A:282:ARG:HD2	5:A:4356:HOH:O	1.99	0.62
1:A:262:VAL:CG2	1:A:264:MET:HE1	2.30	0.61
1:B:37:GLN:H	1:B:37:GLN:HE21	1.47	0.61
1:D:314:TRP:O	1:D:319:ARG:HD3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:4477:HOH:O	1:B:191:PRO:HG2	1.99	0.61
1:A:214:GLU:OE1	1:A:249:HIS:HE1	1.84	0.61
1:B:371:TYR:HD1	1:B:375:ASP:HB2	1.65	0.61
1:C:1:MET:HE2	1:C:3:ILE:CG1	2.30	0.61
1:D:83:TYR:CB	1:D:254:VAL:HG21	2.31	0.61
1:B:314:TRP:CE3	1:B:319:ARG:HD2	2.36	0.60
1:A:293:GLU:HB3	1:C:318:GLU:HG2	1.83	0.60
1:C:133:LYS:HD3	1:C:136:ILE:HD13	1.83	0.60
1:D:93:PRO:HG3	5:D:4130:HOH:O	2.00	0.60
1:B:318:GLU:HG2	1:D:293:GLU:CB	2.31	0.60
1:B:35:ILE:N	1:B:37:GLN:NE2	2.48	0.60
1:C:2:LYS:HB2	1:C:108:ALA:HA	1.84	0.60
1:A:371:TYR:HD1	1:A:375:ASP:HB2	1.67	0.60
1:C:343:LYS:HD2	1:D:343:LYS:HD2	1.84	0.60
1:A:245:ILE:O	1:A:248:ARG:HG2	2.02	0.59
1:D:150:ARG:O	1:D:154:ILE:HD13	2.01	0.59
1:C:343:LYS:CD	1:D:343:LYS:HD2	2.32	0.59
1:D:128:THR:HG22	5:D:4380:HOH:O	2.01	0.59
1:B:393:VAL:O	1:B:395:ARG:NH1	2.35	0.59
1:C:262:VAL:HG11	1:D:371:TYR:OH	2.01	0.59
1:A:133:LYS:HG2	1:A:136:ILE:HB	1.85	0.59
1:A:371:TYR:HB2	1:A:375:ASP:OD1	2.01	0.59
1:C:75:ARG:NH2	5:C:4731:HOH:O	2.35	0.59
1:C:150:ARG:O	1:C:154:ILE:HG13	2.01	0.59
1:D:35:ILE:N	1:D:37:GLN:NE2	2.46	0.59
1:D:37:GLN:H	1:D:37:GLN:HE21	1.51	0.59
1:C:302:SER:HB2	1:C:303:PRO:HD3	1.84	0.58
1:D:174:MET:HE1	1:D:201:ARG:CD	2.33	0.58
1:B:117:GLY:HA2	1:B:122:GLN:NE2	2.18	0.58
1:D:137:LYS:HD3	1:D:137:LYS:N	2.18	0.58
1:B:34:ASP:HA	1:B:37:GLN:HE22	1.69	0.58
1:C:262:VAL:HB	1:C:264:MET:HE1	1.84	0.58
1:C:264:MET:HE3	1:C:264:MET:H	1.69	0.58
1:C:35:ILE:N	1:C:37:GLN:NE2	2.48	0.58
1:D:75:ARG:NH2	5:D:4498:HOH:O	2.35	0.58
1:D:395:ARG:HG3	1:D:395:ARG:NH1	2.18	0.57
1:A:87:GLY:HA2	1:A:179:LEU:HD13	1.85	0.57
1:B:350:GLY:C	1:B:351:ARG:HD2	2.29	0.57
1:B:372:ASP:OD1	1:B:374:LYS:HB3	2.03	0.57
1:A:32:THR:CG2	1:A:41:VAL:HG13	2.34	0.57
1:A:390:ARG:O	1:A:394:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:HH21	1:A:323:GLN:NE2	1.96	0.57
1:B:318:GLU:CG	1:D:293:GLU:CB	2.83	0.57
1:D:67:ARG:HD2	1:D:68:ASP:OD1	2.04	0.57
2:B:1510:ANP:PA	3:B:1520:ARG:HH22	2.27	0.57
1:B:117:GLY:HA2	1:B:122:GLN:HE22	1.69	0.57
1:D:205:ASP:OD1	1:D:207:GLU:OE2	2.23	0.57
1:B:293:GLU:CB	1:D:318:GLU:CG	2.82	0.57
1:C:41:VAL:HG12	1:C:58:ALA:HB1	1.86	0.56
1:B:214:GLU:OE1	1:B:249:HIS:HE1	1.87	0.56
1:D:60:ASP:OD1	1:D:62:LYS:HD3	2.05	0.56
1:A:27:GLU:HG3	1:A:54:SER:OG	2.06	0.56
1:A:21:LYS:HD3	5:A:4491:HOH:O	2.06	0.56
1:C:393:VAL:C	1:C:395:ARG:H	2.12	0.56
1:C:34:ASP:HA	1:C:37:GLN:HE22	1.71	0.56
1:B:359:ARG:HD2	1:B:361:ASP:CG	2.30	0.56
1:B:1:MET:O	1:B:26:ALA:HB1	2.06	0.56
1:B:34:ASP:HB2	1:B:41:VAL:HG21	1.88	0.56
1:C:207:GLU:HA	1:D:342:TYR:OH	2.06	0.56
1:A:382:ILE:HD12	1:C:262:VAL:CG1	2.36	0.55
1:B:360:GLN:HA	1:B:363:VAL:HG22	1.86	0.55
1:C:282:ARG:HD2	5:C:4375:HOH:O	2.06	0.55
1:A:216:VAL:HG21	1:A:245:ILE:HG21	1.88	0.55
1:C:16:ILE:HG23	1:C:141:PRO:HG2	1.87	0.55
1:A:314:TRP:O	1:A:319:ARG:HD3	2.06	0.55
1:B:180:HIS:ND1	1:B:180:HIS:C	2.64	0.55
1:A:93:PRO:HG3	5:A:4177:HOH:O	2.07	0.55
1:C:13:THR:OG1	2:C:2510:ANP:O1G	2.19	0.55
1:C:181:ILE:HG13	1:C:202:MET:HE3	1.87	0.55
1:A:96:ALA:HB3	1:A:128:THR:HG21	1.89	0.55
1:C:40:GLU:CG	1:C:43:GLU:HG3	2.37	0.54
1:D:6:ALA:HB2	1:D:99:LEU:HD11	1.89	0.54
1:D:302:SER:HB2	1:D:303:PRO:HD3	1.88	0.54
1:D:282:ARG:NH1	1:D:282:ARG:HB2	2.23	0.54
1:C:18:LYS:CE	1:C:160:HIS:HB3	2.38	0.54
1:A:157:ALA:HB1	1:A:162:ILE:HB	1.89	0.54
1:C:232:ARG:HG3	1:C:232:ARG:HH11	1.73	0.54
1:B:171:PRO:HG2	5:B:4746:HOH:O	2.06	0.54
1:B:371:TYR:CE1	1:C:382:ILE:HD11	2.43	0.54
1:B:373:GLN:HG2	5:B:4742:HOH:O	2.07	0.54
1:D:338:ARG:HD3	5:D:4424:HOH:O	2.08	0.54
1:B:118:LYS:N	1:B:118:LYS:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:NH2	5:C:4716:HOH:O	2.41	0.54
1:C:51:THR:HG22	1:C:51:THR:O	2.08	0.54
1:D:6:ALA:HB3	2:D:3510:ANP:O2'	2.07	0.54
1:B:126:GLU:HG2	1:B:138:VAL:HG11	1.89	0.53
1:C:32:THR:CG2	1:C:41:VAL:HG13	2.38	0.53
1:A:216:VAL:HG22	5:A:4140:HOH:O	2.08	0.53
1:C:162:ILE:O	1:C:163:PRO:C	2.51	0.53
1:A:302:SER:HB2	1:A:303:PRO:HD3	1.90	0.53
1:D:35:ILE:N	1:D:37:GLN:HE22	2.04	0.53
1:D:394:GLU:O	1:D:395:ARG:O	2.26	0.53
1:C:394:GLU:HA	1:C:394:GLU:OE1	2.08	0.52
1:D:319:ARG:HH21	1:D:323:GLN:HE21	1.55	0.52
1:A:125:PHE:O	1:A:128:THR:HG23	2.08	0.52
1:A:180:HIS:C	1:A:180:HIS:ND1	2.66	0.52
1:C:21:LYS:HD2	1:C:26:ALA:O	2.09	0.52
1:A:41:VAL:HG12	1:A:58:ALA:HB1	1.90	0.52
1:C:179:LEU:O	1:C:272:THR:HG23	2.09	0.52
1:D:176:ALA:CB	1:D:181:ILE:HG12	2.38	0.52
1:D:181:ILE:HG13	1:D:202:MET:HE3	1.92	0.52
1:D:174:MET:HA	1:D:182:SER:O	2.09	0.52
1:D:179:LEU:O	1:D:272:THR:HG23	2.10	0.52
1:C:1:MET:HE2	1:C:3:ILE:HG12	1.92	0.51
1:A:382:ILE:HD12	1:C:262:VAL:HG13	1.93	0.51
1:C:262:VAL:HB	1:C:264:MET:CE	2.41	0.51
1:B:328:HIS:CE1	1:B:331:ARG:HH22	2.28	0.51
1:D:117:GLY:HA2	1:D:122:GLN:NE2	2.26	0.51
1:A:154:ILE:O	1:A:158:GLU:HG3	2.11	0.51
1:B:293:GLU:HB2	1:D:318:GLU:HG3	1.90	0.51
1:B:101:ARG:HD3	5:B:4401:HOH:O	2.11	0.51
1:B:371:TYR:CD1	1:C:382:ILE:HD11	2.45	0.51
1:B:371:TYR:CD1	1:B:375:ASP:HB2	2.46	0.51
1:D:314:TRP:CE3	1:D:319:ARG:HD2	2.46	0.51
1:A:123:VAL:HG22	1:B:380:ILE:CD1	2.26	0.50
1:A:350:GLY:C	1:A:351:ARG:HD2	2.36	0.50
1:C:393:VAL:O	1:C:395:ARG:NH1	2.44	0.50
1:A:298:ARG:C	1:A:298:ARG:HD2	2.36	0.50
1:B:69:PHE:C	1:B:72:PRO:HD2	2.36	0.50
1:C:126:GLU:HG2	1:C:138:VAL:HG11	1.93	0.50
1:A:37:GLN:HG2	5:A:4314:HOH:O	2.11	0.50
1:D:22:GLU:O	1:D:25:ARG:NH1	2.45	0.50
1:B:60:ASP:OD1	1:B:62:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LEU:HD23	1:C:150:ARG:HH21	1.77	0.49
1:C:319:ARG:HH21	1:C:323:GLN:NE2	2.10	0.49
1:A:50:ARG:NH1	5:A:4614:HOH:O	2.45	0.49
1:C:180:HIS:ND1	1:C:180:HIS:C	2.70	0.49
1:C:393:VAL:C	1:C:395:ARG:N	2.66	0.49
1:D:117:GLY:HA2	1:D:122:GLN:HE22	1.77	0.49
1:D:148:GLN:HB2	1:D:152:GLU:OE2	2.12	0.49
1:C:34:ASP:HB2	1:C:41:VAL:HG21	1.94	0.49
1:A:11:LEU:HD23	1:A:150:ARG:HH21	1.77	0.49
1:A:70:VAL:O	1:A:74:MET:HG3	2.13	0.49
1:C:60:ASP:OD1	1:C:62:LYS:HE3	2.13	0.49
1:D:98:HIS:HD2	1:D:101:ARG:NH1	2.11	0.49
1:A:137:LYS:N	1:A:137:LYS:HD3	2.28	0.49
1:B:37:GLN:HG2	5:B:4252:HOH:O	2.11	0.49
1:B:179:LEU:HD23	1:B:179:LEU:O	2.12	0.49
1:C:6:ALA:HB3	2:C:2510:ANP:O2'	2.13	0.48
1:D:370:GLY:O	1:D:371:TYR:HB3	2.12	0.48
1:C:350:GLY:C	1:C:351:ARG:HD2	2.39	0.48
1:B:75:ARG:HG2	1:B:330:ALA:CB	2.43	0.48
1:D:249:HIS:HD2	5:D:4279:HOH:O	1.95	0.48
1:D:10:GLY:HA3	2:D:3510:ANP:O3G	2.13	0.48
1:A:343:LYS:HD2	1:B:343:LYS:CD	2.44	0.48
1:B:298:ARG:HD2	1:B:298:ARG:C	2.38	0.48
1:C:343:LYS:HD2	1:D:343:LYS:CD	2.43	0.48
1:A:248:ARG:HG3	1:A:249:HIS:ND1	2.29	0.48
1:B:87:GLY:HA3	1:B:180:HIS:CD2	2.48	0.48
2:B:1510:ANP:O1A	3:B:1520:ARG:NH2	2.42	0.48
1:D:34:ASP:HA	1:D:37:GLN:HE22	1.78	0.48
1:A:339:LEU:HD12	1:A:339:LEU:N	2.29	0.48
1:C:80:TYR:CD2	1:C:81:GLU:HG3	2.49	0.48
1:C:158:GLU:O	1:C:159:ALA:C	2.57	0.48
1:D:371:TYR:HB2	1:D:375:ASP:OD1	2.13	0.48
1:B:124:ARG:O	1:B:128:THR:HG23	2.13	0.47
1:C:73:MET:CE	1:C:90:ILE:HG12	2.44	0.47
1:C:75:ARG:HG2	1:C:330:ALA:CB	2.44	0.47
1:C:98:HIS:HD2	1:C:101:ARG:NH1	2.12	0.47
1:D:22:GLU:OE2	1:D:160:HIS:NE2	2.46	0.47
1:A:249:HIS:HD2	5:A:4197:HOH:O	1.96	0.47
1:D:93:PRO:HA	1:D:128:THR:HG21	1.96	0.47
1:A:318:GLU:HG3	1:C:293:GLU:HB2	1.97	0.47
1:B:319:ARG:HH21	1:B:323:GLN:NE2	2.08	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ARG:HD2	5:D:4631:HOH:O	2.14	0.47
1:B:345:ASN:HB3	1:B:347:TYR:CE1	2.50	0.47
1:A:7:TYR:CE2	1:A:9:GLY:HA2	2.50	0.47
1:C:189:GLU:O	1:C:191:PRO:HD3	2.15	0.47
1:C:18:LYS:HZ2	1:C:160:HIS:HB3	1.79	0.47
1:C:25:ARG:HB3	1:C:25:ARG:NH1	2.29	0.47
2:D:3510:ANP:PA	3:D:3520:ARG:HH22	2.38	0.47
1:C:93:PRO:HG3	5:C:4212:HOH:O	2.14	0.47
1:C:116:THR:HG21	1:D:365:PHE:CZ	2.50	0.47
