



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 AM UTC

PDB ID : 3WQT / pdb_00003wqt
Title : Staphylococcus aureus FtsA complexed with AMPPNP
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Deposited on : 2014-02-01
Resolution : 2.20 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

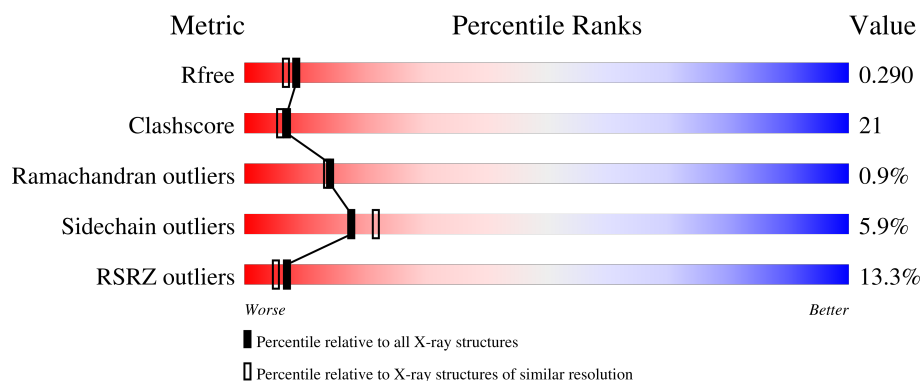
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	484	2% 54% 20% • 24%
1	B	484	23% 35% 32% • 31%
1	C	484	2% 51% 22% • 24%
1	D	484	12% 40% 28% 5% 27%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11614 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 Cell division protein FtsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2871	1811	458	595	7			
1	B	334	Total	C	N	O	S	0	0	0
			2590	1640	412	532	6			
1	C	368	Total	C	N	O	S	0	0	0
			2853	1801	453	592	7			
1	D	352	Total	C	N	O	S	0	0	0
			2733	1729	434	563	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q6GHQ0
A	-14	ASN	-	expression tag	UNP Q6GHQ0
A	-13	HIS	-	expression tag	UNP Q6GHQ0
A	-12	LYS	-	expression tag	UNP Q6GHQ0
A	-11	VAL	-	expression tag	UNP Q6GHQ0
A	-10	HIS	-	expression tag	UNP Q6GHQ0
A	-9	HIS	-	expression tag	UNP Q6GHQ0
A	-8	HIS	-	expression tag	UNP Q6GHQ0
A	-7	HIS	-	expression tag	UNP Q6GHQ0
A	-6	HIS	-	expression tag	UNP Q6GHQ0
A	-5	HIS	-	expression tag	UNP Q6GHQ0
A	-4	ILE	-	expression tag	UNP Q6GHQ0
A	-3	GLU	-	expression tag	UNP Q6GHQ0
A	-2	GLY	-	expression tag	UNP Q6GHQ0
A	-1	ARG	-	expression tag	UNP Q6GHQ0
A	0	HIS	-	expression tag	UNP Q6GHQ0
B	-15	MET	-	expression tag	UNP Q6GHQ0
B	-14	ASN	-	expression tag	UNP Q6GHQ0
B	-13	HIS	-	expression tag	UNP Q6GHQ0
B	-12	LYS	-	expression tag	UNP Q6GHQ0
B	-11	VAL	-	expression tag	UNP Q6GHQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q6GHQ0
B	-9	HIS	-	expression tag	UNP Q6GHQ0
B	-8	HIS	-	expression tag	UNP Q6GHQ0
B	-7	HIS	-	expression tag	UNP Q6GHQ0
B	-6	HIS	-	expression tag	UNP Q6GHQ0
B	-5	HIS	-	expression tag	UNP Q6GHQ0
B	-4	ILE	-	expression tag	UNP Q6GHQ0
B	-3	GLU	-	expression tag	UNP Q6GHQ0
B	-2	GLY	-	expression tag	UNP Q6GHQ0
B	-1	ARG	-	expression tag	UNP Q6GHQ0
B	0	HIS	-	expression tag	UNP Q6GHQ0
C	-15	MET	-	expression tag	UNP Q6GHQ0
C	-14	ASN	-	expression tag	UNP Q6GHQ0
C	-13	HIS	-	expression tag	UNP Q6GHQ0
C	-12	LYS	-	expression tag	UNP Q6GHQ0
C	-11	VAL	-	expression tag	UNP Q6GHQ0
C	-10	HIS	-	expression tag	UNP Q6GHQ0
C	-9	HIS	-	expression tag	UNP Q6GHQ0
C	-8	HIS	-	expression tag	UNP Q6GHQ0
C	-7	HIS	-	expression tag	UNP Q6GHQ0
C	-6	HIS	-	expression tag	UNP Q6GHQ0
C	-5	HIS	-	expression tag	UNP Q6GHQ0
C	-4	ILE	-	expression tag	UNP Q6GHQ0
C	-3	GLU	-	expression tag	UNP Q6GHQ0
C	-2	GLY	-	expression tag	UNP Q6GHQ0
C	-1	ARG	-	expression tag	UNP Q6GHQ0
C	0	HIS	-	expression tag	UNP Q6GHQ0
D	-15	MET	-	expression tag	UNP Q6GHQ0
D	-14	ASN	-	expression tag	UNP Q6GHQ0
D	-13	HIS	-	expression tag	UNP Q6GHQ0
D	-12	LYS	-	expression tag	UNP Q6GHQ0
D	-11	VAL	-	expression tag	UNP Q6GHQ0
D	-10	HIS	-	expression tag	UNP Q6GHQ0
D	-9	HIS	-	expression tag	UNP Q6GHQ0
D	-8	HIS	-	expression tag	UNP Q6GHQ0
D	-7	HIS	-	expression tag	UNP Q6GHQ0
D	-6	HIS	-	expression tag	UNP Q6GHQ0
D	-5	HIS	-	expression tag	UNP Q6GHQ0
D	-4	ILE	-	expression tag	UNP Q6GHQ0
D	-3	GLU	-	expression tag	UNP Q6GHQ0
D	-2	GLY	-	expression tag	UNP Q6GHQ0
D	-1	ARG	-	expression tag	UNP Q6GHQ0

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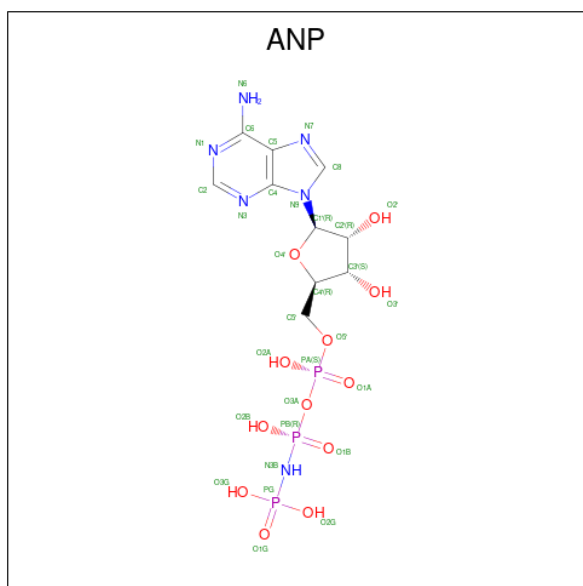
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q6GHQ0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	2	Total Mg 2 2	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	4	Total 4	Cl 4	0	0
4	D	2	Total 2	Cl 2	0	0

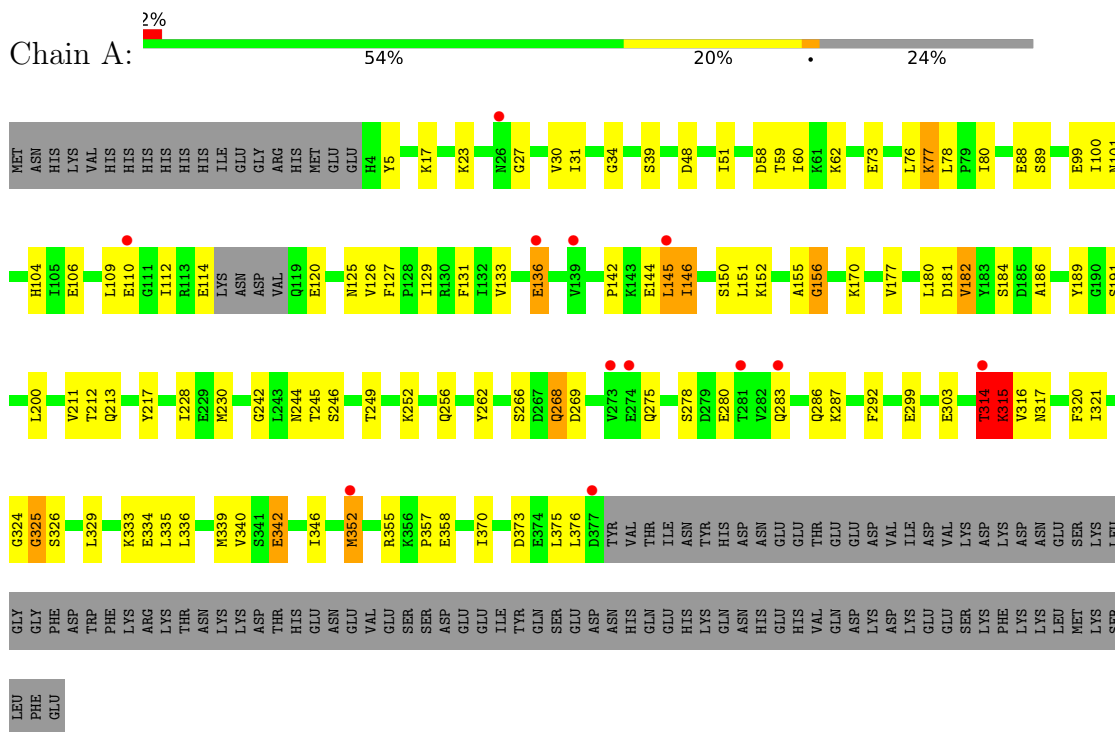
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total 136	O 136	0	0
5	B	49	Total 49	O 49	0	0
5	C	158	Total 158	O 158	0	0
5	D	85	Total 85	O 85	0	0

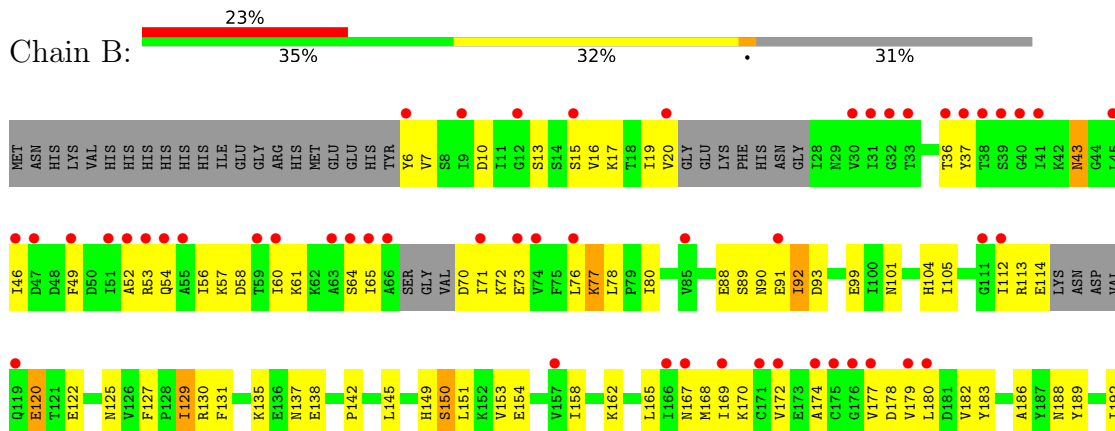
3 Residue-property plots

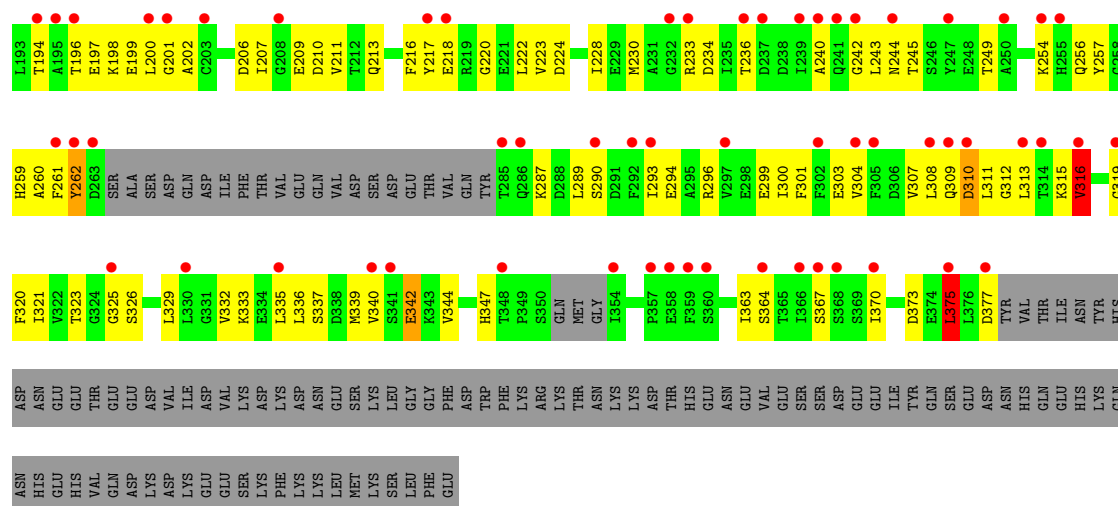
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cell division protein FtsA

