



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:18 PM GMT

PDB ID : 2FJB
Title : Adenosine-5'-phosphosulfatereductase im complex with products
Authors : Schiffer, A.; Fritz, G.; Kroneck, P.M.; Ermler, U.
Deposited on : 2006-01-02
Resolution : 1.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

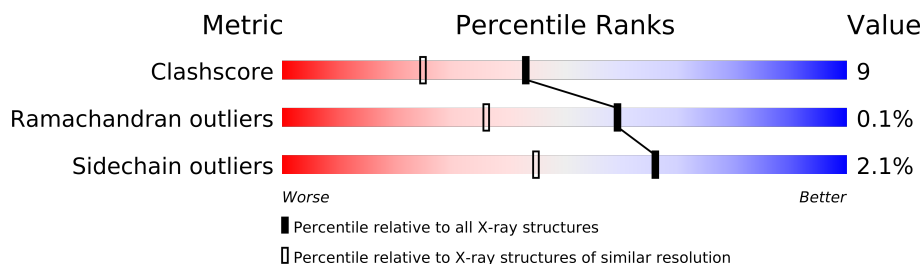
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	643	
1	C	643	
2	B	150	
2	D	150	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14529 atoms, of which 0 are hydrogen and 0 are deuterium.

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 adenylylsulfate reductase, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	6	0
			5187	3358	851	948	30			
1	C	642	Total	C	N	O	S	0	6	0
			5184	3355	851	949	29			

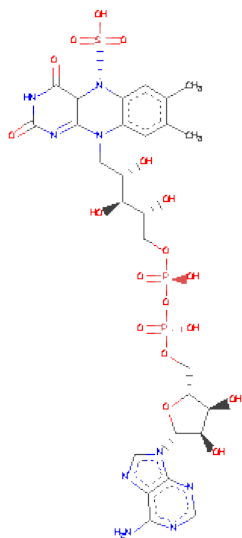
- Molecule 2 is a protein called adenylylsulfate reductase, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	1	0
			1175	747	193	219	16			
2	D	149	Total	C	N	O	S	0	2	0
			1180	750	193	220	17			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

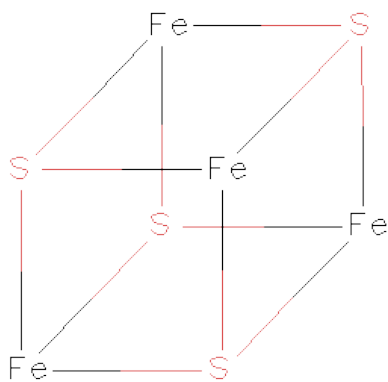
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is (S)-10-((2S,3S,4R)-5-((S)-((S)-(((2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXY-TETRAHYDROFURAN-2-YL)METHOXY)(HYDROXY)PHOSPHORYLOXY)(HYDROXY)PHOSPHORYLOXY)-2,3,4-TRIHYDROXYPENTYL)-7,8-DIMETHYL-2,4-DIOXO-2,3,4,4A-TETRAHYDROBENZO[G]PTERIDINE-5(10H)-SULFONIC ACID (three-letter code: SFD) (formula: C₂₇H₃₅N₉O₁₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			57	27	9	18	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			57	27	9	18	2	1		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



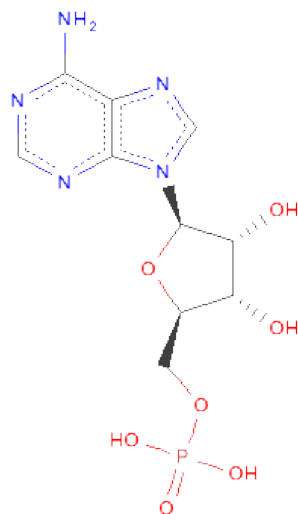
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			8	4	4		
5	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	579	Total	O	0	0
			579	579		
7	B	169	Total	O	0	0
			169	169		
7	C	635	Total	O	0	0
			635	635		
7	D	204	Total	O	0	0
			204	204		