1:A:395:ARG:HH22	1:D:355:LYS:CE	2.27	0.46
1:C:248:ARG:HG3	1:C:249:HIS:CD2	2.49	0.46
1:B:249:HIS:HD2	5:B:4064:HOH:O	1.98	0.46
1:B:370:GLY:HA3	1:C:385:LEU:HD13	1.97	0.46
1:C:6:ALA:HB2	1:C:99:LEU:HD11	1.96	0.46
1:D:162:ILE:O	1:D:163:PRO:C	2.58	0.46
1:C:372:ASP:C	1:C:372:ASP:OD2	2.58	0.46
1:D:10:GLY:HA3	2:D:3510:ANP:PG	2.56	0.46
1:A:117:GLY:H	1:B:373:GLN:NE2	2.13	0.46
1:B:260:ARG:HD2	1:B:264:MET:SD	2.55	0.46
1:B:373:GLN:O	1:B:376:ALA:HB3	2.16	0.46
1:C:209:ALA:O	1:C:343:LYS:NZ	2.47	0.46
1:D:29:ILE:N	1:D:29:ILE:CD1	2.78	0.46
1:D:180:HIS:ND1	1:D:180:HIS:C	2.74	0.46
1:A:74:MET:HE2	5:A:4706:HOH:O	2.15	0.46
1:B:50:ARG:NH1	5:B:4373:HOH:O	2.49	0.46
1:D:154:ILE:O	1:D:158:GLU:HG3	2.16	0.46
1:B:376:ALA:O	1:B:380:ILE:HG12	2.16	0.46
1:C:395:ARG:HG3	1:C:395:ARG:HH11	1.80	0.46
1:D:122:GLN:HE21	1:D:143:ARG:HH11	1.64	0.45
1:D:298:ARG:O	1:D:298:ARG:HD2	2.16	0.45
1:B:328:HIS:CD2	1:D:321:ALA:HA	2.51	0.45
1:C:123:VAL:HG12	1:C:127:LEU:CD1	2.46	0.45
1:C:39:GLU:HG3	1:C:39:GLU:O	2.15	0.45
1:D:136:ILE:C	1:D:137:LYS:HD3	2.41	0.45
1:C:150:ARG:HG2	1:C:154:ILE:HD11	1.98	0.45
1:D:87:GLY:HA2	1:D:179:LEU:HD13	1.99	0.45
1:D:298:ARG:HD2	1:D:298:ARG:C	2.42	0.45
1:A:27:GLU:HG3	1:A:54:SER:CB	2.47	0.45
1:A:382:ILE:HG23	1:C:262:VAL:HG13	1.99	0.45
2:A:510:ANP:PA	3:A:520:ARG:HH22	2.37	0.45
1:C:157:ALA:O	1:C:158:GLU:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:SER:O	1:D:147:PHE:C	2.58	0.45
1:D:350:GLY:C	1:D:351:ARG:HD2	2.41	0.45
1:A:24:TYR:O	1:A:25:ARG:C	2.57	0.45
1:C:67:ARG:NH1	1:C:68:ASP:OD1	2.50	0.45
1:C:122:GLN:HE21	1:C:143:ARG:NH1	2.12	0.45
1:C:80:TYR:CE2	1:C:81:GLU:HG3	2.51	0.45
1:D:174:MET:HE1	1:D:201:ARG:HD2	1.97	0.45
1:D:158:GLU:C	1:D:160:HIS:N	2.74	0.45
1:B:80:TYR:HB3	1:B:84:TYR:HB3	1.99	0.44
1:C:201:ARG:HG3	1:C:201:ARG:HH11	1.82	0.44
1:D:16:ILE:HG23	1:D:141:PRO:HG2	1.98	0.44
1:A:191:PRO:HB2	1:B:351:ARG:HD3	1.99	0.44
1:A:351:ARG:HD3	1:B:191:PRO:HB2	1.98	0.44
1:D:69:PHE:C	1:D:72:PRO:HD2	2.43	0.44
1:A:176:ALA:CB	1:A:181:ILE:HG12	2.47	0.44
1:B:94:LEU:HD13	1:B:94:LEU:C	2.42	0.44
1:A:125:PHE:O	1:A:128:THR:CG2	2.66	0.44
1:B:370:GLY:HA3	1:C:385:LEU:CD1	2.46	0.44
1:A:41:VAL:CG1	1:A:58:ALA:HB1	2.48	0.44
1:A:371:TYR:CD1	1:D:382:ILE:HD11	2.52	0.44
1:C:238:LEU:C	1:C:238:LEU:HD23	2.42	0.44
1:C:1:MET:O	1:C:26:ALA:HB1	2.18	0.44
1:A:98:HIS:HD2	1:A:101:ARG:NH1	2.15	0.44
1:B:174:MET:HG2	1:B:183:TYR:CD2	2.53	0.44
1:C:232:ARG:HG3	1:C:232:ARG:NH1	2.33	0.44
1:D:262:VAL:O	1:D:262:VAL:HG13	2.17	0.44
1:B:32:THR:CG2	1:B:41:VAL:HG13	2.48	0.44
1:D:7:TYR:CE2	1:D:9:GLY:HA2	2.53	0.44
1:A:343:LYS:HD2	1:B:343:LYS:HD3	2.00	0.44
1:C:371:TYR:HA	5:C:4340:HOH:O	2.18	0.44
1:D:150:ARG:HA	1:D:153:MET:HE3	1.99	0.44
1:D:345:ASN:HB3	1:D:347:TYR:CE1	2.53	0.43
1:B:298:ARG:HD2	1:B:298:ARG:O	2.16	0.43
1:C:32:THR:HG22	1:C:41:VAL:HG13	2.00	0.43
1:D:238:LEU:C	1:D:238:LEU:HD23	2.43	0.43
1:D:251:VAL:HG11	1:D:346:VAL:CG2	2.48	0.43
1:D:331:ARG:HE	1:D:331:ARG:HB3	1.49	0.43
1:D:339:LEU:N	1:D:339:LEU:HD12	2.33	0.43
1:A:150:ARG:HA	1:A:153:MET:HE3	2.01	0.43
1:A:191:PRO:HG2	5:B:4445:HOH:O	2.18	0.43
1:A:222:GLU:HB2	5:A:4658:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HB2	1:A:282:ARG:NH1	2.33	0.43
1:D:116:THR:HG23	4:D:3530:SIN:O1	2.19	0.43
1:B:304:LYS:O	1:B:307:GLU:HG2	2.18	0.43
1:C:41:VAL:CG1	1:C:58:ALA:HB1	2.49	0.43
1:A:251:VAL:CG1	1:A:252:GLY:N	2.82	0.43
1:A:328:HIS:CD2	1:C:321:ALA:HA	2.54	0.43
1:B:61:LEU:HD13	1:B:94:LEU:HD11	2.00	0.43
1:C:40:GLU:HG3	1:C:43:GLU:H	1.84	0.43
1:D:181:ILE:HG22	1:D:183:TYR:CE1	2.54	0.43
1:D:394:GLU:O	1:D:395:ARG:C	2.62	0.43
1:A:96:ALA:HB3	1:A:128:THR:CG2	2.47	0.43
1:C:116:THR:HG23	4:C:2530:SIN:O1	2.19	0.43
1:A:179:LEU:O	1:A:272:THR:HG23	2.18	0.43
1:A:371:TYR:CE1	1:D:382:ILE:HD11	2.54	0.43
1:B:351:ARG:N	1:B:351:ARG:CD	2.71	0.43
1:C:12:ASP:O	1:C:16:ILE:HG13	2.19	0.43
1:C:71:PHE:HB2	1:C:72:PRO:HD3	2.01	0.43
1:C:162:ILE:O	1:C:164:VAL:HG13	2.18	0.42
1:C:287:SER:HA	5:C:4779:HOH:O	2.19	0.42
1:D:2:LYS:HB2	1:D:108:ALA:HA	2.01	0.42
1:D:96:ALA:HB3	1:D:128:THR:OG1	2.19	0.42
1:C:117:GLY:HA2	1:C:122:GLN:NE2	2.34	0.42
1:D:70:VAL:O	1:D:74:MET:HG3	2.19	0.42
1:C:17:LEU:C	1:C:17:LEU:HD23	2.44	0.42
1:C:351:ARG:HD3	1:D:191:PRO:HB2	2.01	0.42
1:B:77:GLY:HA2	5:B:4345:HOH:O	2.18	0.42
1:B:359:ARG:HD2	1:B:361:ASP:OD1	2.19	0.42
1:C:150:ARG:N	1:C:151:LYS:HD2	2.35	0.42
1:C:260:ARG:HD2	1:C:264:MET:SD	2.60	0.42
1:C:298:ARG:HD2	1:C:298:ARG:C	2.45	0.42
1:D:17:LEU:O	1:D:21:LYS:HG3	2.19	0.42
1:D:114:GLY:N	2:D:3510:ANP:O3'	2.50	0.42
1:D:371:TYR:HD1	1:D:372:ASP:O	2.02	0.42
1:C:328:HIS:CE1	1:C:331:ARG:HH22	2.36	0.42
1:A:17:LEU:HD23	1:A:17:LEU:C	2.44	0.42
1:A:180:HIS:HB2	1:A:271:GLU:O	2.20	0.42
1:A:204:GLN:NE2	5:A:4668:HOH:O	2.53	0.42
1:B:339:LEU:N	1:B:339:LEU:HD12	2.35	0.42
1:A:382:ILE:CG2	1:C:262:VAL:HG13	2.49	0.42
1:D:203:THR:HB	1:D:250:GLY:HA2	2.02	0.42
1:A:358:TYR:O	1:A:359:ARG:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ARG:HG2	1:C:68:ASP:OD1	2.20	0.42
1:C:373:GLN:H	1:C:373:GLN:CD	2.27	0.42
1:D:13:THR:OG1	2:D:3510:ANP:O1G	2.26	0.42
1:B:282:ARG:HB2	1:B:282:ARG:CZ	2.50	0.42
1:A:379:PHE:HB2	1:D:382:ILE:HG13	2.01	0.42
1:C:394:GLU:OE1	1:C:394:GLU:CA	2.68	0.42
1:A:6:ALA:HB3	2:A:510:ANP:O2'	2.20	0.41
1:B:7:TYR:CE2	1:B:9:GLY:HA2	2.55	0.41
1:C:343:LYS:HD3	1:D:343:LYS:HD2	2.01	0.41
1:C:7:TYR:CE2	1:C:48:ALA:HB2	2.55	0.41
1:C:13:THR:HG23	2:C:2510:ANP:O1G	2.20	0.41
1:B:33:ALA:HB1	1:B:61:LEU:HD12	2.02	0.41
1:B:372:ASP:O	1:B:373:GLN:C	2.62	0.41
1:D:64:GLU:OE1	1:D:98:HIS:HE1	2.03	0.41
1:A:42:GLU:O	1:A:46:GLU:HG3	2.21	0.41
1:B:16:ILE:HG23	1:B:141:PRO:HG2	2.03	0.41
1:B:316:ALA:O	1:B:320:GLU:HG3	2.21	0.41
1:C:109:GLU:CG	1:C:137:LYS:HE3	2.41	0.41
1:C:150:ARG:HA	1:C:153:MET:HE3	2.03	0.41
1:C:27:GLU:CG	1:C:54:SER:OG	2.66	0.41
1:D:18:LYS:HG3	1:D:162:ILE:HD11	2.03	0.41
1:D:251:VAL:CG1	1:D:252:GLY:N	2.83	0.41
1:C:100:VAL:O	1:C:104:GLU:HG3	2.20	0.41
1:C:114:GLY:N	2:C:2510:ANP:O3'	2.54	0.41
1:A:298:ARG:HD2	1:A:298:ARG:O	2.21	0.41
1:B:321:ALA:HA	1:D:328:HIS:CD2	2.56	0.41
1:C:18:LYS:HZ1	1:C:160:HIS:C	2.27	0.41
1:D:73:MET:CE	1:D:90:ILE:HG12	2.51	0.41
1:D:97:LYS:HD2	1:D:315:TYR:OH	2.19	0.41
1:A:238:LEU:C	1:A:238:LEU:HD23	2.46	0.41
3:B:1520:ARG:N	5:B:4065:HOH:O	2.54	0.41
1:D:122:GLN:HG3	1:D:123:VAL:N	2.36	0.41
1:A:319:ARG:NH2	1:A:323:GLN:HE21	2.03	0.41
1:B:122:GLN:HE21	1:B:143:ARG:HH11	1.68	0.41
1:D:128:THR:O	1:D:132:LEU:HG	2.21	0.41
1:C:98:HIS:CD2	1:C:101:ARG:NH1	2.89	0.40
1:D:15:ILE:HG23	1:D:156:TYR:CD2	2.56	0.40
1:B:41:VAL:HG12	1:B:58:ALA:CB	2.40	0.40
1:B:92:ARG:HE	1:B:121:ASP:CG	2.30	0.40
1:D:174:MET:HE1	1:D:201:ARG:HD3	2.00	0.40
1:B:98:HIS:HD2	1:B:101:ARG:NH1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:GLY:HA3	2:C:2510:ANP:PG	2.61	0.40
1:A:260:ARG:HD2	1:A:264:MET:SD	2.61	0.40
1:B:1:MET:HB3	1:B:26:ALA:HB2	2.04	0.40
1:C:373:GLN:HG2	1:C:374:LYS:N	2.37	0.40
1:A:321:ALA:HA	1:C:328:HIS:CD2	2.57	0.40
1:A:371:TYR:HD2	1:A:371:TYR:H	1.70	0.40
1:B:24:TYR:O	1:B:25:ARG:C	2.64	0.40
1:C:357:LEU:HB2	1:D:265:LYS:HE3	2.04	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%)	365 (98%)	8 (2%)	1 (0%)	36	28
1	B	380/400 (95%)	370 (97%)	8 (2%)	2 (0%)	24	16
1	C	380/400 (95%)	367 (97%)	12 (3%)	1 (0%)	36	28
1	D	380/400 (95%)	369 (97%)	9 (2%)	2 (0%)	24	16
All	All	1514/1600 (95%)	1471 (97%)	37 (2%)	6 (0%)	30	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	TYR
1	C	159	ALA
1	A	343	LYS
1	B	373	GLN
1	D	343	LYS
1	D	273	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/319 (95%)	289 (95%)	15 (5%)	22	11
1	B	310/319 (97%)	295 (95%)	15 (5%)	23	12
1	C	310/319 (97%)	293 (94%)	17 (6%)	19	8
1	D	310/319 (97%)	293 (94%)	17 (6%)	19	8
All	All	1234/1276 (97%)	1170 (95%)	64 (5%)	19	9