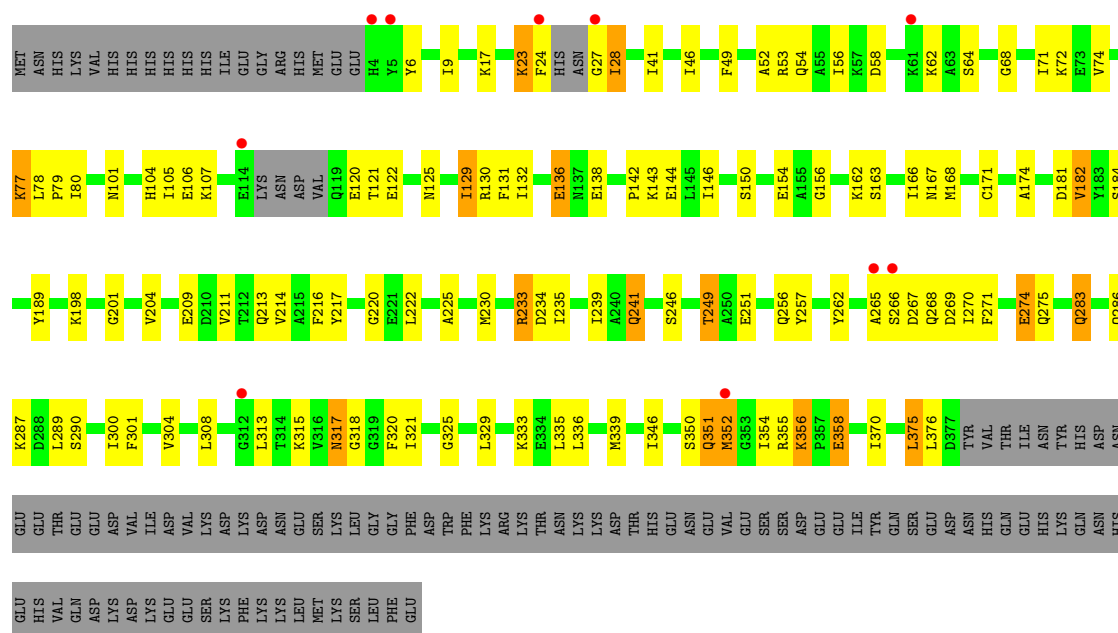


• Molecule 1: Cell division protein FtsA

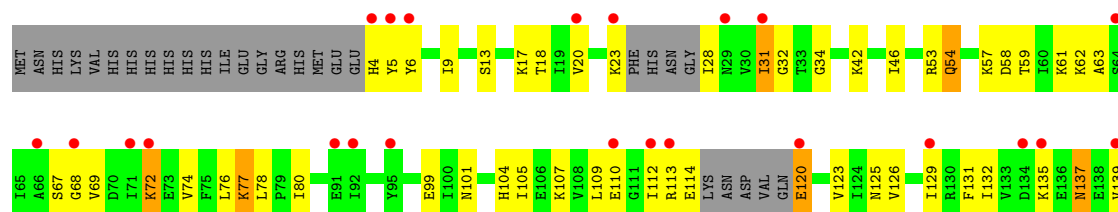


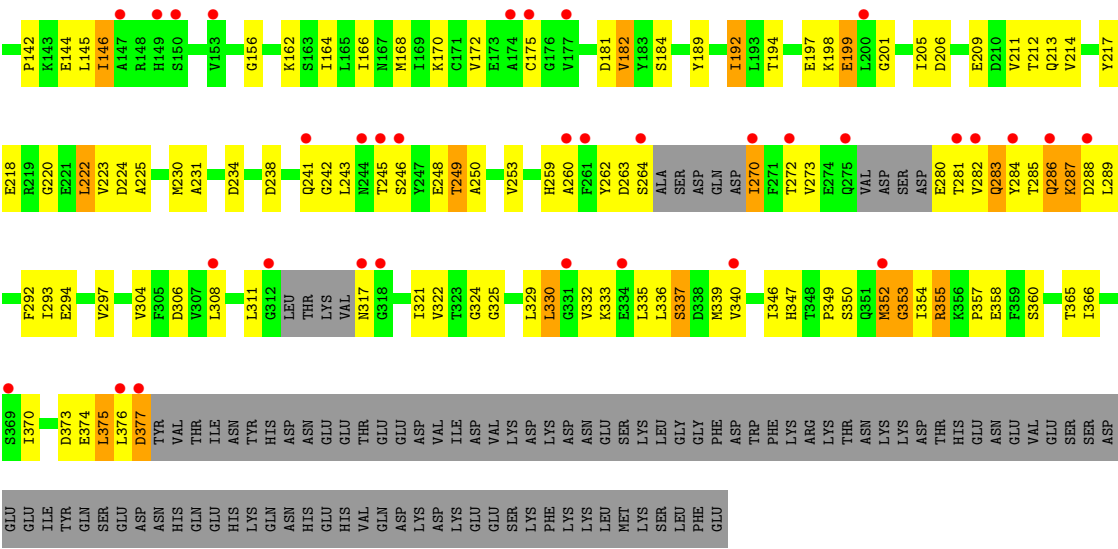


• Molecule 1: Cell division protein FtsA



• Molecule 1: Cell division protein FtsA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.26Å 102.74Å 105.86Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	37.98 – 2.20 37.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (37.98-2.20) 92.4 (37.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.289 0.234 , 0.290	Depositor DCC
R_{free} test set	3989 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11614	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: CL, MG, 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	0.45	0/2910	0.96	12/3935 (0.3%)
1	B	0.34	0/2619	0.87	5/3535 (0.1%)
1	C	0.45	0/2890	0.93	7/3906 (0.2%)
1	D	0.40	0/2766	0.95	10/3733 (0.3%)
All	All	0.41	0/11185	0.93	34/15109 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	353	GLY	N-CA-C	-10.87	100.67	114.37
1	A	129	ILE	N-CA-C	-9.10	102.99	111.45
1	A	150	SER	N-CA-C	7.94	120.20	108.60
1	D	289	LEU	N-CA-C	-7.36	102.95	112.23
1	D	129	ILE	N-CA-C	-7.32	105.97	111.90
1	A	146	ILE	N-CA-C	7.28	119.06	108.58
1	A	314	THR	N-CA-C	-6.93	101.89	110.41
1	C	150	SER	N-CA-C	6.70	118.39	108.60
1	C	351	GLN	N-CA-C	6.61	119.34	110.35
1	D	211	VAL	N-CA-C	6.52	117.86	108.48
1	A	256	GLN	N-CA-C	6.11	117.73	111.14
1	B	211	VAL	N-CA-C	5.94	116.86	108.36
1	C	174	ALA	N-CA-C	-5.92	106.03	113.20
1	D	68	GLY	N-CA-C	-5.85	107.99	115.42
1	D	360	SER	N-CA-C	5.71	117.50	111.28
1	A	325	GLY	N-CA-C	5.59	119.65	112.83
1	B	150	SER	N-CA-C	5.57	117.31	108.79
1	D	365	THR	N-CA-C	-5.50	105.36	111.36
1	A	39	SER	N-CA-C	-5.47	105.83	112.88
1	C	318	GLY	N-CA-C	-5.46	107.55	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	GLY	N-CA-C	-5.37	101.19	112.04
1	C	129	ILE	N-CA-C	-5.35	106.96	111.56
1	A	211	VAL	N-CA-C	5.34	116.17	108.48
1	C	211	VAL	N-CA-C	5.33	116.41	108.46
1	D	145	LEU	N-CA-C	-5.31	101.51	109.95
1	D	146	ILE	N-CA-C	5.28	115.70	107.99
1	D	156	GLY	N-CA-C	-5.22	101.42	110.71
1	B	256	GLN	N-CA-C	5.22	118.80	112.23
1	C	156	GLY	N-CA-C	-5.21	101.51	112.04
1	B	129	ILE	N-CA-C	-5.17	106.65	111.45
1	A	191	SER	N-CA-C	5.16	118.84	112.54
1	A	155	ALA	N-CA-C	5.11	118.06	110.14
1	B	375	LEU	N-CA-C	-5.10	108.80	114.62
1	A	27	GLY	N-CA-C	5.02	117.81	110.63