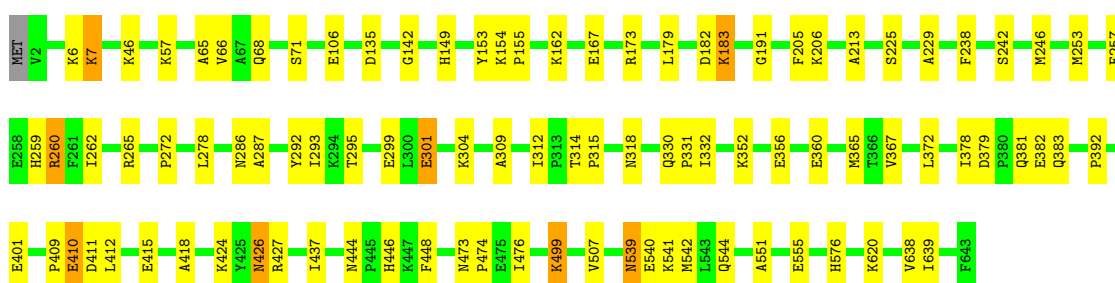
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

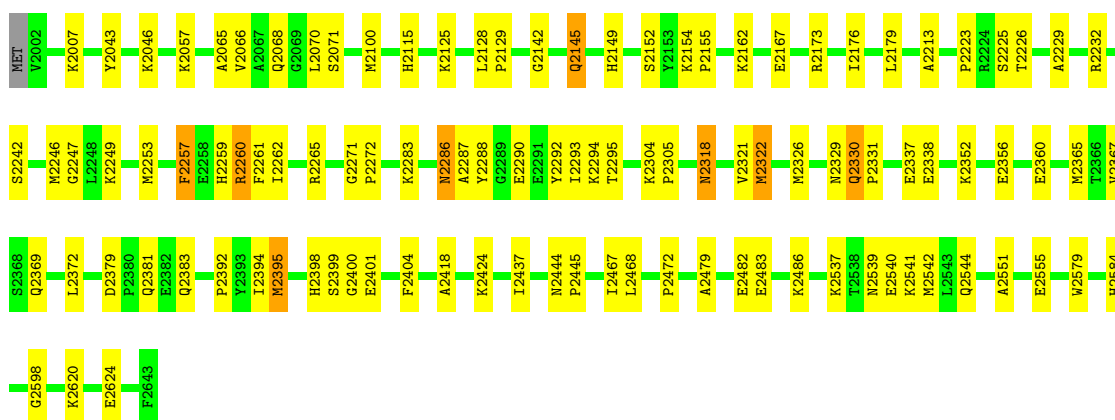
- Molecule 1: adenylylsulfate reductase, subunit A

Chain A:



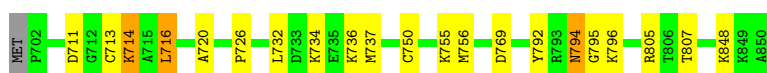
- Molecule 1: adenylylsulfate reductase, subunit A

Chain C:



- Molecule 2: adenylylsulfate reductase, subunit B

Chain B:



- Molecule 2: adenylylsulfate reductase, subunit B

Chain D:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.60Å 113.50Å 193.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70	Depositor
% Data completeness (in resolution range)	90.8 (30.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.168 , 0.192	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SF4, SFD, AMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/5352	0.58	0/7244
1	C	0.34	1/5349 (0.0%)	0.61	4/7241 (0.1%)
2	B	0.31	0/1209	0.63	0/1632
2	D	0.30	0/1218	0.64	0/1642
All	All	0.32	1/13128 (0.0%)	0.60	4/17759 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2330	GLN	C-N	-10.21	1.14	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2329	ASN	O-C-N	-8.68	108.82	122.70
1	C	2329	ASN	C-N-CA	6.83	138.78	121.70
1	C	2329	ASN	CA-C-N	5.97	130.33	117.20
1	C	2330	GLN	O-C-N	5.17	130.92	121.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5187	0	5083	90	1
1	C	5184	0	5077	99	0
2	B	1175	0	1151	23	0
2	D	1180	0	1156	19	1
3	C	1	0	0	0	0
4	A	57	0	31	4	0
4	C	57	0	31	5	0
5	B	16	0	0	1	0
5	D	16	0	0	1	0
6	A	46	0	22	7	0
6	C	23	0	11	1	0
7	A	579	0	0	8	0
7	B	169	0	0	4	0
7	C	635	0	0	8	0
7	D	204	0	0	6	0
All	All	14529	0	12562	225	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (225) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1000:SFD:S	4:A:1000:SFD:N5F	1.97	1.35
4:C:3000:SFD:S	4:C:3000:SFD:N5F	2.09	1.24
2:B:713:CYS:HB3	2:B:716:LEU:HD21	1.25	1.08
1:C:2379:ASP:H	1:C:2383:GLN:HE21	1.03	0.95
1:C:2272:PRO:HG3	1:C:2365:MET:HE3	1.51	0.88
1:C:2379:ASP:H	1:C:2383:GLN:NE2	1.74	0.86
1:C:2259:HIS:HD2	1:C:2401:GLU:H	1.26	0.84
1:A:293:ILE:HG21	6:A:1303:AMP:H2'	1.62	0.81
1:A:259:HIS:HD2	1:A:401:GLU:H	1.27	0.80
4:C:3000:SFD:S	4:C:3000:SFD:C5F	2.70	0.80
1:C:2292:TYR:CE1	1:C:2321[B]:VAL:HG12	2.18	0.79
1:A:539:ASN:ND2	1:A:542[A]:MET:HG3	1.98	0.79
2:B:716:LEU:H	2:B:716:LEU:HD13	1.48	0.79
1:A:183:LYS:O	1:A:183:LYS:HG2	1.82	0.79
4:C:3000:SFD:S	4:C:3000:SFD:C6F	2.72	0.77
1:A:426:ASN:HD21	1:A:427:ARG:HH11	1.32	0.77
4:A:1000:SFD:S	4:A:1000:SFD:C6F	2.73	0.76
1:A:106:GLU:HB3	1:A:639[B]:ILE:HD13	1.66	0.76
1:C:2272:PRO:HG3	1:C:2365:MET:CE	2.14	0.76
1:A:378:ILE:HG12	1:A:383:GLN:HE21	1.51	0.76
1:C:2541:LYS:HA	1:C:2541:LYS:HE2	1.65	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1000:SFD:S	4:A:1000:SFD:C5F	2.76	0.73
2:D:2796:LYS:HE2	2:D:2798:LEU:HD21	1.69	0.73
2:B:711:ASP:OD1	2:B:714:LYS:HG2	1.89	0.72
1:C:2043:TYR:O	1:C:2046:LYS:HE2	1.90	0.72
1:C:2379:ASP:N	1:C:2383:GLN:HE21	1.85	0.70
1:A:225:SER:HB3	1:A:229:ALA:HB3	1.73	0.69
1:A:272:PRO:HG3	1:A:365:MET:CE	2.23	0.69
1:A:6:LYS:HB3	1:A:7:LYS:HD3	1.74	0.69
1:A:162:LYS:HE3	1:A:167:GLU:HB2	1.74	0.69
1:A:292:TYR:OH	6:A:1303:AMP:H2	1.75	0.69
1:C:2330:GLN:HB3	1:C:2331:PRO:HA	1.75	0.68
1:A:272:PRO:HG3	1:A:365:MET:HE3	1.75	0.67