All (64) 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	101	ARG
1	A	151	LYS
1	A	179	LEU
1	A	180	HIS
1	A	188	LEU
1	A	239	LEU
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	62	LYS
1	B	90	ILE
1	B	118	LYS
1	B	146	SER
1	B	165	PRO
1	B	179	LEU
1	B	180	HIS
1	B	182	SER

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Mol	Chain	Res	Type
1	B	188	LEU
1	B	239	LEU
1	B	319	ARG
1	B	351	ARG
1	B	359	ARG
1	B	373	GLN
1	C	37	GLN
1	C	39	GLU
1	C	62	LYS
1	C	90	ILE
1	C	150	ARG
1	C	151	LYS
1	C	179	LEU
1	C	180	HIS
1	C	188	LEU
1	C	197	LYS
1	C	239	LEU
1	C	264	MET
1	C	319	ARG
1	C	351	ARG
1	C	361	ASP
1	C	373	GLN
1	C	394	GLU
1	D	29	ILE
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	319	ARG
1	D	351	ARG
1	D	372	ASP
1	D	395	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	148	GLN
1	A	249	HIS
1	A	323	GLN
1	A	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	C	37	GLN
1	C	98	HIS
1	C	122	GLN
1	C	180	HIS
1	C	323	GLN
1	C	360	GLN
1	C	373	GLN
1	D	37	GLN
1	D	98	HIS
1	D	122	GLN
1	D	148	GLN
1	D	204	GLN
1	D	240	GLN
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$
4	SIN	A	530	-	7,7,7	2.02	3 (42%)	8,8,8	1.39	1 (12%)
3	ARG	D	3520	-	10,11,11	0.70	0	9,13,13	1.33	2 (22%)
4	SIN	D	3530	-	7,7,7	2.16	4 (57%)	8,8,8	1.30	1 (12%)
2	ANP	A	510	-	33,33,33	2.38	10 (30%)	45,52,52	2.65	13 (28%)
2	ANP	B	1510	-	33,33,33	2.12	11 (33%)	45,52,52	2.69	13 (28%)
2	ANP	D	3510	-	33,33,33	2.36	10 (30%)	45,52,52	2.62	12 (26%)
4	SIN	C	2530	-	7,7,7	1.99	3 (42%)	8,8,8	1.24	1 (12%)
4	SIN	B	1530	-	7,7,7	1.99	3 (42%)	8,8,8	1.14	0
3	ARG	B	1520	-	10,11,11	0.73	0	9,13,13	0.87	0
3	ARG	C	2520	-	10,11,11	0.73	0	9,13,13	1.30	1 (11%)
3	ARG	A	520	-	10,11,11	0.75	0	9,13,13	0.97	1 (11%)
2	ANP	C	2510	-	33,33,33	2.26	10 (30%)	45,52,52	2.64	13 (28%)