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	2871	0	2813	74	0
1	B	2590	0	2567	158	0
1	C	2853	0	2799	104	0
1	D	2733	0	2688	137	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	31	0	13	2	0
3	B	31	0	13	6	0
3	C	31	0	13	2	0
3	D	31	0	13	3	0
4	A	2	0	0	1	0
4	B	1	0	0	0	0
4	C	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	1	0
5	A	136	0	0	2	0
5	B	49	0	0	7	0
5	C	158	0	0	7	0
5	D	85	0	0	7	0
All	All	11614	0	10919	463	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 (463) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ASN:HD22	1:C:317:ASN:H	1.05	1.01
1:C:101:ASN:H	1:C:104:HIS:HD2	1.13	0.95
1:C:335:LEU:HG	1:C:339:MET:HE2	1.49	0.93
1:D:101:ASN:H	1:D:104:HIS:HD2	1.15	0.93
1:A:329:LEU:HD13	3:A:503:ANP:H2	1.54	0.89
1:B:213:GLN:HB2	5:B:649:HOH:O	1.73	0.87
1:D:17:LYS:HE2	1:D:358:GLU:HB2	1.56	0.87
4:C:504:CL:CL	5:C:680:HOH:O	2.30	0.85
1:C:265:ALA:HB3	1:C:287:LYS:HG2	1.57	0.84
1:B:167:ASN:HB3	5:B:647:HOH:O	1.78	0.83
1:A:80:ILE:H	1:A:213:GLN:NE2	1.77	0.83
1:D:58:ASP:O	1:D:62:LYS:HG2	1.79	0.83
1:B:335:LEU:HG	1:B:339:MET:HE2	1.61	0.82
1:A:142:PRO:O	1:A:145:LEU:HD22	1.81	0.81
1:D:352:MET:HA	1:D:355:ARG:HG3	1.63	0.81
1:B:61:LYS:O	1:B:65:ILE:HG13	1.81	0.81
1:A:314:THR:HG23	5:A:706:HOH:O	1.79	0.81
1:C:130:ARG:HD2	1:C:138:GLU:OE1	1.81	0.80
1:C:317:ASN:H	1:C:317:ASN:ND2	1.80	0.80
1:A:246:SER:OG	1:A:249:THR:HG22	1.82	0.79
1:D:101:ASN:H	1:D:104:HIS:CD2	1.98	0.79
1:A:125:ASN:HD21	1:A:184:SER:H	1.31	0.78
4:D:504:CL:CL	5:D:673:HOH:O	2.37	0.78
1:C:80:ILE:H	1:C:213:GLN:NE2	1.81	0.78
1:D:329:LEU:HD13	3:D:503:ANP:H2	1.66	0.77
1:C:246:SER:OG	1:C:249:THR:HG23	1.85	0.76
1:D:32:GLY:HA3	1:D:67:SER:HB3	1.67	0.76
1:C:130:ARG:NH2	1:C:130:ARG:HB2	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LYS:HB3	1:C:220:GLY:HA2	1.69	0.75
1:B:88:GLU:HG2	1:B:112:ILE:HG23	1.70	0.74
1:D:101:ASN:N	1:D:104:HIS:HD2	1.86	0.73
1:B:101:ASN:H	1:B:104:HIS:HD2	1.37	0.73
1:B:309:GLN:HG3	1:C:27:GLY:HA2	1.70	0.72
1:D:53:ARG:NH2	1:D:54:GLN:HE21	1.87	0.72
1:B:7:VAL:HG22	1:B:20:VAL:HG22	1.70	0.72
1:D:352:MET:SD	1:D:353:GLY:N	2.62	0.72
1:A:77:LYS:C	1:A:77:LYS:HD2	2.15	0.71
1:A:352:MET:HA	1:A:355:ARG:HE	1.55	0.71
1:D:242:GLY:HA3	1:D:292:PHE:CZ	2.26	0.71
1:D:246:SER:OG	1:D:249:THR:HG22	1.90	0.71
1:B:80:ILE:H	1:B:213:GLN:NE2	1.88	0.70
1:C:17:LYS:HE2	1:C:358:GLU:HB2	1.74	0.70
1:D:4:HIS:CG	1:D:5:TYR:H	2.08	0.70
1:D:336:LEU:O	1:D:340:VAL:HG22	1.91	0.70
1:A:245:THR:OG1	1:A:249:THR:HG21	1.93	0.69
1:D:270:ILE:N	1:D:270:ILE:HD12	2.07	0.69
1:C:125:ASN:HD21	1:C:184:SER:H	1.39	0.69
1:B:80:ILE:H	1:B:213:GLN:HE22	1.39	0.69
1:D:241:GLN:HG3	5:D:676:HOH:O	1.92	0.69
1:C:41:ILE:HD13	1:C:46:ILE:HA	1.73	0.68
1:C:335:LEU:HG	1:C:339:MET:CE	2.22	0.68
1:A:335:LEU:HG	1:A:339:MET:CE	2.23	0.68
1:A:101:ASN:H	1:A:104:HIS:HD2	1.41	0.68
1:D:168:MET:O	1:D:172:VAL:HG23	1.95	0.67
1:B:46:ILE:HG13	1:B:168:MET:HE2	1.75	0.67
1:B:52:ALA:O	1:B:56:ILE:HG13	1.95	0.67
1:D:57:LYS:HE2	1:D:61:LYS:HZ1	1.60	0.66
1:A:23:LYS:HD3	1:A:370:ILE:HG23	1.78	0.65
1:B:43:ASN:N	1:B:43:ASN:HD22	1.93	0.65
1:D:6:TYR:CE2	1:D:370:ILE:HG12	2.32	0.65
1:D:262:TYR:C	1:D:264:SER:H	2.05	0.65
1:B:49:PHE:CE2	1:B:170:LYS:HE3	2.32	0.64
1:B:183:TYR:HB3	1:B:188:ASN:HD21	1.63	0.64
1:B:46:ILE:HD11	1:B:168:MET:HG3	1.80	0.64
1:A:112:ILE:C	1:A:114:GLU:H	2.05	0.64
1:C:120:GLU:HG3	1:C:121:THR:HG23	1.78	0.64
1:D:120:GLU:O	1:D:162:LYS:HB2	1.98	0.64
1:D:57:LYS:HE2	1:D:61:LYS:NZ	2.12	0.63
1:C:267:ASP:HB2	1:C:287:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ILE:O	1:C:72:LYS:HD2	1.98	0.63
1:D:53:ARG:NH2	1:D:54:GLN:HG2	2.14	0.63
1:D:352:MET:HB2	1:D:355:ARG:CZ	2.29	0.63
1:B:210:ASP:OD1	1:B:233:ARG:HD3	1.98	0.63
1:D:262:TYR:HB2	1:D:294:GLU:OE2	1.99	0.63
1:A:335:LEU:HG	1:A:339:MET:HE3	1.80	0.62
1:B:307:VAL:HA	1:B:310:ASP:OD2	1.99	0.62
1:B:73:GLU:HB3	1:B:180:LEU:HD21	1.82	0.62
1:A:244:ASN:HD22	1:A:275:GLN:NE2	1.98	0.61
1:D:105:ILE:HG21	1:D:375:LEU:CD2	2.30	0.61
1:D:125:ASN:HD21	1:D:184:SER:H	1.47	0.61
1:D:270:ILE:HA	1:D:285:THR:HA	1.82	0.61
1:B:189:TYR:HB2	1:B:217:TYR:OH	2.00	0.61
1:B:196:THR:HG22	1:B:200:LEU:HD12	1.82	0.61
1:B:293:ILE:CG2	1:B:329:LEU:HD21	2.31	0.61
1:C:274:GLU:HG2	1:C:275:GLN:N	2.14	0.61
1:D:262:TYR:O	1:D:287:LYS:HE3	1.99	0.61
1:D:373:ASP:O	1:D:377:ASP:HB2	2.00	0.61
1:B:234:ASP:HB3	1:B:296:ARG:HH21	1.65	0.61
1:D:18:THR:HB	1:D:59:THR:HG22	1.81	0.61
1:C:266:SER:OG	1:C:286:GLN:HB3	2.02	0.60
1:C:315:LYS:HE3	1:C:317:ASN:HD21	1.65	0.60
1:D:125:ASN:ND2	1:D:184:SER:H	2.00	0.60
1:B:64:SER:HB2	1:B:71:ILE:HD13	1.83	0.60
1:B:92:ILE:HG22	1:B:151:LEU:HB3	1.81	0.60
1:B:333:LYS:HE3	1:B:344:VAL:O	2.01	0.60
1:C:46:ILE:HG13	5:C:680:HOH:O	2.02	0.60
1:B:6:TYR:CZ	1:B:370:ILE:HG12	2.37	0.60
1:A:189:TYR:HB2	1:A:217:TYR:OH	2.02	0.60
1:B:216:PHE:HB3	1:B:313:LEU:HD13	1.83	0.60
1:D:6:TYR:CZ	1:D:370:ILE:HG12	2.37	0.59
1:B:13:SER:N	3:B:502:ANP:HNB1	1.99	0.59
1:D:285:THR:OG1	1:D:288:ASP:HB2	2.02	0.59
1:B:320:PHE:CE2	1:B:340:VAL:HG21	2.36	0.59
1:B:197:GLU:HB3	1:B:202:ALA:HB2	1.83	0.59
1:C:235:ILE:O	1:C:239:ILE:HG13	2.01	0.59
1:A:352:MET:O	1:A:352:MET:SD	2.61	0.59
1:C:329:LEU:HD13	3:C:502:ANP:H2	1.84	0.59
1:C:301:PHE:HD2	1:C:339:MET:HE1	1.66	0.59
1:D:77:LYS:HD3	5:D:640:HOH:O	2.02	0.59
1:B:122:GLU:HB2	1:B:162:LYS:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLN:HG2	5:C:685:HOH:O	2.02	0.59
1:B:194:THR:OG1	1:B:197:GLU:HG3	2.03	0.59
1:B:312:GLY:HA3	1:C:350:SER:HB2	1.83	0.59
1:C:317:ASN:HD22	1:C:317:ASN:N	1.87	0.59
1:D:280:GLU:HG2	1:D:281:THR:H	1.68	0.59
1:B:309:GLN:CG	1:C:27:GLY:HA2	2.33	0.58
1:B:206:ASP:HB3	5:B:649:HOH:O	2.03	0.58
1:D:31:ILE:HD13	1:D:31:ILE:H	1.69	0.58
1:B:188:ASN:HB3	1:B:364:SER:OG	2.03	0.58
1:D:72:LYS:NZ	1:D:72:LYS:HB2	2.18	0.58
1:B:179:VAL:HG23	1:B:179:VAL:O	2.04	0.58
1:B:335:LEU:HG	1:B:339:MET:CE	2.33	0.58
1:D:242:GLY:O	1:D:243:LEU:HD23	2.04	0.58
1:D:245:THR:HG21	1:D:273:VAL:HG21	1.86	0.58
1:D:280:GLU:HG2	1:D:281:THR:N	2.19	0.58
1:A:352:MET:HB3	1:A:355:ARG:HH21	1.69	0.57
1:B:207:ILE:HB	1:B:326:SER:HB2	1.85	0.57
1:D:250:ALA:O	1:D:253:VAL:HG22	2.03	0.57
1:B:46:ILE:HD12	5:B:647:HOH:O	2.02	0.57
1:C:125:ASN:ND2	1:C:184:SER:H	2.01	0.57
1:A:60:ILE:HD13	1:A:177:VAL:HG11	1.85	0.57
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.69	0.57
1:D:109:LEU:HD22	1:D:126:VAL:HG12	1.87	0.57
1:B:168:MET:O	1:B:172:VAL:HG23	2.04	0.57
1:D:248:GLU:CD	1:D:248:GLU:H	2.11	0.57
1:A:125:ASN:ND2	1:A:184:SER:H	2.01	0.57
1:D:105:ILE:HD11	1:D:142:PRO:HG2	1.87	0.57
1:B:172:VAL:O	1:B:177:VAL:HG12	2.05	0.56
1:D:282:VAL:HG12	1:D:283:GLN:N	2.21	0.56
1:D:321:ILE:HD12	1:D:321:ILE:N	2.21	0.56
1:B:127:PHE:CE2	1:B:129:ILE:HD11	2.40	0.56
1:C:49:PHE:CZ	1:C:171:CYS:HA	2.41	0.56
1:D:53:ARG:HG2	1:D:175:CYS:SG	2.46	0.56
1:B:112:ILE:C	1:B:114:GLU:H	2.12	0.56
1:A:326:SER:O	1:A:329:LEU:HB2	2.05	0.56
1:A:17:LYS:HE3	1:A:358:GLU:O	2.06	0.56
1:C:130:ARG:HB2	1:C:130:ARG:HH21	1.70	0.56
1:A:316:VAL:HB	1:A:342:GLU:OE1	2.05	0.55
1:A:320:PHE:CE2	1:A:340:VAL:HG21	2.41	0.55
1:D:201:GLY:HA2	1:D:218:GLU:HG2	1.88	0.55
1:B:216:PHE:CD1	1:B:313:LEU:HD13	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLY:O	1:A:357:PRO:HB2	2.05	0.55
1:B:122:GLU:OE2	1:B:162:LYS:HE3	2.07	0.55
1:C:266:SER:O	1:C:267:ASP:HB3	2.07	0.55
1:D:67:SER:C	1:D:69:VAL:H	2.14	0.55
1:B:342:GLU:CD	1:B:342:GLU:H	2.13	0.55
1:D:4:HIS:CD2	1:D:5:TYR:H	2.24	0.55
1:D:370:ILE:O	1:D:374:GLU:HG3	2.05	0.55
1:B:167:ASN:HD22	1:B:167:ASN:N	2.04	0.55
1:C:77:LYS:HD2	1:C:77:LYS:C	2.32	0.55
1:B:70:ASP:O	1:B:72:LYS:HE2	2.07	0.55
1:D:166:ILE:O	1:D:170:LYS:HB2	2.07	0.55
1:D:105:ILE:HG21	1:D:375:LEU:HD22	1.88	0.55
1:B:194:THR:O	1:B:198:LYS:HG3	2.07	0.54
1:B:129:ILE:HB	1:B:154:GLU:O	2.08	0.54
1:B:209:GLU:CG	1:B:233:ARG:HB2	2.37	0.54
1:D:262:TYR:O	1:D:264:SER:N	2.37	0.54
1:D:325:GLY:HA3	3:D:503:ANP:O5'	2.07	0.54
1:B:135:LYS:HD3	1:C:269:ASP:CG	2.32	0.54
1:C:189:TYR:HB2	1:C:217:TYR:OH	2.08	0.54
1:A:133:VAL:HG21	1:A:145:LEU:HD21	1.89	0.54
1:B:77:LYS:O	1:B:77:LYS:HD3	2.08	0.54
1:B:321:ILE:HD12	1:B:321:ILE:N	2.23	0.54
1:D:214:VAL:HG21	1:D:304:VAL:HG13	1.90	0.54
1:B:78:LEU:HG	1:B:182:VAL:CG2	2.37	0.54
1:B:196:THR:HG22	1:B:200:LEU:CD1	2.38	0.54
1:C:101:ASN:H	1:C:104:HIS:CD2	2.06	0.54
1:C:131:PHE:CD2	1:C:142:PRO:HD3	2.43	0.54
1:A:78:LEU:HD12	1:A:182:VAL:CG1	2.38	0.54
1:D:260:ALA:O	1:D:294:GLU:HB2	2.08	0.54
1:C:230:MET:HA	1:C:234:ASP:OD2	2.08	0.53
1:B:92:ILE:HD13	1:B:93:ASP:N	2.23	0.53
1:D:222:LEU:HD23	1:D:223:VAL:N	2.24	0.53
1:C:122:GLU:HB2	1:C:162:LYS:HD3	1.91	0.53
1:D:286:GLN:C	1:D:288:ASP:H	2.16	0.53
1:D:375:LEU:HD13	1:D:376:LEU:CD1	2.39	0.53
1:A:170:LYS:NZ	1:B:99:GLU:OE2	2.33	0.53
1:B:315:LYS:CB	1:C:352:MET:HG2	2.39	0.53
1:D:99:GLU:CG	1:D:144:GLU:HA	2.38	0.53
1:D:249:THR:O	1:D:253:VAL:HG13	2.07	0.53
1:B:315:LYS:HB2	1:C:352:MET:HG2	1.90	0.53
1:D:201:GLY:HA2	1:D:217:TYR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HD12	1:A:146:ILE:N	2.23	0.53
1:B:201:GLY:HA2	1:B:217:TYR:O	2.09	0.53
1:B:90:ASN:HB2	1:B:112:ILE:HG12	1.90	0.53
1:B:57:LYS:HE3	1:B:61:LYS:HE3	1.91	0.52
1:B:101:ASN:N	1:B:104:HIS:HD2	2.07	0.52
1:D:346:ILE:HD12	1:D:346:ILE:N	2.25	0.52
1:B:76:LEU:HD22	1:B:172:VAL:HG21	1.90	0.52
1:B:10:ASP:O	1:B:16:VAL:HA	2.09	0.52
1:D:350:SER:O	1:D:355:ARG:NH1	2.42	0.52
1:C:49:PHE:CD1	1:D:144:GLU:HG3	2.45	0.52
1:B:150:SER:HB3	5:B:645:HOH:O	2.10	0.52
1:B:57:LYS:HE3	1:B:61:LYS:CE	2.39	0.51
1:B:308:LEU:HB3	1:B:313:LEU:O	2.09	0.51
1:D:304:VAL:O	1:D:308:LEU:HG	2.09	0.51
1:A:242:GLY:HA3	1:A:292:PHE:CZ	2.45	0.51
1:B:46:ILE:CD1	1:B:168:MET:HG3	2.41	0.51
1:C:320:PHE:C	1:C:321:ILE:HD12	2.36	0.51
1:A:333:LYS:HB2	1:A:346:ILE:CD1	2.40	0.51
1:A:242:GLY:HA3	1:A:292:PHE:CE1	2.45	0.51
1:B:13:SER:N	3:B:502:ANP:N3B	2.58	0.51
1:B:209:GLU:HG3	1:B:233:ARG:HB2	1.93	0.51
1:D:107:LYS:O	1:D:110:GLU:HG2	2.10	0.51
1:C:9:ILE:HD12	1:C:74:VAL:HG21	1.93	0.51
1:D:335:LEU:HG	1:D:339:MET:HE3	1.92	0.51
1:B:71:ILE:N	1:B:71:ILE:HD12	2.26	0.51
1:B:240:ALA:HA	1:B:245:THR:HG23	1.93	0.51
1:B:261:PHE:HA	1:B:294:GLU:OE2	2.11	0.51
1:C:143:LYS:O	1:C:144:GLU:HB2	2.09	0.51
1:A:78:LEU:HD12	1:A:182:VAL:HG11	1.92	0.51
1:B:125:ASN:HB2	1:B:158:ILE:HB	1.93	0.51
1:B:153:VAL:O	1:B:153:VAL:HG13	2.10	0.51
1:D:20:VAL:HG11	1:D:69:VAL:HG21	1.92	0.51
1:C:333:LYS:HB2	1:C:346:ILE:CD1	2.41	0.51
1:D:352:MET:HB2	1:D:355:ARG:NH2	2.25	0.51
1:C:189:TYR:HB3	1:C:204:VAL:HG21	1.92	0.51
1:D:192:ILE:HG13	1:D:347:HIS:CD2	2.45	0.51
1:B:15:SER:HB2	1:B:36:THR:O	2.11	0.51
1:B:77:LYS:HD3	1:B:77:LYS:C	2.35	0.51
1:D:286:GLN:HG3	1:D:287:LYS:N	2.26	0.51