1:C:2286:ASN:C	1:C:2286:ASN:HD22	1.97	0.67
1:C:2379:ASP:OD2	1:C:2381:GLN:HG2	1.94	0.67
1:C:2115:HIS:HD2	2:D:2834:GLU:OE2	1.78	0.67
1:C:2260:ARG:HH21	1:C:2584:HIS:HE1	1.43	0.67
1:A:539:ASN:HD21	1:A:542[A]:MET:HG3	1.61	0.65
6:A:1302:AMP:HN61	6:A:1303:AMP:H8	1.44	0.65
1:C:2225:SER:HB3	1:C:2229:ALA:HB3	1.77	0.64
6:A:1302:AMP:N6	6:A:1303:AMP:H8	1.95	0.64
1:C:2145:GLN:H	1:C:2145:GLN:NE2	1.97	0.63
1:C:2352:LYS:O	1:C:2356:GLU:HG3	1.98	0.62
2:D:2718:ARG:HD2	7:D:5259:HOH:O	1.99	0.62
1:A:539:ASN:HD22	1:A:539:ASN:C	2.02	0.62
1:A:66:VAL:HG12	1:A:66:VAL:O	2.00	0.62
2:B:794:ASN:C	2:B:794:ASN:HD22	2.03	0.62
1:A:309:ALA:O	1:A:312:ILE:HD13	1.99	0.62
2:B:794:ASN:ND2	2:B:796:LYS:H	1.98	0.62
1:C:2286:ASN:ND2	1:C:2288:TYR:H	1.98	0.61
1:A:379:ASP:OD2	1:A:381:GLN:HG2	1.99	0.61
1:A:253:MET:HG2	1:A:620:LYS:HB2	1.82	0.61
1:A:551:ALA:O	1:A:555:GLU:HG3	2.01	0.61
2:B:734:LYS:H	2:B:734:LYS:HD2	1.65	0.61
1:C:2179:LEU:HG	1:C:2246[B]:MET:HB2	1.83	0.60
1:A:259:HIS:CD2	1:A:401:GLU:H	2.16	0.60
1:A:499:LYS:HB2	1:A:499:LYS:NZ	2.17	0.60
1:A:71:SER:CB	1:A:365:MET:HE2	2.32	0.59
1:C:2259:HIS:HD2	1:C:2401:GLU:N	1.96	0.59
1:C:2330:GLN:HA	1:C:2331:PRO:C	2.21	0.59
1:C:2259:HIS:CD2	1:C:2401:GLU:HG2	2.36	0.59
1:A:293:ILE:HD13	6:A:1303:AMP:H3'	1.83	0.59
1:A:378:ILE:HG12	1:A:383:GLN:NE2	2.16	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2066:VAL:O	1:C:2066:VAL:HG12	2.03	0.59
1:A:352:LYS:O	1:A:356:GLU:HG3	2.03	0.58
1:A:418:ALA:O	1:A:424:LYS:HE3	2.03	0.58
1:A:542[A]:MET:SD	7:A:5808:HOH:O	2.57	0.58
1:A:542[B]:MET:SD	1:C:2331:PRO:HG3	2.43	0.58
1:A:301:GLU:HG2	1:A:304:LYS:HZ3	1.68	0.58
1:A:415:GLU:HG2	7:A:7460:HOH:O	2.04	0.57
1:C:2551:ALA:O	1:C:2555:GLU:HG3	2.05	0.57
1:A:183:LYS:O	1:A:183:LYS:CG	2.50	0.57
1:A:71:SER:HB2	1:A:365:MET:HE2	1.86	0.57
1:C:2257:PHE:O	1:C:2584:HIS:HD2	1.87	0.57
1:C:2262:ILE:HD11	1:C:2392:PRO:HG3	1.87	0.57
1:A:68:GLN:HE22	1:A:367:VAL:H	1.53	0.56
1:C:2294:LYS:HD3	7:C:7500:HOH:O	2.04	0.56
1:C:2293:ILE:HG23	7:C:5361:HOH:O	2.04	0.56
1:C:2539:ASN:OD1	1:C:2542[A]:MET:HG3	2.06	0.56
1:A:331:PRO:HG3	1:C:2542[B]:MET:SD	2.45	0.56
1:C:2337:GLU:HG2	1:C:2338:GLU:N	2.20	0.56
1:A:71:SER:OG	1:A:365:MET:HE2	2.06	0.55
1:C:2292:TYR:HA	1:C:2295:THR:OG1	2.07	0.55
1:C:2260:ARG:HH21	1:C:2584:HIS:CE1	2.25	0.55
1:A:46:LYS:HD2	7:B:7167:HOH:O	2.06	0.55
1:C:2057:LYS:O	1:C:2173:ARG:HA	2.08	0.54
1:A:7:LYS:HE3	7:B:7116:HOH:O	2.08	0.54
1:A:287:ALA:HB1	1:C:2541:LYS:HG3	1.89	0.54
1:A:154:LYS:HB3	1:A:155:PRO:HD3	1.88	0.54
1:A:179:LEU:HG	1:A:246[B]:MET:HB2	1.90	0.53
1:A:57:LYS:O	1:A:173:ARG:HA	2.08	0.53
1:C:2283:LYS:HD2	7:C:7053:HOH:O	2.09	0.53
2:B:755:LYS:HB3	2:B:756:MET:HE1	1.91	0.53
1:C:2115:HIS:HE1	7:D:5004:HOH:O	1.92	0.53
1:A:473:ASN:N	1:A:474:PRO:HD3	2.24	0.52
1:A:301:GLU:O	1:A:304:LYS:HG3	2.10	0.52
1:A:179:LEU:HG	1:A:246[A]:MET:HB3	1.90	0.52
1:A:149:HIS:HD2	1:A:360:GLU:OE2	1.92	0.52