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	SIN	A	530	-	-	4/5/5/5	-
3	ARG	D	3520	-	-	4/11/11/11	-
4	SIN	D	3530	-	-	4/5/5/5	-
2	ANP	A	510	-	-	7/18/38/38	0/3/3/3
2	ANP	B	1510	-	-	8/18/38/38	0/3/3/3
2	ANP	D	3510	-	-	7/18/38/38	0/3/3/3
4	SIN	C	2530	-	-	4/5/5/5	-
4	SIN	B	1530	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ARG	B	1520	-	-	3/11/11/11	-
3	ARG	C	2520	-	-	1/11/11/11	-
3	ARG	A	520	-	-	5/11/11/11	-
2	ANP	C	2510	-	-	8/18/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3510	ANP	PB-O3A	7.60	1.68	1.59
2	A	510	ANP	PB-O3A	7.47	1.68	1.59
2	C	2510	ANP	PB-O3A	7.45	1.68	1.59
2	B	1510	ANP	PB-O3A	5.29	1.65	1.59
2	A	510	ANP	PA-O3A	4.56	1.64	1.59
2	D	3510	ANP	PA-O3A	4.53	1.64	1.59
2	D	3510	ANP	PB-O1B	4.36	1.52	1.46
2	A	510	ANP	PB-O1B	4.27	1.52	1.46
2	C	2510	ANP	PB-O1B	4.23	1.52	1.46
2	B	1510	ANP	PB-O1B	4.15	1.52	1.46
2	B	1510	ANP	PA-O3A	3.90	1.63	1.59
2	B	1510	ANP	C3'-C4'	-3.52	1.44	1.53
2	C	2510	ANP	PA-O3A	3.48	1.63	1.59
2	A	510	ANP	C3'-C4'	-3.43	1.44	1.53
2	C	2510	ANP	C3'-C4'	-3.34	1.44	1.53
2	A	510	ANP	PG-N3B	3.21	1.71	1.63
2	A	510	ANP	PB-O2B	-3.19	1.48	1.56
2	A	510	ANP	C5-N7	-3.14	1.33	1.39
2	D	3510	ANP	C3'-C4'	-3.10	1.45	1.53
2	C	2510	ANP	PB-O2B	-3.05	1.48	1.56
2	D	3510	ANP	PB-O2B	-3.02	1.48	1.56
4	D	3530	SIN	O2-C1	-3.01	1.20	1.30
4	A	530	SIN	C3-C4	2.98	1.57	1.50
4	A	530	SIN	O2-C1	-2.90	1.21	1.30
2	C	2510	ANP	C5-N7	-2.89	1.33	1.39
4	D	3530	SIN	C3-C4	2.89	1.57	1.50
2	D	3510	ANP	PG-O1G	2.89	1.50	1.46
2	D	3510	ANP	C5-N7	-2.86	1.33	1.39
4	D	3530	SIN	O4-C4	-2.84	1.21	1.30
2	B	1510	ANP	C5-N7	-2.83	1.33	1.39
4	C	2530	SIN	O4-C4	-2.83	1.21	1.30
2	B	1510	ANP	PB-O2B	-2.79	1.49	1.56
4	C	2530	SIN	O2-C1	-2.77	1.21	1.30
4	C	2530	SIN	C3-C4	2.76	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2510	ANP	PG-O1G	2.74	1.50	1.46
4	B	1530	SIN	O2-C1	-2.72	1.21	1.30
4	B	1530	SIN	C3-C4	2.68	1.56	1.50
2	D	3510	ANP	PB-N3B	-2.68	1.56	1.63
4	A	530	SIN	O4-C4	-2.68	1.22	1.30
2	A	510	ANP	C1'-N9	2.67	1.53	1.46
2	D	3510	ANP	C1'-N9	2.64	1.53	1.46
4	B	1530	SIN	O4-C4	-2.64	1.22	1.30
2	A	510	ANP	C2-N1	2.63	1.38	1.33
2	A	510	ANP	PG-O1G	2.61	1.50	1.46
2	B	1510	ANP	C1'-N9	2.52	1.53	1.46
2	C	2510	ANP	C1'-N9	2.50	1.53	1.46
2	D	3510	ANP	C2-N1	2.49	1.38	1.33
2	B	1510	ANP	PG-O1G	2.46	1.49	1.46
2	C	2510	ANP	PB-N3B	-2.37	1.57	1.63
2	B	1510	ANP	PG-N3B	2.33	1.69	1.63
2	B	1510	ANP	C2-N1	2.32	1.38	1.33
2	C	2510	ANP	C2-N1	2.29	1.38	1.33
2	B	1510	ANP	PB-N3B	-2.17	1.57	1.63
4	D	3530	SIN	C2-C1	2.11	1.55	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1510	ANP	O1B-PB-N3B	-8.11	99.83	111.77
2	A	510	ANP	O1B-PB-N3B	-7.76	100.34	111.77
2	C	2510	ANP	O1B-PB-N3B	-7.64	100.53	111.77
2	D	3510	ANP	O1B-PB-N3B	-7.50	100.72	111.77
2	B	1510	ANP	C5-C4-N3	-7.11	116.92	126.72
2	D	3510	ANP	C5-C4-N3	-7.11	116.93	126.72
2	C	2510	ANP	C5-C4-N3	-7.05	117.01	126.72
2	A	510	ANP	C5-C4-N3	-7.04	117.02	126.72
2	B	1510	ANP	O3A-PB-N3B	7.00	126.02	106.59
2	C	2510	ANP	N3-C4-N9	6.41	138.07	127.17
2	A	510	ANP	N3-C4-N9	6.38	138.02	127.17
2	D	3510	ANP	N3-C4-N9	6.31	137.91	127.17
2	A	510	ANP	O3A-PB-N3B	6.20	123.79	106.59
2	B	1510	ANP	N3-C4-N9	6.15	137.63	127.17
2	C	2510	ANP	O3A-PB-N3B	5.69	122.39	106.59
2	D	3510	ANP	O3A-PB-N3B	5.53	121.94	106.59
2	C	2510	ANP	C2-N3-C4	4.11	121.86	111.83
2	D	3510	ANP	C2-N3-C4	4.09	121.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1510	ANP	C2-N3-C4	4.07	121.78	111.83
2	C	2510	ANP	C4'-O4'-C1'	4.05	118.42	109.47
2	D	3510	ANP	C4'-O4'-C1'	4.01	118.31	109.47
2	A	510	ANP	C2-N3-C4	3.98	121.56	111.83
2	A	510	ANP	C4'-O4'-C1'	3.68	117.59	109.47
2	B	1510	ANP	C4'-O4'-C1'	3.66	117.55	109.47
2	B	1510	ANP	PA-O5'-C5'	-3.42	101.78	121.35
2	C	2510	ANP	C3'-C2'-C1'	3.35	107.80	101.46
2	A	510	ANP	O4'-C1'-C2'	-3.33	99.50	106.62
2	B	1510	ANP	O4'-C1'-C2'	-3.30	99.56	106.62
2	C	2510	ANP	O4'-C1'-C2'	-3.28	99.61	106.62
2	A	510	ANP	N3-C2-N1	-3.26	123.64	128.58
2	C	2510	ANP	N3-C2-N1	-3.24	123.67	128.58
2	D	3510	ANP	O4'-C1'-C2'	-3.24	99.68	106.62
2	D	3510	ANP	C3'-C2'-C1'	3.22	107.56	101.46
2	D	3510	ANP	N3-C2-N1	-3.20	123.74	128.58
2	A	510	ANP	PA-O5'-C5'	-3.16	103.26	121.35
2	D	3510	ANP	O1G-PG-N3B	-3.15	107.13	111.77
2	A	510	ANP	C3'-C2'-C1'	3.12	107.36	101.46
2	A	510	ANP	C6-C5-C4	3.03	121.31	117.18
2	D	3510	ANP	C6-C5-C4	2.95	121.20	117.18
2	C	2510	ANP	PA-O5'-C5'	-2.92	104.59	121.35
2	B	1510	ANP	N3-C2-N1	-2.90	124.19	128.58
2	B	1510	ANP	C6-C5-C4	2.90	121.13	117.18
2	C	2510	ANP	C6-C5-C4	2.86	121.09	117.18
2	B	1510	ANP	C3'-C2'-C1'	2.82	106.79	101.46
2	B	1510	ANP	C5'-C4'-C3'	-2.76	105.28	115.21
2	D	3510	ANP	PA-O5'-C5'	-2.70	105.91	121.35
3	C	2520	ARG	CB-CA-C	-2.56	103.67	110.45
4	A	530	SIN	C3-C2-C1	2.52	120.35	113.67
3	D	3520	ARG	CB-CA-C	-2.40	104.08	110.45
2	C	2510	ANP	O1G-PG-N3B	-2.37	108.28	111.77
3	D	3520	ARG	CG-CB-CA	2.29	120.62	113.22
2	B	1510	ANP	O1G-PG-N3B	-2.29	108.40	111.77
4	D	3530	SIN	C3-C2-C1	2.23	119.58	113.67
2	A	510	ANP	C5'-C4'-C3'	-2.16	107.44	115.21
4	C	2530	SIN	C3-C2-C1	2.16	119.39	113.67
3	A	520	ARG	CG-CD-NE	2.13	118.16	112.20
2	A	510	ANP	C6-C5-N7	-2.08	128.08	132.09
2	C	2510	ANP	C2'-C3'-C4'	2.03	106.53	102.61