1:B:131:PHE:CD2	1:B:142:PRO:HD3	2.47	0.50
1:C:64:SER:O	1:C:68:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ARG:HH22	1:D:54:GLN:HE21	1.57	0.50
1:D:105:ILE:HD11	1:D:142:PRO:CG	2.42	0.50
1:B:259:HIS:HB3	1:B:290:SER:OG	2.11	0.50
1:D:222:LEU:HD23	1:D:222:LEU:C	2.36	0.50
1:A:145:LEU:HD23	1:A:145:LEU:O	2.12	0.50
1:D:78:LEU:HG	1:D:182:VAL:HG13	1.93	0.50
1:D:375:LEU:HD22	1:D:376:LEU:HD12	1.94	0.50
1:B:300:ILE:O	1:B:304:VAL:HG23	2.12	0.50
1:B:316:VAL:HG12	1:B:319:GLY:O	2.12	0.50
1:C:249:THR:HG21	1:C:274:GLU:OE2	2.11	0.50
1:C:58:ASP:O	1:C:62:LYS:HG3	2.12	0.50
1:C:356:LYS:HB3	1:C:358:GLU:OE1	2.12	0.50
1:A:320:PHE:HE2	1:A:340:VAL:HG21	1.75	0.49
1:B:216:PHE:CB	1:B:313:LEU:HD13	2.41	0.49
1:C:78:LEU:CD1	1:C:182:VAL:HG11	2.42	0.49
1:B:168:MET:HE3	5:B:646:HOH:O	2.11	0.49
1:A:131:PHE:CD2	1:A:142:PRO:HD3	2.47	0.49
1:C:71:ILE:C	1:C:72:LYS:HD2	2.37	0.49
1:A:336:LEU:O	1:A:340:VAL:HG12	2.12	0.49
1:D:34:GLY:C	1:D:59:THR:HG23	2.37	0.49
1:A:80:ILE:H	1:A:213:GLN:HE22	1.60	0.49
1:D:28:ILE:HD13	1:D:366:ILE:HG22	1.95	0.49
1:D:131:PHE:HB2	1:D:139:VAL:O	2.13	0.49
1:D:4:HIS:CG	1:D:5:TYR:N	2.77	0.49
1:D:181:ASP:OD1	1:D:182:VAL:N	2.37	0.49
1:D:324:GLY:O	1:D:357:PRO:HB2	2.13	0.49
1:A:321:ILE:N	1:A:321:ILE:HD12	2.28	0.49
1:C:129:ILE:HB	1:C:154:GLU:O	2.12	0.49
1:C:201:GLY:HA2	1:C:217:TYR:O	2.13	0.48
1:D:270:ILE:N	1:D:270:ILE:CD1	2.76	0.48
1:B:293:ILE:HG21	1:B:329:LEU:HD21	1.95	0.48
1:A:109:LEU:HD22	1:A:126:VAL:HG12	1.94	0.48
1:B:186:ALA:O	1:B:222:LEU:HD22	2.12	0.48
1:D:80:ILE:HD13	1:D:225:ALA:HB1	1.95	0.48
1:A:262:TYR:CE1	1:A:287:LYS:HG2	2.49	0.48
1:A:325:GLY:HA3	3:A:503:ANP:O5'	2.13	0.48
1:C:78:LEU:HD12	1:C:182:VAL:HG11	1.96	0.48
1:C:101:ASN:N	1:C:104:HIS:HD2	1.96	0.48
1:C:265:ALA:CB	1:C:287:LYS:HG2	2.37	0.48
1:D:243:LEU:HD22	1:D:284:TYR:CE1	2.48	0.48
1:C:333:LYS:HB2	1:C:346:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLU:HG3	1:D:144:GLU:HA	1.96	0.48
1:D:329:LEU:O	1:D:332:VAL:HG23	2.13	0.48
1:B:13:SER:HB3	3:B:502:ANP:PG	2.53	0.48
1:B:13:SER:HB3	3:B:502:ANP:N3B	2.29	0.48
1:B:206:ASP:CB	5:B:649:HOH:O	2.60	0.48
1:C:301:PHE:CD2	1:C:339:MET:HE1	2.46	0.48
1:B:105:ILE:HG21	1:B:375:LEU:HD22	1.95	0.48
1:D:80:ILE:H	1:D:213:GLN:NE2	2.12	0.48
1:B:88:GLU:CG	1:B:112:ILE:HG23	2.41	0.48
1:D:245:THR:HB	1:D:249:THR:CG2	2.44	0.48
1:D:105:ILE:HG21	1:D:375:LEU:HD21	1.95	0.48
1:D:333:LYS:O	1:D:337:SER:HB2	2.14	0.48
1:B:46:ILE:HD11	1:B:168:MET:CG	2.44	0.47
1:B:120:GLU:CD	1:B:120:GLU:H	2.22	0.47
1:B:234:ASP:HB3	1:B:296:ARG:HE	1.79	0.47
1:B:240:ALA:HA	1:B:245:THR:CG2	2.44	0.47
1:C:52:ALA:O	1:C:56:ILE:HG13	2.15	0.47
1:B:236:THR:OG1	1:B:254:LYS:HE3	2.15	0.47
1:D:285:THR:O	1:D:288:ASP:HB3	2.14	0.47
1:A:5:TYR:CE1	1:A:31:ILE:HD13	2.50	0.47
1:D:230:MET:HA	1:D:234:ASP:OD2	2.14	0.47
1:A:106:GLU:HB2	1:A:376:LEU:HD22	1.96	0.47
1:A:127:PHE:CZ	1:A:156:GLY:HA3	2.50	0.47
1:B:53:ARG:HD2	1:B:174:ALA:HB1	1.96	0.47
1:D:135:LYS:NZ	1:D:135:LYS:HB3	2.30	0.47
1:B:260:ALA:O	1:B:294:GLU:HB2	2.14	0.47
1:C:130:ARG:HH21	1:C:130:ARG:CB	2.28	0.47
1:D:270:ILE:HG13	1:D:285:THR:HG22	1.96	0.47
1:B:49:PHE:HE2	1:B:170:LYS:HE3	1.77	0.47
1:A:77:LYS:HD2	1:A:78:LEU:N	2.30	0.46
1:B:91:GLU:OE1	1:B:135:LYS:NZ	2.43	0.46
1:D:107:LYS:HA	1:D:110:GLU:HG2	1.97	0.46
1:A:100:ILE:HD12	1:A:151:LEU:HD22	1.98	0.46
1:B:101:ASN:H	1:B:104:HIS:CD2	2.25	0.46
1:D:20:VAL:HG23	1:D:63:ALA:HB1	1.98	0.46
1:B:73:GLU:HB3	1:B:180:LEU:CD2	2.44	0.46
1:B:262:TYR:CE1	1:B:287:LYS:HB3	2.50	0.46
1:C:308:LEU:HB3	1:C:313:LEU:O	2.15	0.46
1:B:54:GLN:O	1:B:58:ASP:OD1	2.34	0.46
1:D:209:GLU:O	1:D:231:ALA:HB3	2.15	0.46
1:D:262:TYR:C	1:D:264:SER:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:SER:HB3	1:B:37:TYR:CD1	2.50	0.46
1:D:243:LEU:HD22	1:D:284:TYR:CD1	2.51	0.46
1:A:73:GLU:HB3	1:A:180:LEU:HG	1.98	0.46
1:A:200:LEU:O	1:A:317:ASN:HB2	2.16	0.46
1:B:188:ASN:O	1:B:364:SER:HB2	2.15	0.46
1:B:242:GLY:O	1:B:243:LEU:HD23	2.15	0.46
1:C:214:VAL:O	1:C:225:ALA:HB1	2.16	0.46
1:C:325:GLY:HA3	3:C:502:ANP:O5'	2.16	0.46
1:D:9:ILE:HD12	1:D:74:VAL:HG21	1.98	0.46
1:D:31:ILE:HD13	1:D:31:ILE:N	2.31	0.46
1:B:127:PHE:HE2	1:B:129:ILE:HD11	1.81	0.46
1:C:168:MET:HE3	5:C:754:HOH:O	2.15	0.46
1:D:246:SER:H	1:D:249:THR:CG2	2.28	0.46
1:A:320:PHE:C	1:A:321:ILE:HD12	2.41	0.46
1:B:7:VAL:HG21	1:B:71:ILE:HG13	1.96	0.46
1:B:224:ASP:OD1	1:B:311:LEU:HD22	2.16	0.46
1:D:282:VAL:CG1	1:D:283:GLN:N	2.79	0.46
1:A:230:MET:HE1	1:A:299:GLU:OE2	2.16	0.45
1:B:112:ILE:C	1:B:114:GLU:N	2.75	0.45
1:B:336:LEU:HA	1:B:339:MET:HE3	1.97	0.45
1:C:246:SER:HG	1:C:249:THR:HG23	1.81	0.45
1:D:280:GLU:N	5:D:670:HOH:O	2.48	0.45
1:D:317:ASN:N	5:D:666:HOH:O	2.49	0.45
1:B:301:PHE:CD2	1:B:339:MET:HE1	2.51	0.45
1:A:77:LYS:C	1:A:77:LYS:CD	2.83	0.45
1:D:132:ILE:N	1:D:132:ILE:HD12	2.31	0.45
1:C:239:ILE:HD13	1:C:289:LEU:HD11	1.99	0.45
1:D:224:ASP:OD1	1:D:311:LEU:HD22	2.17	0.45
1:D:164:ILE:O	1:D:168:MET:HG2	2.16	0.45
1:A:100:ILE:O	1:A:144:GLU:N	2.46	0.45
1:B:198:LYS:HB3	1:B:220:GLY:HA2	1.99	0.45
1:D:46:ILE:HG13	5:D:673:HOH:O	2.17	0.45
1:D:238:ASP:O	1:D:242:GLY:N	2.46	0.45
1:A:112:ILE:C	1:A:114:GLU:N	2.73	0.45
1:C:300:ILE:O	1:C:304:VAL:HG23	2.17	0.45
1:B:6:TYR:O	1:B:20:VAL:HA	2.16	0.45
1:C:132:ILE:HD13	1:C:138:GLU:HA	1.99	0.45
1:B:57:LYS:HG2	1:B:61:LYS:HE3	1.98	0.45
1:C:270:ILE:HG22	1:C:271:PHE:N	2.32	0.45
1:C:321:ILE:HD12	1:C:321:ILE:N	2.31	0.45
1:D:322:VAL:O	1:D:346:ILE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:THR:O	1:A:315:LYS:HB3	2.16	0.44
1:B:336:LEU:O	1:B:340:VAL:HG12	2.17	0.44
1:D:272:THR:HG22	1:D:273:VAL:N	2.33	0.44
1:B:218:GLU:H	1:B:223:VAL:HG23	1.81	0.44
1:D:349:PRO:HB2	1:D:354:ILE:O	2.16	0.44
1:C:266:SER:O	1:C:267:ASP:CB	2.65	0.44
1:C:283:GLN:HG2	5:C:706:HOH:O	2.17	0.44
1:B:243:LEU:O	1:B:244:ASN:C	2.60	0.44
1:B:296:ARG:O	1:B:299:GLU:HB3	2.16	0.44
1:C:79:PRO:HA	1:C:213:GLN:HE22	1.81	0.44
1:B:198:LYS:HE2	1:B:220:GLY:O	2.17	0.44
1:B:218:GLU:OE1	1:C:355:ARG:NH2	2.44	0.44
1:D:199:GLU:HG2	1:D:220:GLY:N	2.33	0.44
1:B:73:GLU:OE1	1:B:178:ASP:HB2	2.17	0.44
1:B:13:SER:HB3	3:B:502:ANP:HNB1	1.83	0.43
1:B:165:LEU:O	1:B:169:ILE:HG13	2.18	0.43
1:B:216:PHE:CD1	1:B:313:LEU:HD22	2.53	0.43
1:B:234:ASP:HB3	1:B:296:ARG:NH2	2.31	0.43
1:B:19:ILE:HG22	1:B:20:VAL:N	2.33	0.43
1:A:278:SER:C	1:A:280:GLU:H	2.27	0.43
1:C:163:SER:O	1:C:167:ASN:ND2	2.51	0.43
1:C:317:ASN:ND2	1:C:317:ASN:N	2.52	0.43
1:A:30:VAL:O	1:A:352:MET:HE1	2.18	0.43
1:A:58:ASP:O	1:A:62:LYS:HG3	2.17	0.43
1:B:56:ILE:O	1:B:60:ILE:HG13	2.19	0.43
1:D:198:LYS:HG2	1:D:220:GLY:HA2	2.00	0.43
1:B:261:PHE:O	1:B:262:TYR:C	2.61	0.43
1:C:53:ARG:NH1	1:C:54:GLN:NE2	2.66	0.43
1:D:13:SER:N	3:D:503:ANP:HNB1	2.17	0.43
1:B:303:GLU:O	1:B:307:VAL:HG23	2.19	0.43
1:D:189:TYR:HB2	1:D:217:TYR:OH	2.19	0.43
1:A:275:GLN:NE2	5:A:619:HOH:O	2.43	0.42
1:B:321:ILE:CG2	1:B:347:HIS:HB2	2.49	0.42
1:C:23:LYS:O	1:C:24:PHE:C	2.62	0.42
1:C:78:LEU:HD12	1:C:182:VAL:CG1	2.49	0.42
1:B:301:PHE:HD2	1:B:339:MET:HE1	1.85	0.42
1:C:146:ILE:HD12	1:C:146:ILE:N	2.34	0.42
1:C:266:SER:C	1:C:268:GLN:H	2.27	0.42
1:A:48:ASP:OD1	1:A:51:ILE:HG13	2.19	0.42
1:A:120:GLU:HG3	1:C:270:ILE:HB	2.01	0.42
1:C:256:GLN:HG2	1:C:257:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PHE:CD1	1:C:313:LEU:HD13	2.54	0.42
1:D:206:ASP:O	1:D:212:THR:HA	2.20	0.42
1:A:152:LYS:HE3	4:A:505:CL:CL	2.57	0.42
1:B:364:SER:HA	1:B:367:SER:HB3	2.02	0.42
1:A:217:TYR:CD1	1:A:217:TYR:N	2.86	0.42
1:B:131:PHE:O	1:B:138:GLU:HA	2.20	0.42
1:D:72:LYS:HB2	1:D:72:LYS:HZ2	1.82	0.42
1:D:222:LEU:C	1:D:222:LEU:CD2	2.93	0.42
1:A:186:ALA:O	1:A:217:TYR:OH	2.29	0.42
1:B:89:SER:HA	1:B:153:VAL:O	2.20	0.42
1:C:80:ILE:H	1:C:213:GLN:HE22	1.64	0.42
1:C:106:GLU:OE1	1:C:376:LEU:HD13	2.19	0.42
1:D:205:ILE:CD1	1:D:304:VAL:HG11	2.50	0.42
1:B:120:GLU:O	1:B:162:LYS:HG3	2.20	0.42
1:B:206:ASP:HA	1:B:323:THR:O	2.20	0.42
1:B:325:GLY:HA3	3:B:502:ANP:O5'	2.19	0.42
1:C:6:TYR:CE2	1:C:23:LYS:HG2	2.54	0.42
1:C:262:TYR:CD1	1:C:262:TYR:C	2.98	0.42
1:D:28:ILE:N	5:D:677:HOH:O	2.53	0.42
1:A:88:GLU:OE1	1:A:89:SER:N	2.40	0.41
1:B:129:ILE:HG22	1:B:130:ARG:NH1	2.34	0.41
1:B:209:GLU:HG2	1:B:233:ARG:HB2	2.01	0.41
1:D:31:ILE:O	1:D:67:SER:HA	2.20	0.41
1:D:112:ILE:C	1:D:114:GLU:H	2.26	0.41
1:A:228:ILE:HD13	1:A:303:GLU:HB3	2.03	0.41
1:B:92:ILE:HD13	1:B:93:ASP:H	1.84	0.41
1:B:228:ILE:HD13	1:B:303:GLU:HB3	2.02	0.41
1:C:28:ILE:HD11	1:C:370:ILE:HD12	2.03	0.41
1:D:293:ILE:O	1:D:297:VAL:HG23	2.21	0.41
1:A:99:GLU:HG2	1:A:144:GLU:HA	2.00	0.41
1:C:6:TYR:HE1	5:C:694:HOH:O	2.03	0.41
1:C:267:ASP:HB2	1:C:287:LYS:CE	2.47	0.41
1:D:34:GLY:O	1:D:59:THR:HG23	2.20	0.41
1:D:194:THR:OG1	1:D:197:GLU:HG3	2.20	0.41
1:D:259:HIS:CD2	1:D:330:LEU:HD22	2.55	0.41
1:A:78:LEU:CD1	1:A:182:VAL:HG11	2.50	0.41
1:B:137:ASN:C	1:B:137:ASN:HD22	2.28	0.41
1:B:329:LEU:O	1:B:332:VAL:HG23	2.20	0.41
1:B:373:ASP:O	1:B:377:ASP:OD2	2.39	0.41
1:D:113:ARG:HG2	1:D:123:VAL:HG11	2.03	0.41
1:A:106:GLU:O	1:A:110:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ILE:H	1:B:168:MET:HE2	1.85	0.41
1:B:192:ILE:HB	1:B:347:HIS:NE2	2.36	0.41
1:B:257:TYR:O	1:B:289:LEU:HD23	2.21	0.41
1:C:53:ARG:HH12	1:C:54:GLN:HE22	1.68	0.41
1:C:105:ILE:HG21	1:C:375:LEU:CD2	2.51	0.41
1:C:262:TYR:HA	1:C:290:SER:OG	2.21	0.41
1:B:167:ASN:O	1:B:170:LYS:HB3	2.21	0.41
1:C:209:GLU:O	1:C:233:ARG:HB3	2.21	0.41
1:C:315:LYS:HE3	1:C:317:ASN:ND2	2.34	0.41
1:C:336:LEU:HA	1:C:339:MET:HE3	2.03	0.41
1:D:286:GLN:C	1:D:288:ASP:N	2.79	0.41
1:A:34:GLY:C	1:A:59:THR:HG23	2.46	0.40
1:A:100:ILE:HB	1:A:142:PRO:O	2.21	0.40
1:A:266:SER:HB3	1:A:286:GLN:NE2	2.36	0.40
1:A:268:GLN:OE1	1:A:268:GLN:HA	2.21	0.40
1:C:351:GLN:HB2	1:C:354:ILE:HD11	2.02	0.40
1:B:73:GLU:HB3	1:B:180:LEU:CG	2.52	0.40
1:C:129:ILE:HD11	5:C:742:HOH:O	2.21	0.40
1:C:166:ILE:CG2	1:D:146:ILE:HD12	2.52	0.40
1:D:245:THR:HB	1:D:249:THR:HG21	2.04	0.40
1:A:146:ILE:N	1:A:146:ILE:CD1	2.85	0.40
1:B:149:HIS:HB3	1:C:268:GLN:HB3	2.04	0.40
1:B:262:TYR:N	1:B:294:GLU:OE2	2.51	0.40
1:D:248:GLU:CD	1:D:248:GLU:N	2.79	0.40
1:B:76:LEU:O	1:B:182:VAL:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	366/484 (76%)	350 (96%)	14 (4%)	2 (0%)	24 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	322/484 (66%)	297 (92%)	21 (6%)	4 (1%)	10	8
1	C	362/484 (75%)	343 (95%)	17 (5%)	2 (1%)	21	23
1	D	340/484 (70%)	308 (91%)	28 (8%)	4 (1%)	10	8
All	All	1390/1936 (72%)	1298 (93%)	80 (6%)	12 (1%)	14	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	137	ASN
1	D	263	ASP
1	A	136	GLU
1	A	315	LYS
1	B	262	TYR
1	D	286	GLN
1	B	230	MET
1	C	28	ILE
1	C	136	GLU
1	B	113	ARG
1	D	287	LYS
1	B	316	VAL