1:C:2259:HIS:CD2	1:C:2401:GLU:H	2.17	0.52
1:C:2537:LYS:HD3	7:C:7570:HOH:O	2.09	0.52
1:A:410:GLU:HG2	7:A:5772:HOH:O	2.10	0.52
2:D:2716:LEU:HD13	7:D:5903:HOH:O	2.10	0.51
1:A:426:ASN:ND2	1:A:427:ARG:HH11	2.06	0.51
1:C:2261:PHE:CE1	1:C:2399:SER:HB2	2.46	0.51
1:A:383:GLN:HG2	7:A:5771:HOH:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2226:THR:HA	7:C:7128:HOH:O	2.11	0.51
2:D:2720:ALA:HB3	5:D:3110:SF4:S1	2.51	0.51
1:A:259:HIS:HD2	1:A:401:GLU:N	2.03	0.50
6:A:1302:AMP:H5'1	7:A:5375:HOH:O	2.09	0.50
1:C:2318:ASN:O	1:C:2321[B]:VAL:HG22	2.11	0.50
1:A:206:LYS:HE2	1:A:476:ILE:CD1	2.41	0.50
1:C:2479:ALA:O	1:C:2483:GLU:HG3	2.11	0.50
1:C:2394:ILE:C	1:C:2395:MET:HG3	2.31	0.50
1:A:541:LYS:HG3	1:C:2287:ALA:HB1	1.94	0.50
1:C:2068:GLN:HE22	1:C:2367:VAL:H	1.60	0.49
1:C:2162:LYS:NZ	1:C:2167:GLU:HB3	2.26	0.49
1:C:2360:GLU:HB2	2:D:2802:PHE:CE2	2.48	0.49
2:D:2834:GLU:HB3	2:D:2835:PRO:HA	1.93	0.49
1:A:68:GLN:HG2	2:B:750:CYS:HB2	1.94	0.49
2:D:2715:ALA:C	2:D:2716:LEU:HD12	2.32	0.49
1:C:2125:LYS:HE2	7:D:7230:HOH:O	2.12	0.49
1:A:272:PRO:HG3	1:A:365:MET:HE1	1.94	0.49
1:C:2418:ALA:O	1:C:2424:LYS:HE3	2.13	0.49
1:C:2176:ILE:HG22	1:C:2246[A]:MET:SD	2.53	0.48
1:C:2286:ASN:C	1:C:2286:ASN:ND2	2.66	0.48
2:B:755:LYS:CB	2:B:756:MET:HE1	2.43	0.48
1:C:2129:PRO:HB2	1:C:2149:HIS:HB2	1.95	0.48
1:A:286:ASN:HA	1:A:332[A]:ILE:HD13	1.95	0.48
2:B:792:TYR:HB2	2:B:796:LYS:HB3	1.96	0.47
1:A:213:ALA:HB2	1:A:437:ILE:HD11	1.95	0.47
1:C:2179:LEU:HG	1:C:2246[A]:MET:HB3	1.97	0.47
1:C:2271:GLY:H	1:C:2369:GLN:HE21	1.63	0.47
1:C:2322[A]:MET:HB3	1:C:2326:MET:HE2	1.97	0.47
1:A:301:GLU:HG2	1:A:304:LYS:NZ	2.30	0.47
2:D:2734:LYS:O	2:D:2737[A]:MET:HE2	2.15	0.47
1:A:65:ALA:HB1	4:A:1000:SFD:H3F3	1.97	0.47
2:B:732:LEU:HD12	7:B:7565:HOH:O	2.14	0.47
1:C:2071[A]:SER:OG	1:C:2365:MET:HE2	2.15	0.47
1:A:259:HIS:CD2	1:A:401:GLU:HG2	2.50	0.47
2:D:2787:MET:HE2	7:D:7195:HOH:O	2.14	0.47
1:A:7:LYS:N	1:A:7:LYS:HD3	2.30	0.46
1:C:2286:ASN:ND2	1:C:2290:GLU:H	2.13	0.46
1:C:2540:GLU:O	1:C:2544:GLN:HG3	2.15	0.46
1:A:372:LEU:C	1:A:372:LEU:HD23	2.36	0.46
1:C:2152:SER:C	1:C:2155:PRO:HD2	2.36	0.46
1:A:142:GLY:HA3	1:A:278:LEU:HD13	1.98	0.46
2:B:794:ASN:HD22	2:B:795:GLY:N	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2068:GLN:HG2	2:D:2750:CYS:HB2	1.98	0.46
2:B:736:LYS:O	2:B:737:MET:HB2	2.15	0.46
1:A:499:LYS:HB2	1:A:499:LYS:HZ2	1.80	0.46
2:B:713:CYS:C	2:B:716:LEU:HD11	2.35	0.46
1:C:2259:HIS:CD2	1:C:2400:GLY:HA2	2.51	0.46
1:C:2330:GLN:CB	1:C:2331:PRO:HA	2.43	0.46
1:C:2066:VAL:HG13	1:C:2070:LEU:HG	1.97	0.46
1:C:2242:SER:O	1:C:2246[A]:MET:HG3	2.16	0.46
2:B:794:ASN:HD22	2:B:796:LYS:H	1.59	0.45
1:A:242:SER:OG	1:A:576:HIS:HD2	1.99	0.45
1:A:262:ILE:N	1:A:262:ILE:HD12	2.32	0.45
1:C:2262:ILE:HD13	1:C:2392:PRO:HA	1.98	0.45
1:A:314:THR:N	1:A:315:PRO:HD2	2.31	0.45
1:C:2145:GLN:N	1:C:2145:GLN:NE2	2.63	0.45