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	510	ANP	PG-N3B-PB-O1B
2	A	510	ANP	PA-O3A-PB-O2B
2	B	1510	ANP	PB-N3B-PG-O1G
2	B	1510	ANP	PG-N3B-PB-O1B
2	B	1510	ANP	PG-N3B-PB-O3A
2	C	2510	ANP	PG-N3B-PB-O1B
2	C	2510	ANP	PG-N3B-PB-O3A
2	C	2510	ANP	PA-O3A-PB-O2B
2	D	3510	ANP	PG-N3B-PB-O1B
2	D	3510	ANP	PG-N3B-PB-O3A
3	A	520	ARG	N-CA-CB-CG
3	A	520	ARG	NH1-CZ-NE-CD
3	A	520	ARG	NH2-CZ-NE-CD
3	B	1520	ARG	N-CA-CB-CG
3	D	3520	ARG	N-CA-CB-CG
2	B	1510	ANP	C3'-C4'-C5'-O5'
2	D	3510	ANP	C3'-C4'-C5'-O5'
3	D	3520	ARG	NE-CD-CG-CB
3	C	2520	ARG	NE-CD-CG-CB
3	B	1520	ARG	NE-CD-CG-CB
2	A	510	ANP	C3'-C4'-C5'-O5'
2	B	1510	ANP	O4'-C4'-C5'-O5'
2	C	2510	ANP	C3'-C4'-C5'-O5'
2	D	3510	ANP	O4'-C4'-C5'-O5'
2	C	2510	ANP	O4'-C4'-C5'-O5'
2	A	510	ANP	O4'-C4'-C5'-O5'
3	A	520	ARG	NE-CD-CG-CB
3	A	520	ARG	C-CA-CB-CG
3	D	3520	ARG	C-CA-CB-CG
2	A	510	ANP	PB-O3A-PA-O2A
2	B	1510	ANP	PB-O3A-PA-O2A
2	C	2510	ANP	PB-O3A-PA-O2A
2	D	3510	ANP	PB-O3A-PA-O2A
3	D	3520	ARG	CG-CD-NE-CZ
4	B	1530	SIN	C2-C3-C4-O4
4	C	2530	SIN	C2-C3-C4-O4
4	A	530	SIN	C2-C3-C4-O4
4	D	3530	SIN	C2-C3-C4-O4
4	B	1530	SIN	O2-C1-C2-C3
4	D	3530	SIN	O2-C1-C2-C3
4	A	530	SIN	O2-C1-C2-C3
4	C	2530	SIN	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	1530	SIN	C2-C3-C4-O3
4	A	530	SIN	C2-C3-C4-O3
4	C	2530	SIN	C2-C3-C4-O3
4	D	3530	SIN	C2-C3-C4-O3
4	B	1530	SIN	O1-C1-C2-C3
3	B	1520	ARG	C-CA-CB-CG
4	C	2530	SIN	O1-C1-C2-C3
4	D	3530	SIN	O1-C1-C2-C3
4	A	530	SIN	O1-C1-C2-C3
2	A	510	ANP	PA-O3A-PB-O1B
2	B	1510	ANP	PA-O3A-PB-O1B
2	C	2510	ANP	PA-O3A-PB-O1B
2	D	3510	ANP	PA-O3A-PB-O1B
2	A	510	ANP	PB-O3A-PA-O1A
2	B	1510	ANP	PB-O3A-PA-O1A
2	C	2510	ANP	PB-O3A-PA-O1A
2	D	3510	ANP	PB-O3A-PA-O1A

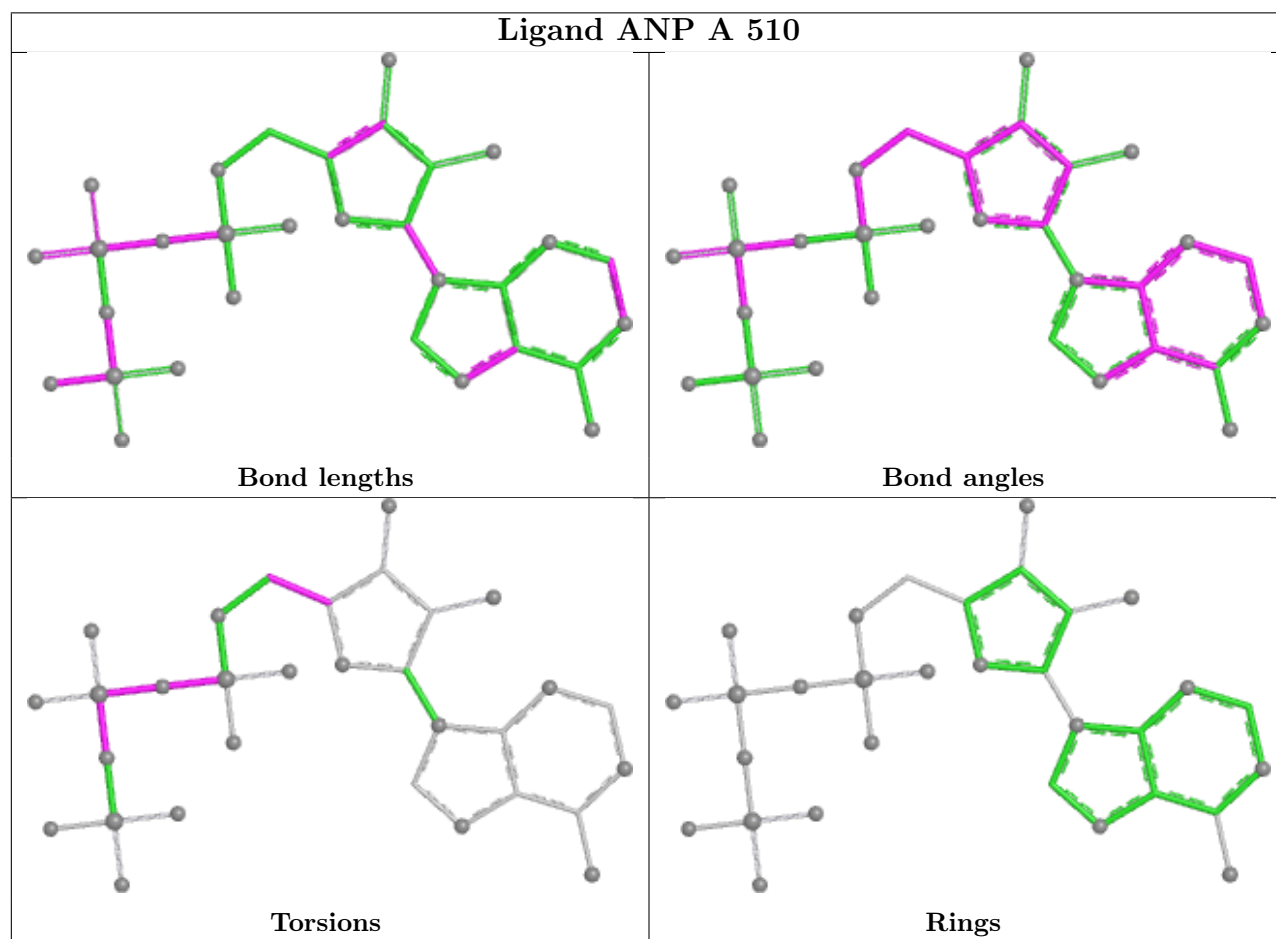
There are no ring outliers.