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	321/432 (74%)	303 (94%)	18 (6%)	19	24
1	B	290/432 (67%)	276 (95%)	14 (5%)	23	30
1	C	319/432 (74%)	301 (94%)	18 (6%)	19	24
1	D	305/432 (71%)	282 (92%)	23 (8%)	12	14
All	All	1235/1728 (72%)	1162 (94%)	73 (6%)	18	22

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	77	LYS
1	A	136	GLU
1	A	145	LEU
1	A	181	ASP
1	A	182	VAL
1	A	212	THR
1	A	252	LYS
1	A	268	GLN
1	A	269	ASP
1	A	283	GLN
1	A	314	THR
1	A	315	LYS
1	A	334	GLU
1	A	342	GLU
1	A	352	MET
1	A	373	ASP
1	A	375	LEU
1	B	17	LYS
1	B	43	ASN
1	B	77	LYS
1	B	92	ILE
1	B	120	GLU
1	B	145	LEU
1	B	199	GLU
1	B	249	THR
1	B	310	ASP
1	B	316	VAL
1	B	337	SER
1	B	342	GLU
1	B	363	ILE
1	B	375	LEU
1	C	23	LYS
1	C	77	LYS
1	C	107	LYS
1	C	136	GLU
1	C	181	ASP
1	C	182	VAL
1	C	222	LEU
1	C	233	ARG
1	C	241	GLN
1	C	249	THR
1	C	251	GLU