1:A:409:PRO:HG2	1:A:412:LEU:HB2	1.99	0.45
1:C:2154:LYS:HB3	1:C:2155:PRO:HD3	1.99	0.44
1:A:541:LYS:HE2	7:A:7185:HOH:O	2.17	0.44
1:C:2318:ASN:O	1:C:2322[B]:MET:HG2	2.17	0.44
1:C:2304:LYS:HA	1:C:2305:PRO:HA	1.83	0.44
1:C:2065:ALA:HB1	4:C:3000:SFD:H3F3	2.00	0.44
1:A:6:LYS:HB3	1:A:7:LYS:CD	2.44	0.44
1:A:411:ASP:O	2:B:848:LYS:NZ	2.48	0.44
1:A:507:VAL:CG1	2:D:2704:PHE:HB3	2.48	0.44
1:C:2468:LEU:HD12	2:D:2826:LEU:CD2	2.48	0.44
1:C:2232:ARG:HD2	2:D:2767:TYR:CE1	2.53	0.43
1:A:540:GLU:O	1:A:544:GLN:HG3	2.17	0.43
1:C:2142:GLY:H	1:C:2145:GLN:NE2	2.15	0.43
1:C:2467:ILE:HA	1:C:2472:PRO:HD2	2.00	0.43
2:B:720:ALA:HB3	5:B:1110:SF4:S1	2.58	0.43
2:D:2714:LYS:HD3	2:D:2737[B]:MET:CE	2.48	0.43
1:A:68:GLN:NE2	1:A:367:VAL:H	2.17	0.43
1:C:2162:LYS:HB2	7:C:7257:HOH:O	2.18	0.43
1:C:2318:ASN:O	1:C:2321[A]:VAL:HG12	2.19	0.43
1:C:2229:ALA:HA	2:D:2767:TYR:CD2	2.53	0.43
2:B:713:CYS:CA	2:B:716:LEU:HD11	2.48	0.42
1:C:2223:PRO:HD2	7:C:7128:HOH:O	2.19	0.42
1:C:2249:LYS:HE2	1:C:2579:TRP:CH2	2.54	0.42
1:C:2253:MET:HG2	1:C:2620:LYS:HB2	2.01	0.42
1:A:383:GLN:NE2	7:A:5495:HOH:O	2.52	0.42
1:C:2322[A]:MET:SD	1:C:2598:GLY:HA2	2.59	0.42
2:D:2725:CYS:HA	2:D:2726:PRO:HD3	1.87	0.42
1:C:2046:LYS:NZ	7:C:5959:HOH:O	2.51	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:734:LYS:HE3	7:B:7564:HOH:O	2.19	0.42
1:C:2260:ARG:NH2	1:C:2584:HIS:HE1	2.15	0.42
1:A:265:ARG:NH2	6:A:1302:AMP:O1P	2.52	0.42
1:C:2068:GLN:NE2	1:C:2367:VAL:H	2.18	0.42
1:C:2162:LYS:HE2	1:C:2167:GLU:HB3	2.02	0.42
1:A:191:GLY:HA3	1:A:205:PHE:O	2.20	0.41
1:A:446:HIS:HA	1:A:448:PHE:CE1	2.55	0.41
1:A:260:ARG:HG3	1:A:392:PRO:HB3	2.02	0.41
1:C:2247:GLY:HA3	1:C:2404:PHE:CZ	2.55	0.41
1:A:292:TYR:HA	1:A:295:THR:OG1	2.20	0.41
1:A:411:ASP:O	2:B:848:LYS:CE	2.68	0.41
1:C:2265:ARG:NH2	6:C:1301:AMP:O1P	2.53	0.41
2:D:2716:LEU:HD11	7:D:7228:HOH:O	2.20	0.41
1:A:330:GLN:HB3	1:A:331:PRO:HA	2.03	0.41
2:B:805:ARG:HG2	2:B:807:THR:H	1.86	0.41
1:C:2398:HIS:NE2	4:C:3000:SFD:O2	2.46	0.41
1:A:638:VAL:HB	1:A:639[B]:ILE:HD12	2.03	0.41
1:A:238:PHE:CE2	2:B:726:PRO:HB2	2.56	0.41
1:C:2322[B]:MET:HB3	1:C:2326:MET:HE2	2.02	0.41
1:C:2142:GLY:CA	1:C:2145:GLN:HE22	2.34	0.41
1:A:206:LYS:HE2	1:A:476:ILE:HD11	2.02	0.41
1:C:2142:GLY:H	1:C:2145:GLN:HE21	1.69	0.41
1:A:381:GLN:HG3	1:A:382:GLU:HG2	2.03	0.41
7:A:6087:HOH:O	2:B:756:MET:HE3	2.20	0.41
1:C:2261:PHE:CD1	1:C:2399:SER:HB2	2.55	0.41
2:D:2736:LYS:O	2:D:2737[B]:MET:HB2	2.20	0.41
1:C:2372:LEU:C	1:C:2372:LEU:HD23	2.40	0.41
1:C:2213:ALA:HB2	1:C:2437:ILE:HD11	2.03	0.41
1:C:2482:GLU:HG3	1:C:2486:LYS:NZ	2.36	0.40
1:A:378:ILE:HA	1:A:383:GLN:NE2	2.35	0.40
1:C:2100:MET:SD	1:C:2445:PRO:HG3	2.61	0.40
1:C:2128:LEU:HA	1:C:2129:PRO:HD3	1.96	0.40
1:A:539:ASN:ND2	1:A:539:ASN:C	2.73	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:182:ASP:OD1	2:D:2836:GLU:OE2[2_655]	2.11	0.09