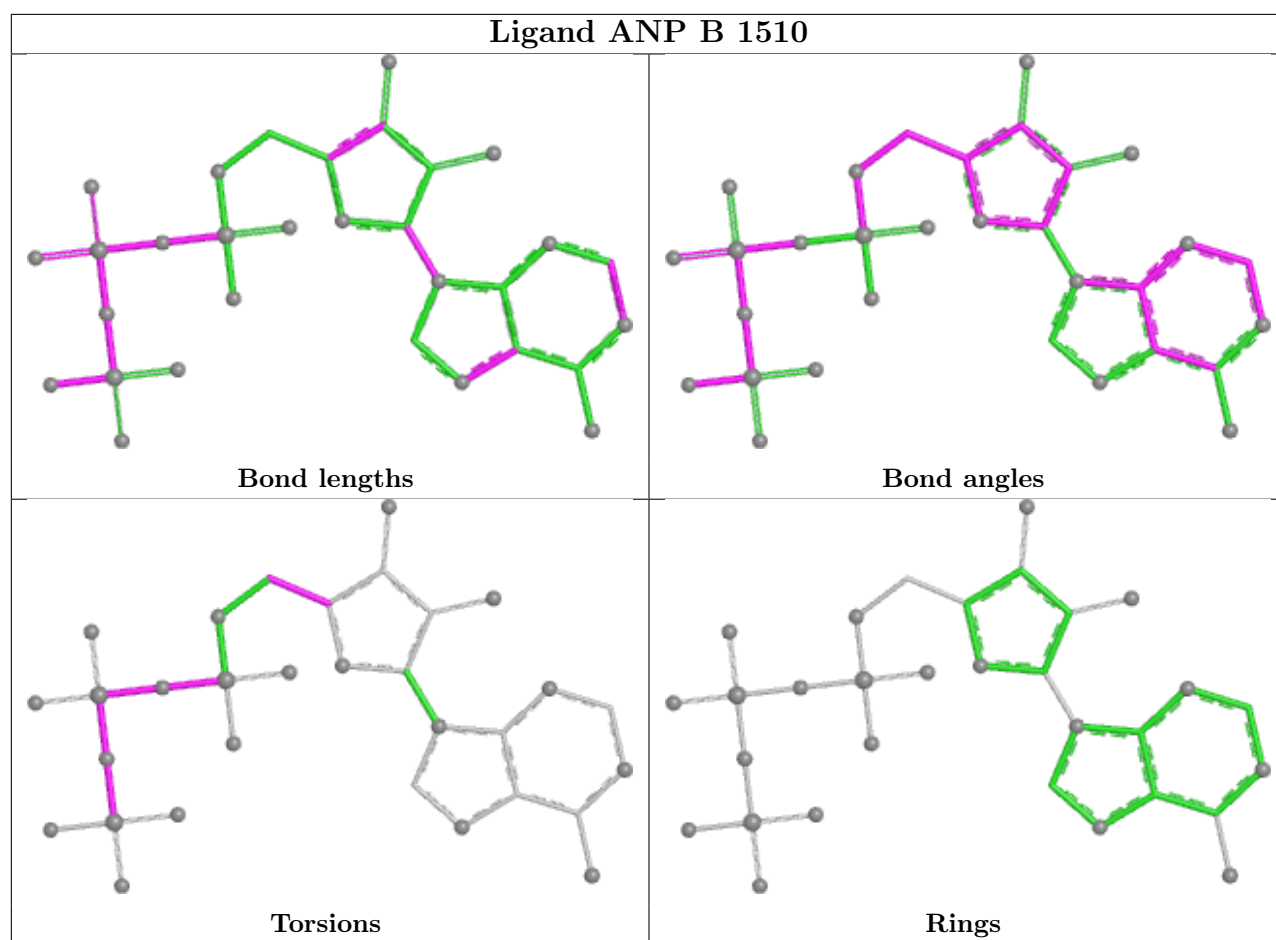
9 monomers are involved in 18 short contacts:

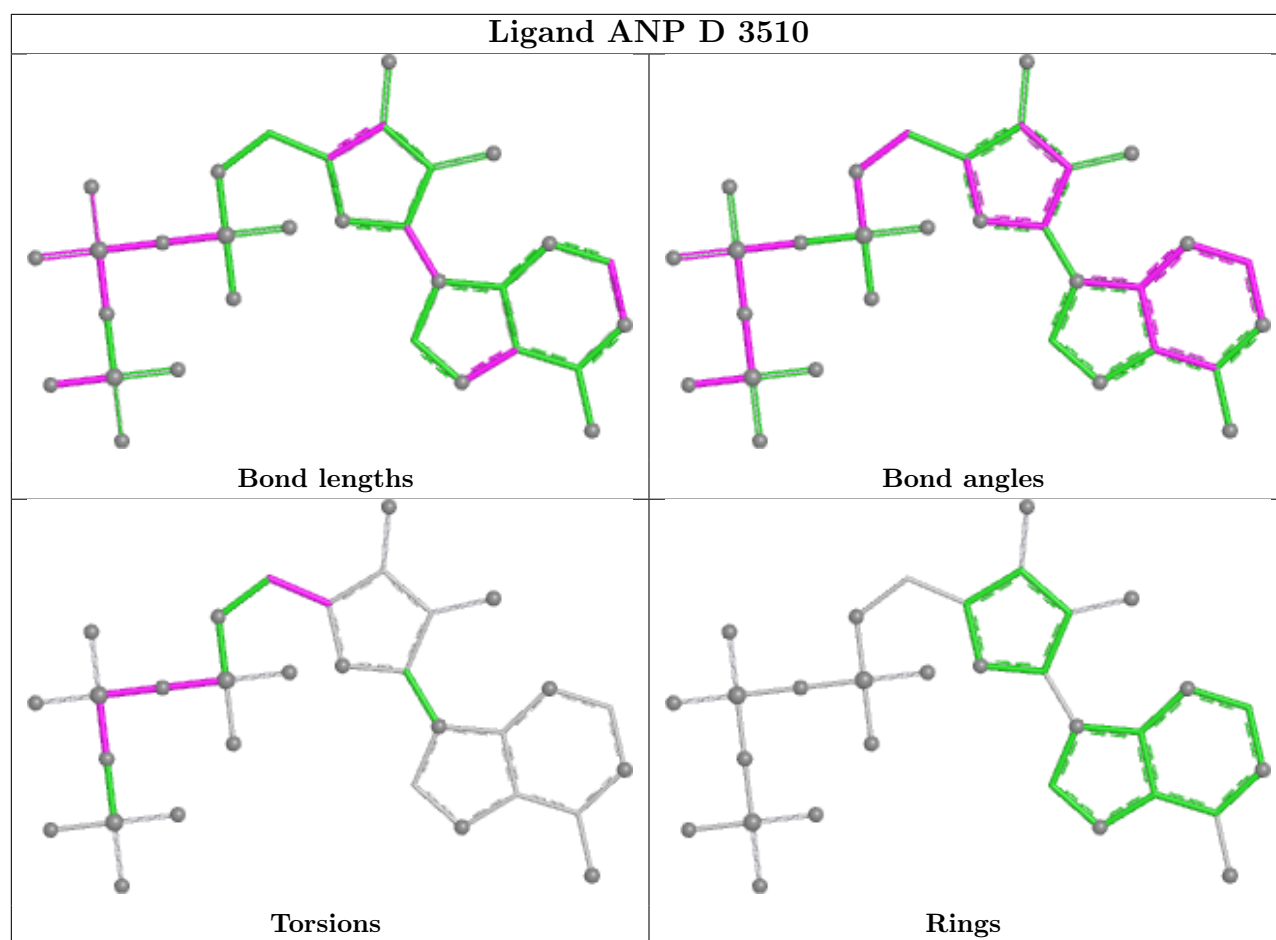
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3520	ARG	1	0
4	D	3530	SIN	1	0
2	A	510	ANP	2	0
2	B	1510	ANP	2	0
2	D	3510	ANP	6	0
4	C	2530	SIN	1	0
3	B	1520	ARG	3	0
3	A	520	ARG	1	0
2	C	2510	ANP	5	0