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Mol	Chain	Res	Type
1	C	274	GLU
1	C	283	GLN
1	C	317	ASN
1	C	352	MET
1	C	356	LYS
1	C	358	GLU
1	C	375	LEU
1	D	23	LYS
1	D	31	ILE
1	D	42	LYS
1	D	54	GLN
1	D	72	LYS
1	D	76	LEU
1	D	77	LYS
1	D	120	GLU
1	D	137	ASN
1	D	182	VAL
1	D	192	ILE
1	D	199	GLU
1	D	222	LEU
1	D	249	THR
1	D	270	ILE
1	D	283	GLN
1	D	306	ASP
1	D	330	LEU
1	D	337	SER
1	D	352	MET
1	D	355	ARG
1	D	375	LEU
1	D	377	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	54	GLN
1	A	90	ASN
1	A	104	HIS
1	A	119	GLN
1	A	125	ASN
1	A	137	ASN
1	A	213	GLN

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Mol	Chain	Res	Type
1	A	244	ASN
1	A	256	GLN
1	A	275	GLN
1	A	286	GLN
1	A	309	GLN
1	A	317	ASN
1	B	43	ASN
1	B	54	GLN
1	B	90	ASN
1	B	104	HIS
1	B	137	ASN
1	B	161	GLN
1	B	167	ASN
1	B	188	ASN
1	B	213	GLN
1	B	256	GLN
1	B	286	GLN
1	B	317	ASN
1	C	35	GLN
1	C	54	GLN
1	C	90	ASN
1	C	104	HIS
1	C	119	GLN
1	C	125	ASN
1	C	137	ASN
1	C	161	GLN
1	C	213	GLN
1	C	317	ASN
1	D	4	HIS
1	D	29	ASN
1	D	35	GLN
1	D	54	GLN
1	D	90	ASN
1	D	104	HIS
1	D	125	ASN
1	D	167	ASN
1	D	213	GLN

5.3.3 RNA ⓘ

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 19 ligands modelled in this entry, 15 are monoatomic - leaving 4 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$
3	ANP	D	503	2	33,33,33	2.52	8 (24%)	45,52,52	1.90	10 (22%)
3	ANP	B	502	2	33,33,33	3.15	8 (24%)	45,52,52	1.87	8 (17%)
3	ANP	A	503	2	33,33,33	2.83	7 (21%)	45,52,52	1.90	9 (20%)
3	ANP	C	502	2	33,33,33	2.31	9 (27%)	45,52,52	1.80	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	D	503	2	-	3/18/38/38	0/3/3/3
3	ANP	B	502	2	-	3/18/38/38	0/3/3/3
3	ANP	A	503	2	-	6/18/38/38	0/3/3/3
3	ANP	C	502	2	-	3/18/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ANP	PG-O1G	10.74	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ANP	PB-O1B	10.72	1.62	1.46
3	D	503	ANP	PG-O1G	10.65	1.62	1.46
3	A	503	ANP	PG-O1G	10.02	1.61	1.46
3	C	502	ANP	PG-O1G	9.67	1.60	1.46
3	A	503	ANP	PB-O1B	9.63	1.60	1.46
3	D	503	ANP	PA-O3A	5.61	1.65	1.59
3	B	502	ANP	PA-O3A	5.32	1.65	1.59
3	C	502	ANP	PA-O3A	4.35	1.64	1.59
3	A	503	ANP	PB-O3A	4.05	1.64	1.59
3	B	502	ANP	PB-O3A	4.00	1.64	1.59
3	C	502	ANP	PB-O3A	3.56	1.63	1.59
3	B	502	ANP	PB-O2B	-3.20	1.48	1.56
3	A	503	ANP	PG-O3G	-3.11	1.48	1.56
3	D	503	ANP	PG-O2G	-3.05	1.48	1.56
3	B	502	ANP	PG-N3B	3.02	1.71	1.63
3	A	503	ANP	PA-O3A	3.01	1.62	1.59
3	D	503	ANP	PB-O3A	2.97	1.62	1.59
3	B	502	ANP	PG-O3G	-2.86	1.49	1.56
3	A	503	ANP	PB-O2B	-2.85	1.49	1.56
3	D	503	ANP	PA-O1A	2.68	1.60	1.50
3	C	502	ANP	PG-O2G	-2.61	1.49	1.56
3	C	502	ANP	PA-O1A	2.57	1.59	1.50
3	A	503	ANP	PG-N3B	2.56	1.70	1.63
3	D	503	ANP	PB-N3B	2.45	1.69	1.63
3	C	502	ANP	PB-N3B	2.27	1.69	1.63
3	C	502	ANP	C5-C4	2.20	1.43	1.39
3	C	502	ANP	PG-N3B	2.07	1.68	1.63
3	C	502	ANP	C5-N7	-2.06	1.35	1.39
3	B	502	ANP	PB-N3B	2.05	1.68	1.63
3	D	503	ANP	C5-N7	-2.03	1.35	1.39
3	D	503	ANP	C6-N6	2.03	1.39	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	ANP	C5-C4-N3	-5.29	119.44	126.72
3	B	502	ANP	C5-C4-N3	-5.27	119.46	126.72
3	D	503	ANP	C5-C4-N3	-5.12	119.67	126.72
3	C	502	ANP	C5-C4-N3	-5.05	119.77	126.72
3	B	502	ANP	N3-C2-N1	-4.80	121.32	128.58
3	D	503	ANP	N3-C2-N1	-4.69	121.48	128.58
3	A	503	ANP	N3-C2-N1	-4.61	121.60	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	ANP	N3-C2-N1	-4.53	121.73	128.58
3	A	503	ANP	N3-C4-N9	4.51	134.84	127.17
3	B	502	ANP	N3-C4-N9	4.51	134.83	127.17
3	D	503	ANP	N3-C4-N9	4.32	134.51	127.17
3	C	502	ANP	N3-C4-N9	4.24	134.37	127.17
3	B	502	ANP	C2-N3-C4	3.88	121.31	111.83
3	A	503	ANP	C5-N7-C8	3.82	109.46	103.45
3	D	503	ANP	C5-N7-C8	3.81	109.44	103.45
3	C	502	ANP	C5-N7-C8	3.79	109.40	103.45
3	D	503	ANP	C2-N3-C4	3.78	121.07	111.83
3	A	503	ANP	C2-N3-C4	3.77	121.04	111.83
3	B	502	ANP	C5-N7-C8	3.74	109.32	103.45
3	C	502	ANP	C2-N3-C4	3.68	120.83	111.83
3	A	503	ANP	O1B-PB-N3B	-3.35	106.83	111.77
3	D	503	ANP	C4-C5-N7	-3.04	107.11	110.58
3	C	502	ANP	C4-C5-N7	-3.01	107.14	110.58
3	A	503	ANP	C4-C5-N7	-2.97	107.19	110.58
3	B	502	ANP	C4-C5-N7	-2.87	107.30	110.58
3	A	503	ANP	N9-C8-N7	-2.75	110.03	113.94
3	C	502	ANP	N9-C8-N7	-2.74	110.04	113.94
3	D	503	ANP	N9-C8-N7	-2.66	110.16	113.94
3	B	502	ANP	N9-C8-N7	-2.64	110.19	113.94
3	D	503	ANP	O2A-PA-O3A	2.33	113.58	107.27
3	B	502	ANP	PA-O5'-C5'	-2.25	108.47	121.35
3	D	503	ANP	O4'-C1'-N9	2.21	112.33	108.09
3	C	502	ANP	PA-O5'-C5'	-2.13	109.17	121.35
3	A	503	ANP	O2B-PB-O3A	2.07	111.54	104.64
3	D	503	ANP	O2G-PG-O1G	-2.01	108.40	113.45

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	ANP	PB-N3B-PG-O1G
3	A	503	ANP	C5'-O5'-PA-O1A
3	A	503	ANP	C5'-O5'-PA-O3A
3	B	502	ANP	PB-N3B-PG-O1G
3	C	502	ANP	PG-N3B-PB-O1B
3	D	503	ANP	PG-N3B-PB-O1B
3	A	503	ANP	C3'-C4'-C5'-O5'
3	A	503	ANP	PG-N3B-PB-O3A
3	C	502	ANP	PG-N3B-PB-O3A

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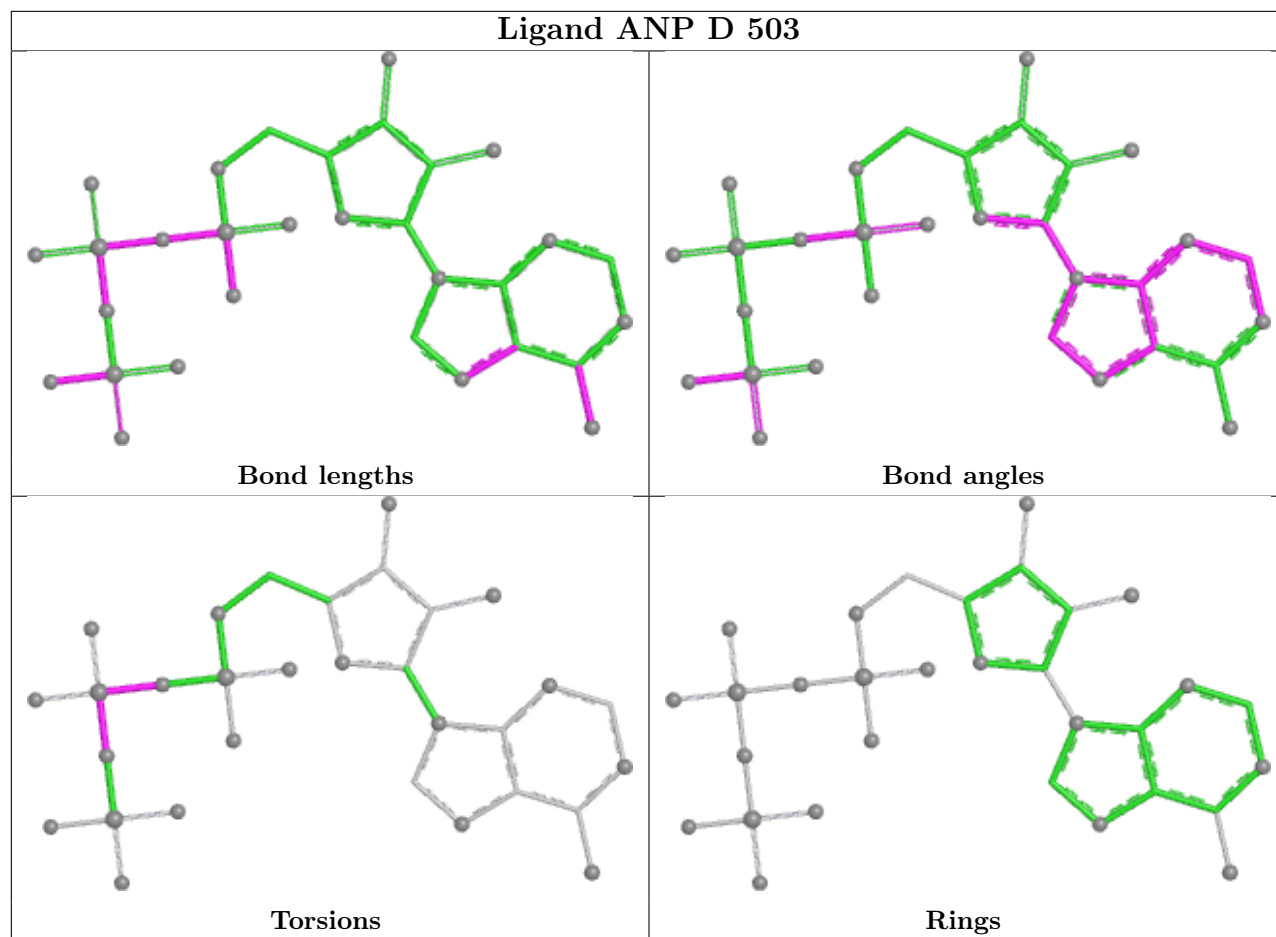
Mol	Chain	Res	Type	Atoms
3	D	503	ANP	PG-N3B-PB-O3A
3	B	502	ANP	C5'-O5'-PA-O1A
3	A	503	ANP	O4'-C4'-C5'-O5'
3	B	502	ANP	C3'-C4'-C5'-O5'
3	C	502	ANP	PA-O3A-PB-O1B
3	D	503	ANP	PA-O3A-PB-O1B