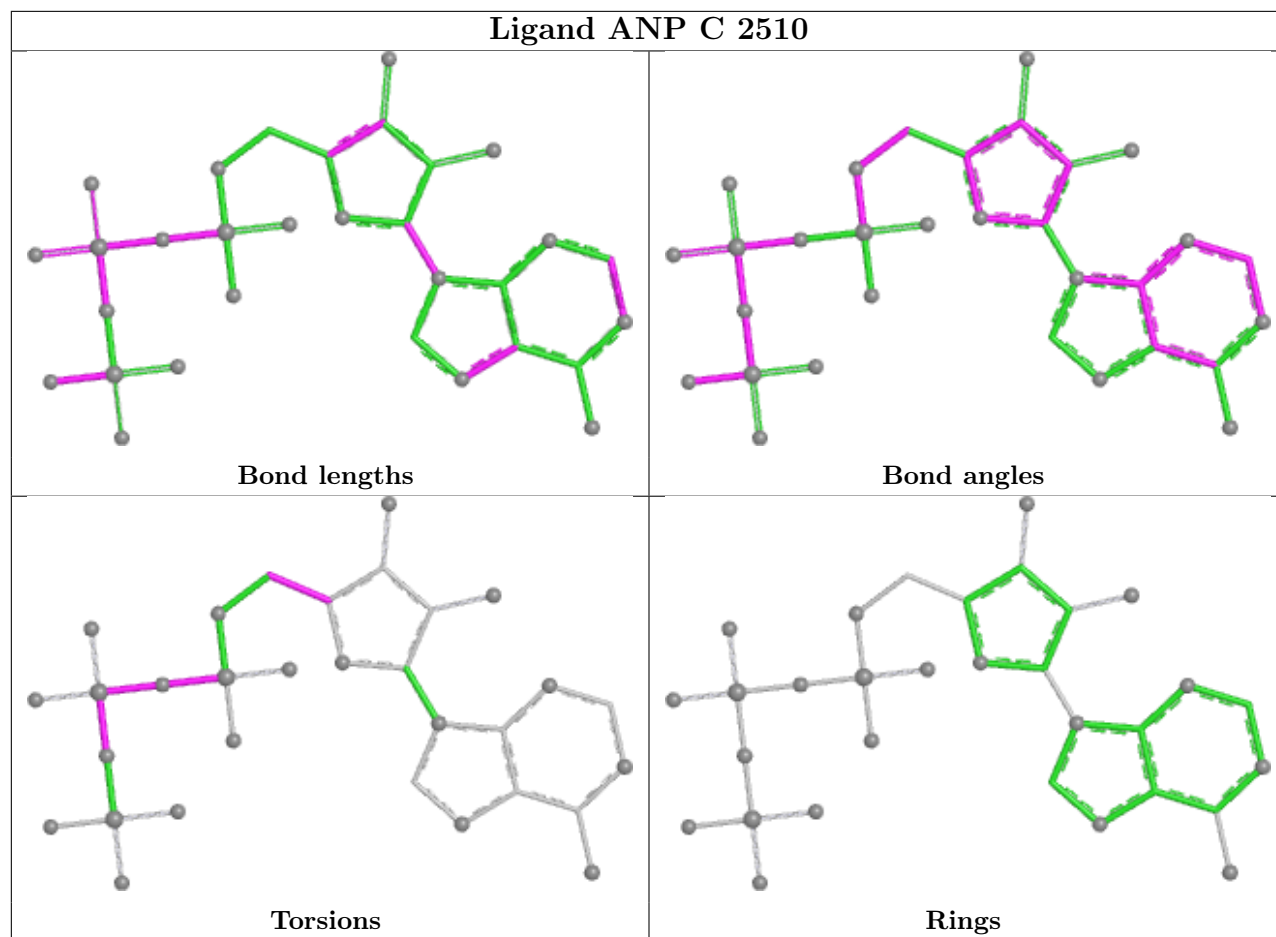
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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%)	0.12	16 (4%)	40	47	20, 27, 49, 75	0
1	B	386/400 (96%)	0.07	18 (4%)	36	42	20, 28, 47, 71	0
1	C	386/400 (96%)	0.58	43 (11%)	10	12	21, 31, 59, 77	0
1	D	386/400 (96%)	0.40	22 (5%)	29	34	22, 31, 55, 76	0
All	All	1538/1600 (96%)	0.29	99 (6%)	25	29	20, 29, 55, 77	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	TYR	9.3
1	A	370	GLY	6.9
1	B	371	TYR	6.7
1	B	365	PHE	6.3
1	C	39	GLU	6.1
1	C	395	ARG	5.4
1	A	165	PRO	5.3
1	C	165	PRO	5.3
1	A	395	ARG	5.1
1	B	361	ASP	5.0
1	C	161	GLY	5.0
1	C	159	ALA	4.7
1	B	395	ARG	4.6
1	D	395	ARG	4.6
1	C	49	LEU	4.5
1	C	365	PHE	4.2
1	D	371	TYR	4.2
1	B	118	LYS	4.2
1	C	373	GLN	4.1
1	D	161	GLY	4.1
1	A	359	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	364	SER	3.8
1	C	370	GLY	3.8
1	B	165	PRO	3.7
1	D	159	ALA	3.6
1	D	370	GLY	3.6
1	C	43	GLU	3.6
1	D	365	PHE	3.6
1	C	394	GLU	3.5
1	C	205	ASP	3.5
1	C	38	GLY	3.5
1	C	155	ALA	3.5
1	C	361	ASP	3.5
1	A	41	VAL	3.4
1	C	164	VAL	3.4
1	C	157	ALA	3.4
1	D	165	PRO	3.3
1	B	370	GLY	3.3
1	D	157	ALA	3.3
1	D	205	ASP	3.3
1	B	151	LYS	3.2
1	C	372	ASP	3.2
1	A	104	GLU	3.1
1	D	164	VAL	3.1
1	D	155	ALA	3.1
1	C	25	ARG	3.0
1	C	158	GLU	3.0
1	C	26	ALA	3.0
1	C	22	GLU	3.0
1	C	104	GLU	3.0
1	C	162	ILE	3.0
1	D	201	ARG	2.9
1	B	372	ASP	2.9
1	C	154	ILE	2.9
1	D	373	GLN	2.8
1	C	137	LYS	2.8
1	D	374	LYS	2.8
1	A	372	ASP	2.7
1	B	360	GLN	2.7
1	D	40	GLU	2.6
1	B	364	SER	2.6
1	C	148	GLN	2.6
1	C	371	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	90	ILE	2.6
1	A	373	GLN	2.5
1	C	151	LYS	2.5
1	C	48	ALA	2.5
1	D	148	GLN	2.5
1	C	1	MET	2.5
1	B	373	GLN	2.4
1	A	151	LYS	2.4
1	D	363	VAL	2.4
1	A	159	ALA	2.3
1	C	90	ILE	2.3
1	A	161	GLY	2.3
1	C	208	GLU	2.3
1	C	53	ALA	2.3
1	C	40	GLU	2.3
1	D	39	GLU	2.3
1	C	50	ARG	2.2
1	C	44	ALA	2.2
1	A	388	ARG	2.2
1	C	10	GLY	2.2
1	B	359	ARG	2.2
1	C	51	THR	2.2
1	B	394	GLU	2.2
1	B	374	LYS	2.2
1	A	216	VAL	2.1
1	C	21	LYS	2.1
1	A	40	GLU	2.1
1	D	207	GLU	2.1
1	D	151	LYS	2.1
1	C	54	SER	2.0
1	C	9	GLY	2.0
1	B	148	GLN	2.0
1	B	362	LEU	2.0
1	D	372	ASP	2.0
1	A	197	LYS	2.0
1	C	41	VAL	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

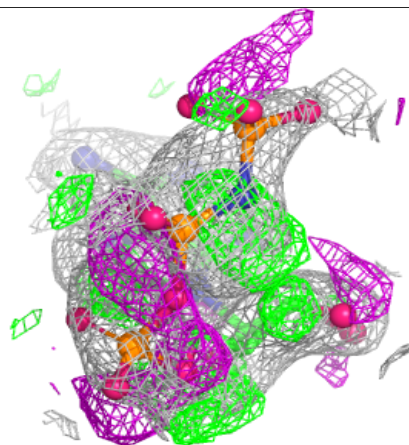
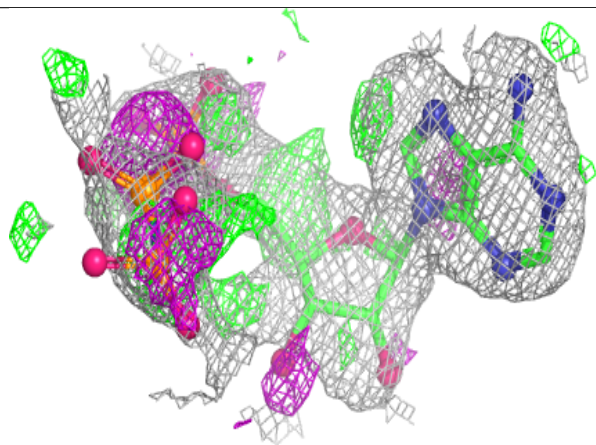
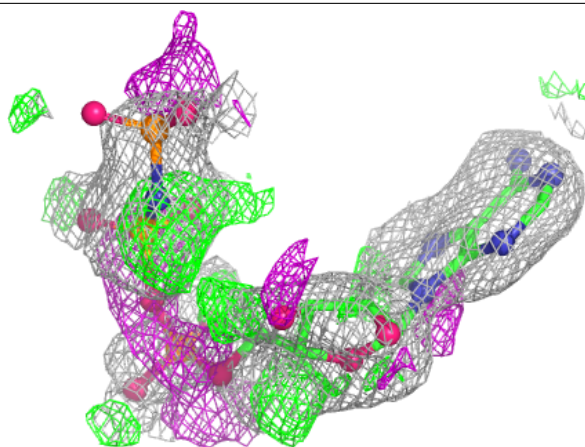
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ANP	D	3510	31/31	0.73	0.20	35,47,76,79	0
4	SIN	A	530	8/8	0.77	0.17	33,37,40,41	0
4	SIN	B	1530	8/8	0.77	0.16	35,37,40,41	0
2	ANP	C	2510	31/31	0.79	0.17	28,44,74,78	0
2	ANP	A	510	31/31	0.80	0.16	26,38,66,68	0
4	SIN	C	2530	8/8	0.80	0.12	29,33,36,38	0
2	ANP	B	1510	31/31	0.81	0.17	25,33,67,71	0
3	ARG	C	2520	12/12	0.82	0.16	28,35,49,52	0
3	ARG	B	1520	12/12	0.82	0.13	17,28,43,44	0
4	SIN	D	3530	8/8	0.82	0.15	33,34,42,43	0
3	ARG	A	520	12/12	0.83	0.14	19,27,38,43	0
3	ARG	D	3520	12/12	0.84	0.14	25,32,44,50	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.