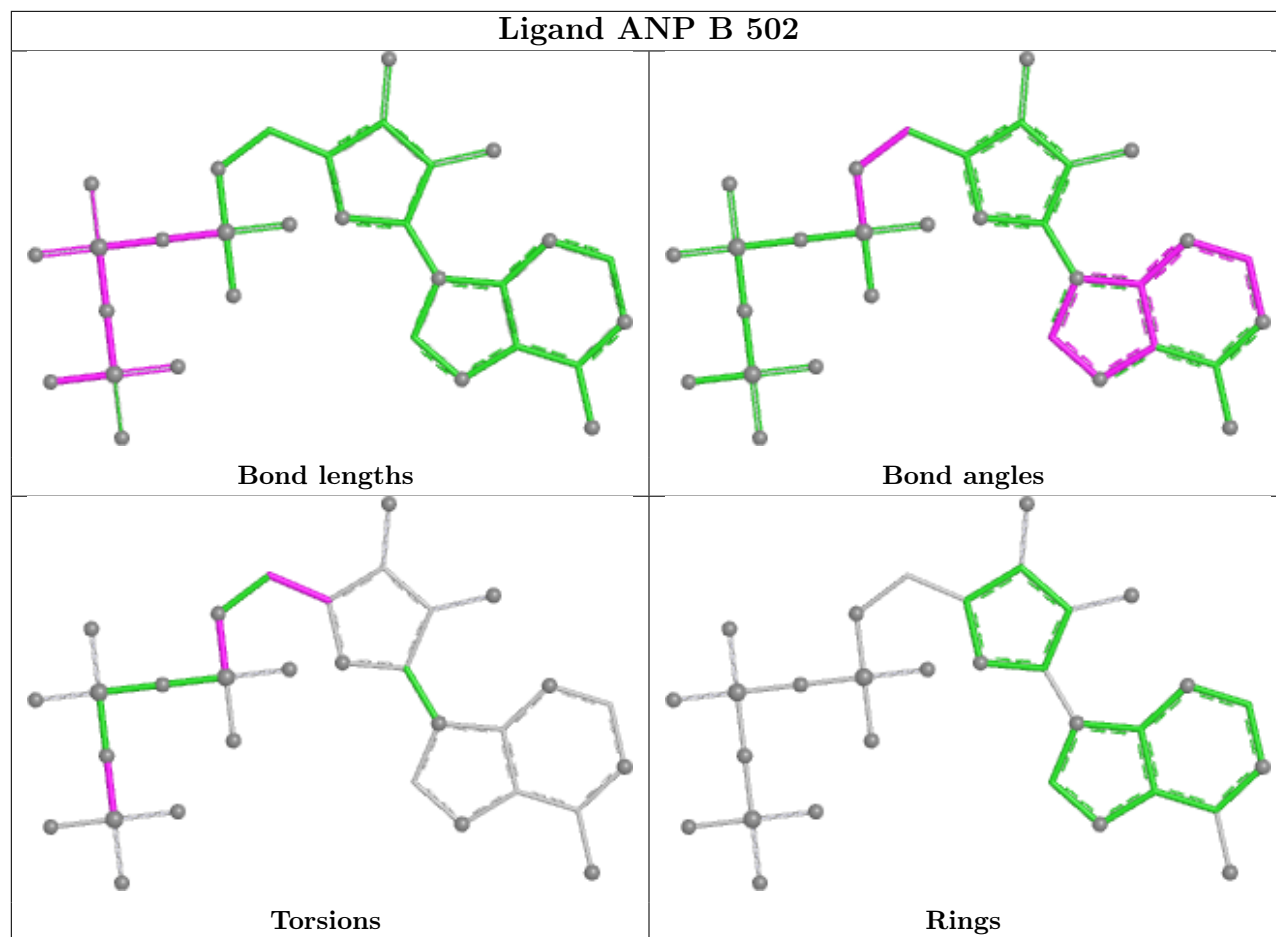
There are no ring outliers.

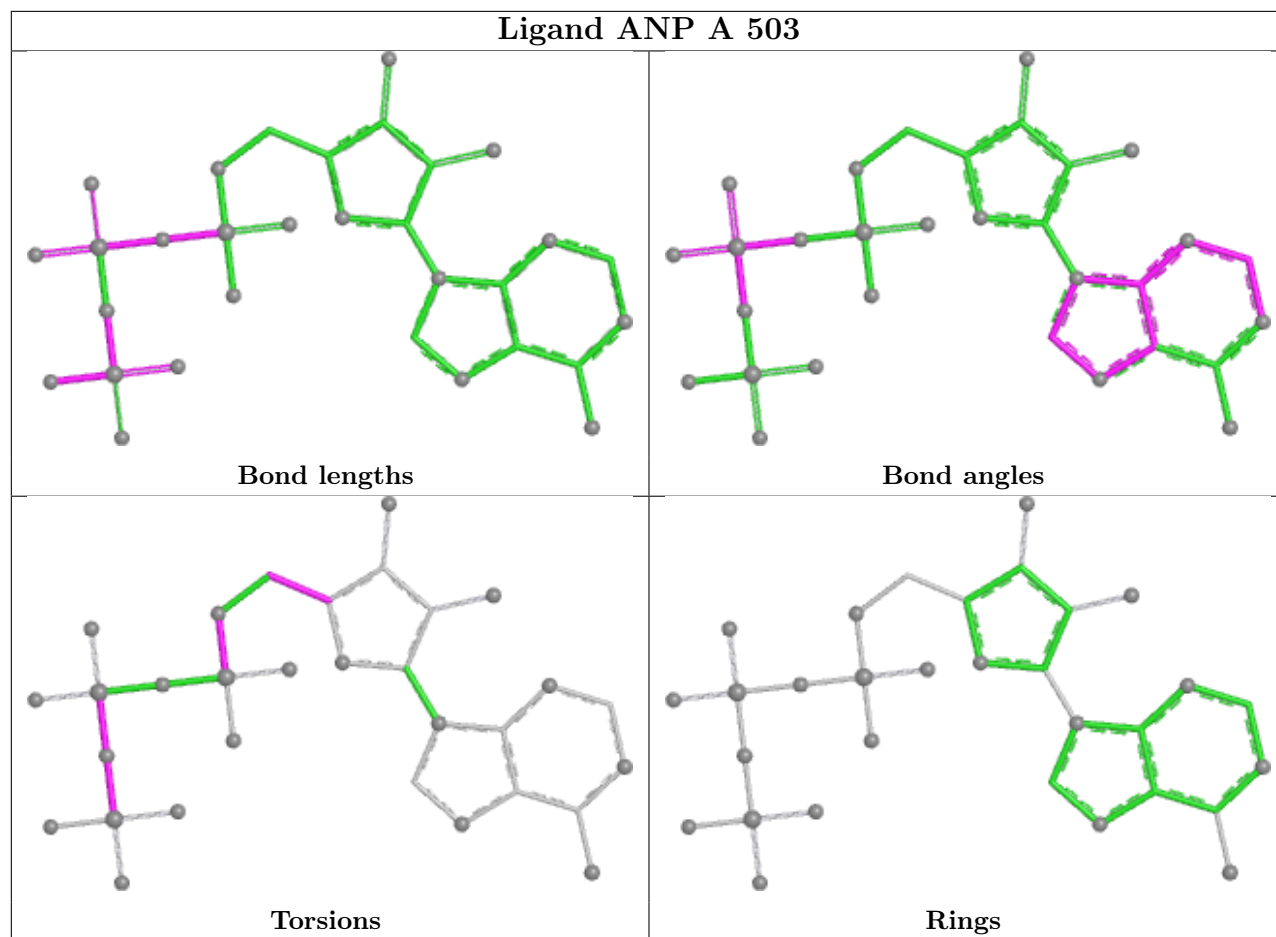
4 monomers are involved in 13 short contacts:

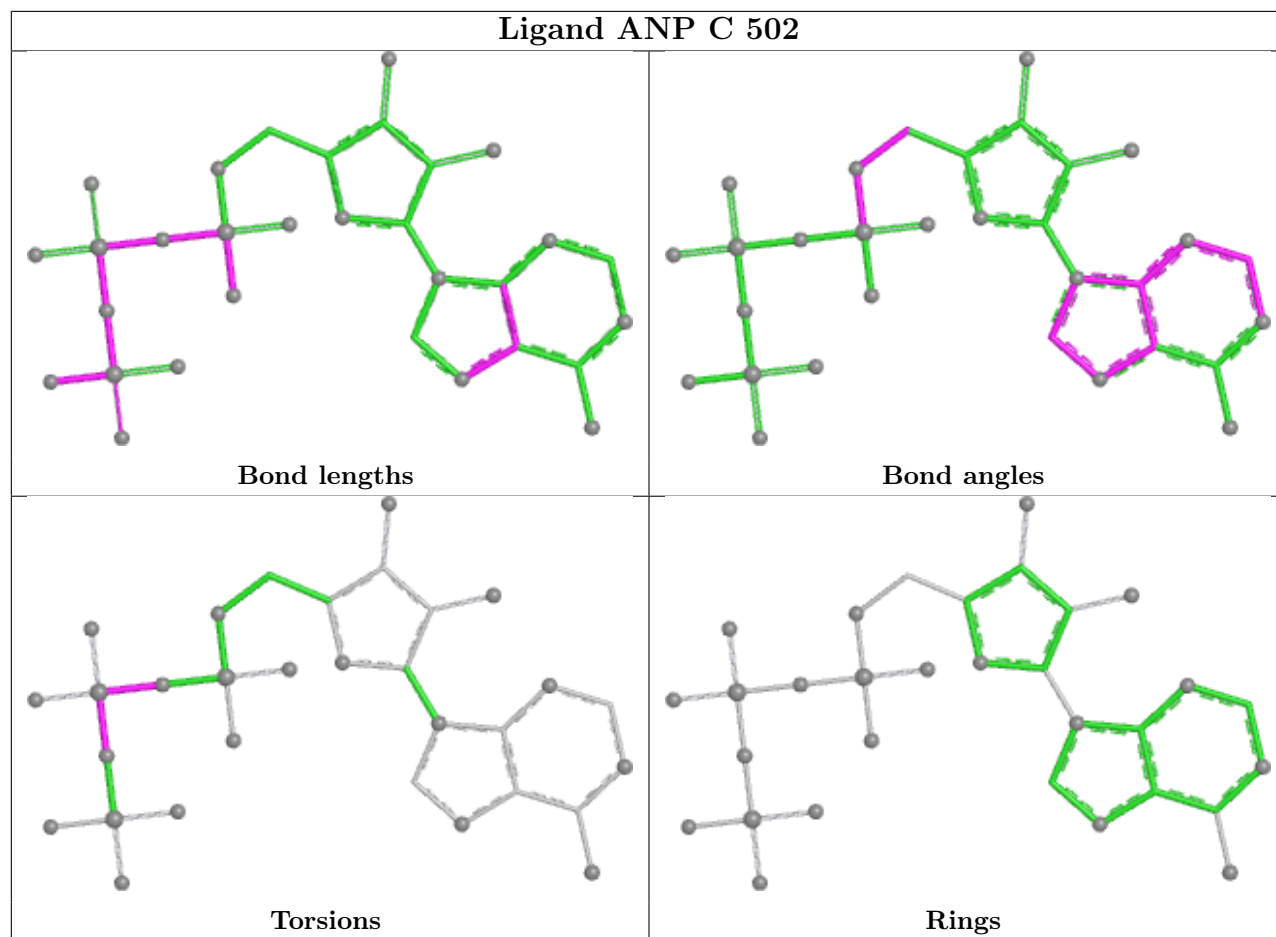
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	ANP	3	0
3	B	502	ANP	6	0
3	A	503	ANP	2	0
3	C	502	ANP	2	0

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









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	370/484 (76%)	0.21	12 (3%) 50 47	21, 37, 57, 73	0
1	B	334/484 (69%)	1.60	110 (32%) 1 0	37, 67, 88, 99	0
1	C	368/484 (76%)	0.25	10 (2%) 56 53	21, 36, 58, 72	0
1	D	352/484 (72%)	1.12	57 (16%) 4 3	28, 52, 77, 93	0
All	All	1424/1936 (73%)	0.77	189 (13%) 7 5	21, 45, 79, 99	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	PHE	4.9
1	B	177	VAL	4.7
1	D	270	ILE	4.3
1	D	308	LEU	4.3
1	C	266	SER	4.3
1	D	264	SER	4.2
1	B	195	ALA	4.1
1	D	4	HIS	4.1
1	B	60	ILE	4.0
1	C	352	MET	3.9
1	B	66	ALA	3.9
1	B	292	PHE	3.9
1	B	237	ASP	3.8
1	C	265	ALA	3.7
1	A	314	THR	3.7
1	B	263	ASP	3.7
1	D	275	GLN	3.7
1	B	179	VAL	3.7
1	B	290	SER	3.7
1	D	288	ASP	3.6
1	B	6	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	352	MET	3.5
1	B	171	CYS	3.5
1	D	23	LYS	3.4
1	D	334	GLU	3.4
1	B	33	THR	3.4
1	B	377	ASP	3.4
1	B	325	GLY	3.4
1	C	24	PHE	3.3
1	B	250	ALA	3.3
1	B	38	THR	3.3
1	B	217	TYR	3.3
1	B	37	TYR	3.2
1	B	176	GLY	3.2
1	B	285	THR	3.2
1	B	54	GLN	3.2
1	D	281	THR	3.2
1	B	167	ASN	3.1
1	B	310	ASP	3.1
1	D	66	ALA	3.1
1	A	352	MET	3.1
1	B	174	ALA	3.1
1	D	282	VAL	3.1
1	D	261	PHE	3.1
1	A	377	ASP	3.1
1	D	318	GLY	3.1
1	B	47	ASP	3.0
1	B	340	VAL	3.0
1	B	112	ILE	3.0
1	D	177	VAL	3.0
1	D	340	VAL	3.0
1	B	247	TYR	3.0
1	B	39	SER	3.0
1	B	30	VAL	3.0
1	B	51	ILE	2.9
1	B	40	GLY	2.9
1	B	241	GLN	2.9
1	B	194	THR	2.9
1	D	71	ILE	2.9
1	A	110	GLU	2.8
1	D	245	THR	2.8
1	B	201	GLY	2.8
1	B	31	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	331	GLY	2.8
1	B	262	TYR	2.8
1	A	139	VAL	2.8
1	D	31	ILE	2.8
1	D	5	TYR	2.8
1	B	254	LYS	2.8
1	B	233	ARG	2.8
1	B	169	ILE	2.7
1	B	239	ILE	2.7
1	B	330	LEU	2.7
1	D	110	GLU	2.7
1	D	95	TYR	2.7
1	B	12	GLY	2.7
1	B	313	LEU	2.7
1	B	309	GLN	2.7
1	B	85	VAL	2.7
1	B	236	THR	2.7
1	B	308	LEU	2.7
1	D	149	HIS	2.6
1	D	72	LYS	2.6
1	D	91	GLU	2.6
1	A	273	VAL	2.6
1	B	293	ILE	2.6
1	B	354	ILE	2.6
1	D	68	GLY	2.6
1	D	175	CYS	2.6
1	B	73	GLU	2.6
1	B	166	ILE	2.6
1	B	240	ALA	2.6
1	C	27	GLY	2.6
1	B	46	ILE	2.6
1	D	112	ILE	2.6
1	B	175	CYS	2.6
1	B	111	GLY	2.6
1	B	305	PHE	2.6
1	B	45	LEU	2.5
1	B	319	GLY	2.5
1	B	302	PHE	2.5
1	B	74	VAL	2.5
1	B	255	HIS	2.5
1	D	317	ASN	2.5
1	D	139	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	260	ALA	2.5
1	C	4	HIS	2.5
1	B	203	CYS	2.4
1	B	375	LEU	2.4
1	D	150	SER	2.4
1	A	136	GLU	2.4
1	C	114	GLU	2.4
1	B	32	GLY	2.4
1	B	15	SER	2.4
1	D	92	ILE	2.4
1	D	376	LEU	2.4
1	B	52	ALA	2.3
1	B	55	ALA	2.3
1	B	368	SER	2.3
1	B	20	VAL	2.3
1	B	358	GLU	2.3
1	B	119	GLN	2.3
1	B	286	GLN	2.3
1	B	180	LEU	2.3
1	D	134	ASP	2.3
1	A	281	THR	2.3
1	D	272	THR	2.3
1	B	64	SER	2.3
1	D	113	ARG	2.3
1	B	41	ILE	2.3
1	B	157	VAL	2.3
1	C	312	GLY	2.3
1	B	341	SER	2.3
1	D	64	SER	2.3
1	D	120	GLU	2.3
1	D	286	GLN	2.3
1	D	377	ASP	2.2
1	B	242	GLY	2.2
1	B	91	GLU	2.2
1	B	348	THR	2.2
1	C	5	TYR	2.2
1	D	147	ALA	2.2
1	D	369	SER	2.2
1	B	76	LEU	2.2
1	D	153	VAL	2.2
1	B	53	ARG	2.2
1	B	357	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	6	TYR	2.2
1	D	284	TYR	2.2
1	B	370	ILE	2.2
1	D	200	LEU	2.2
1	D	20	VAL	2.2
1	D	312	GLY	2.2
1	B	172	VAL	2.2
1	D	241	GLN	2.2
1	B	196	THR	2.2
1	B	364	SER	2.2
1	D	246	SER	2.2
1	A	145	LEU	2.1
1	B	200	LEU	2.1
1	B	366	ILE	2.1
1	A	26	ASN	2.1
1	B	304	VAL	2.1
1	B	316	VAL	2.1
1	D	244	ASN	2.1
1	B	218	GLU	2.1
1	B	208	GLY	2.1
1	C	61	LYS	2.1
1	D	129	ILE	2.1
1	B	359	PHE	2.1
1	B	232	GLY	2.1
1	B	36	THR	2.1
1	B	314	THR	2.1
1	B	367	SER	2.1
1	D	29	ASN	2.1
1	B	59	THR	2.0
1	B	63	ALA	2.0
1	B	244	ASN	2.0
1	B	335	LEU	2.0
1	B	9	ILE	2.0
1	B	71	ILE	2.0
1	B	297	VAL	2.0
1	B	261	PHE	2.0
1	D	135	LYS	2.0
1	A	274	GLU	2.0
1	B	360	SER	2.0
1	D	174	ALA	2.0
1	A	283	GLN	2.0
1	B	65	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

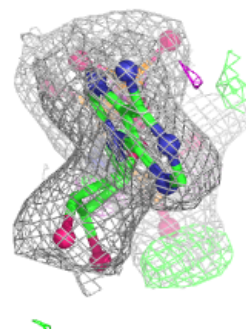
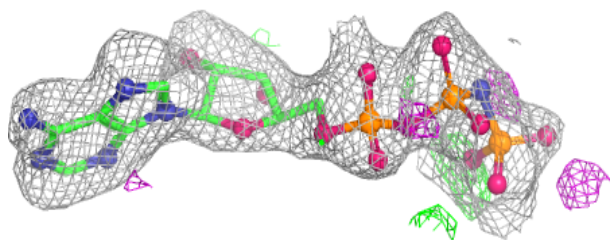
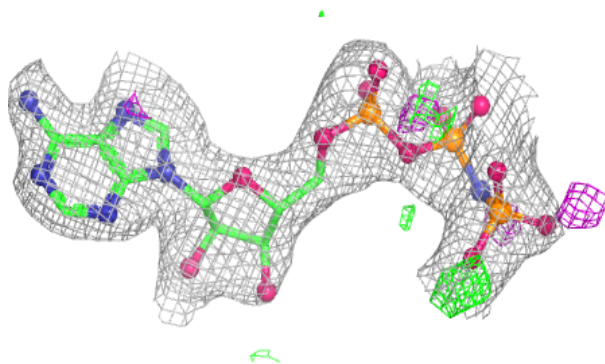
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	501	1/1	0.82	0.20	72,72,72,72	0
4	CL	B	503	1/1	0.84	0.14	80,80,80,80	0
3	ANP	B	502	31/31	0.89	0.13	46,56,58,58	0
4	CL	C	505	1/1	0.94	0.10	48,48,48,48	0
4	CL	D	505	1/1	0.94	0.07	38,38,38,38	0
2	MG	D	502	1/1	0.95	0.05	46,46,46,46	0
2	MG	A	502	1/1	0.96	0.10	45,45,45,45	0
3	ANP	D	503	31/31	0.97	0.06	21,30,34,35	0
4	CL	C	506	1/1	0.97	0.06	50,50,50,50	0
4	CL	C	504	1/1	0.97	0.05	33,33,33,33	0
3	ANP	C	502	31/31	0.98	0.06	21,27,29,30	0
3	ANP	A	503	31/31	0.98	0.06	20,31,36,37	0
4	CL	A	505	1/1	0.98	0.05	45,45,45,45	0
4	CL	D	504	1/1	0.98	0.06	43,43,43,43	0
2	MG	A	501	1/1	0.98	0.03	23,23,23,23	0
2	MG	D	501	1/1	0.99	0.04	33,33,33,33	0
2	MG	C	501	1/1	0.99	0.01	23,23,23,23	0
4	CL	C	503	1/1	0.99	0.04	20,20,20,20	0
4	CL	A	504	1/1	0.99	0.05	34,34,34,34	0

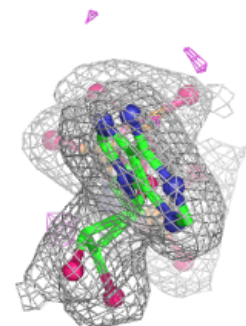
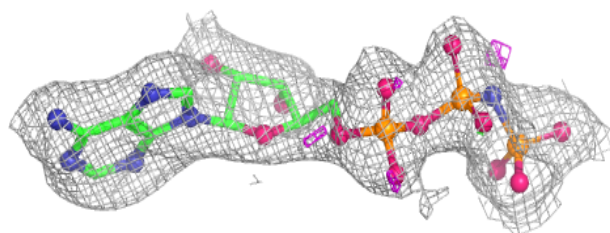
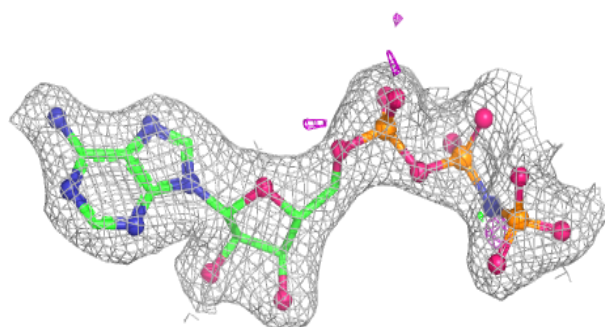
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 502:

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

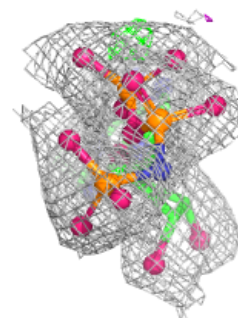
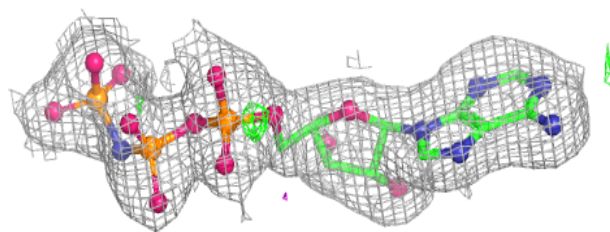
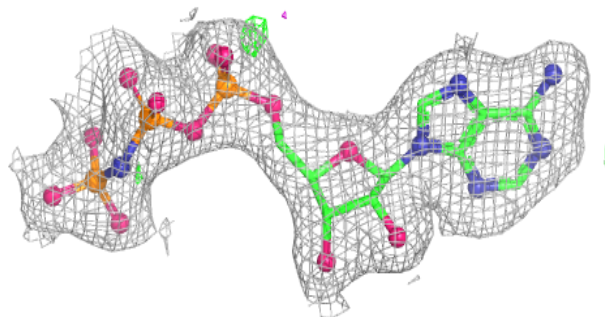
**Electron density around ANP D 503:**

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

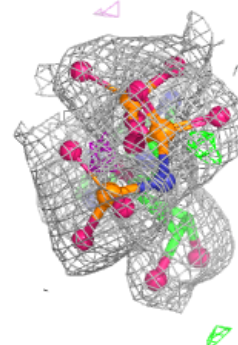
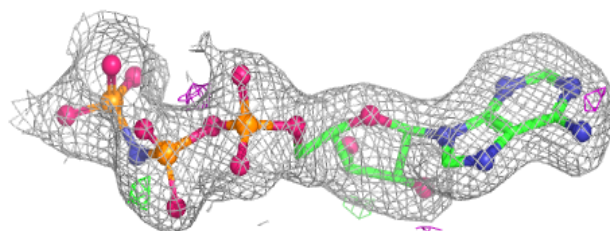
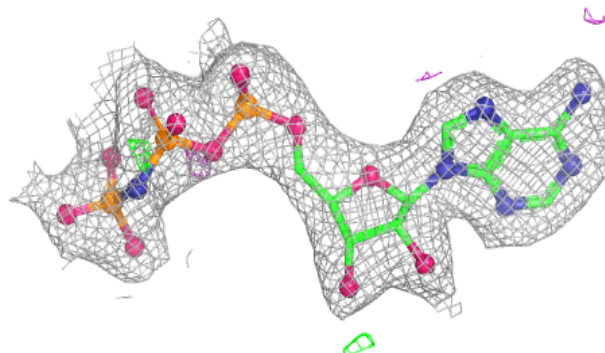


Electron density around ANP C 502:

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

**Electron density around ANP A 503:**

$2mF_o-DF_c$ (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.