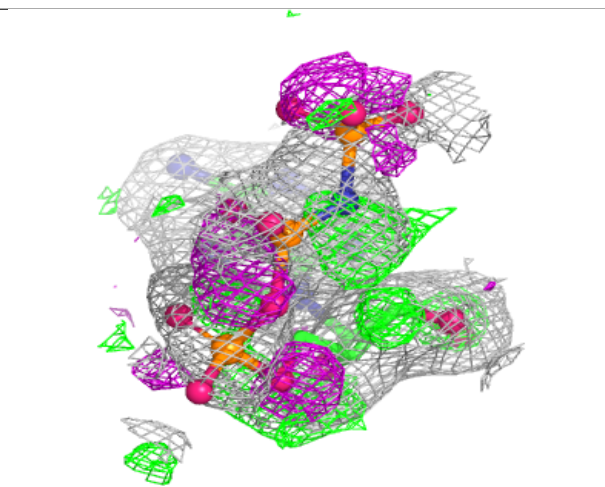
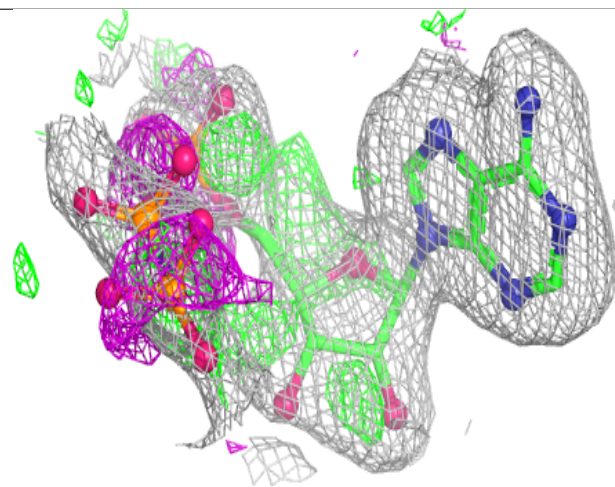
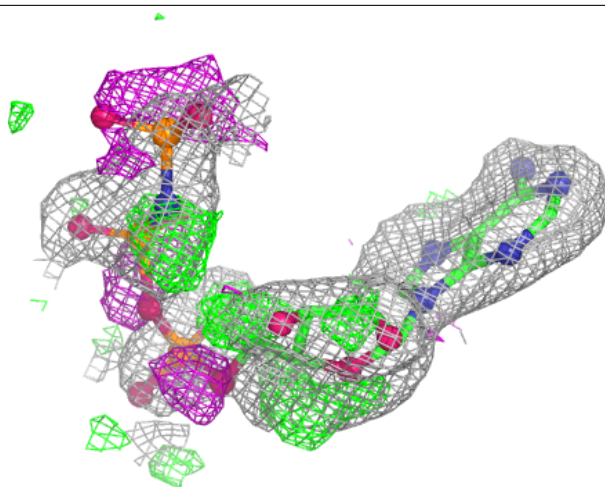
Electron density around ANP D 3510:

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



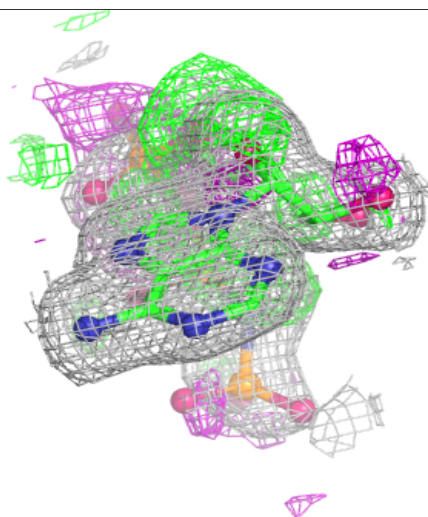
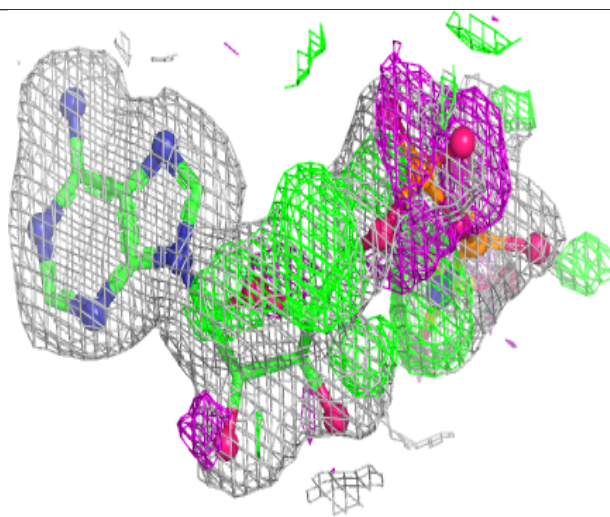
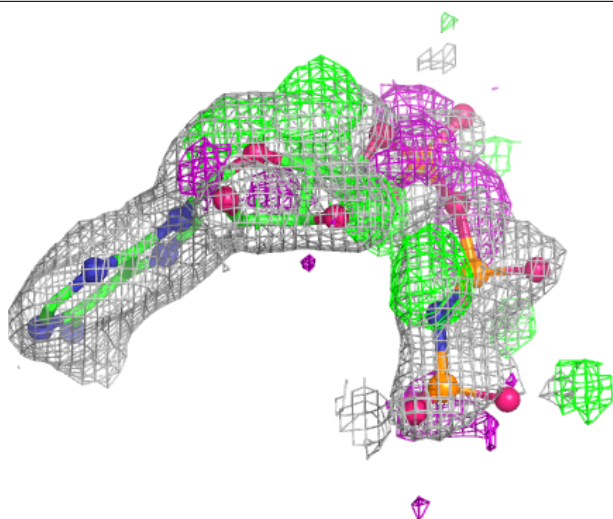
Electron density around ANP C 2510:

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



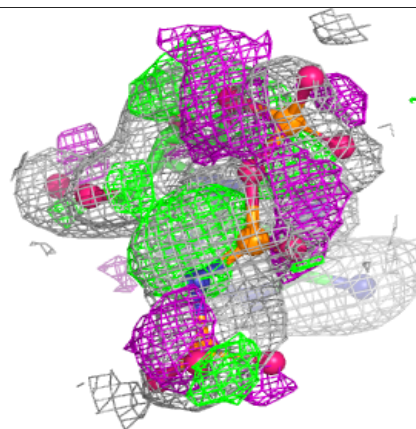
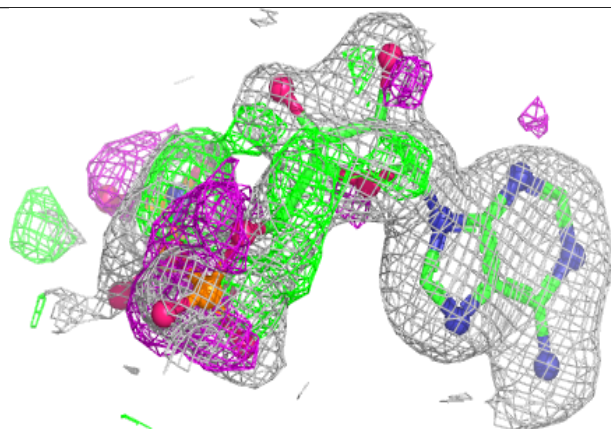
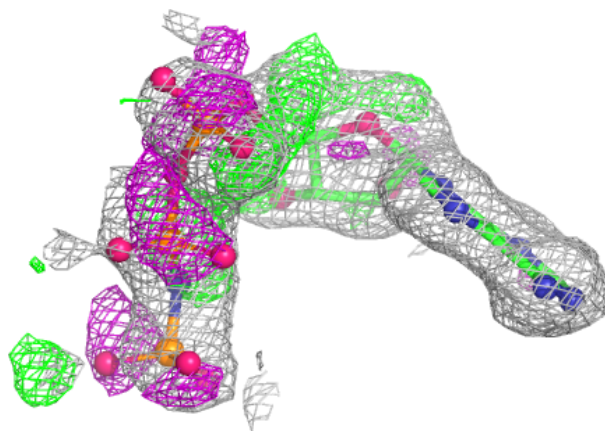
Electron density around ANP A 510:

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



Electron density around ANP B 1510:

$2mF_o-DF_c$ (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.