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	646/643 (100%)	626 (97%)	20 (3%)	0	100	100
1	C	646/643 (100%)	627 (97%)	19 (3%)	0	100	100
2	B	148/150 (99%)	142 (96%)	5 (3%)	1 (1%)	30	10
2	D	149/150 (99%)	147 (99%)	2 (1%)	0	100	100
All	All	1589/1586 (100%)	1542 (97%)	46 (3%)	1 (0%)	59	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	714	LYS

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	531/526 (101%)	517 (97%)	14 (3%)	59	35
1	C	531/526 (101%)	520 (98%)	11 (2%)	66	45
2	B	130/130 (100%)	127 (98%)	3 (2%)	63	41
2	D	131/130 (101%)	130 (99%)	1 (1%)	89	81
All	All	1323/1312 (101%)	1294 (98%)	29 (2%)	66	43

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	135	ASP

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Mol	Chain	Res	Type
1	A	153	TYR
1	A	183	LYS
1	A	257	PHE
1	A	260	ARG
1	A	299	GLU
1	A	301	GLU
1	A	318	ASN
1	A	410	GLU
1	A	426	ASN
1	A	444	ASN
1	A	499	LYS
1	A	539	ASN
1	C	2007	LYS
1	C	2145	GLN
1	C	2257	PHE
1	C	2260	ARG
1	C	2286	ASN
1	C	2318	ASN
1	C	2322[A]	MET
1	C	2322[B]	MET
1	C	2395	MET
1	C	2444	ASN
1	C	2624	GLU
2	B	716	LEU
2	B	769	ASP
2	B	794	ASN
2	D	2769	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	149	HIS
1	A	259	HIS
1	A	310	GLN
1	A	318	ASN
1	A	381	GLN
1	A	383	GLN
1	A	426	ASN
1	A	497	GLN
1	A	539	ASN
1	A	576	HIS

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Mol	Chain	Res	Type
1	C	2068	GLN
1	C	2074	ASN
1	C	2115	HIS
1	C	2145	GLN
1	C	2259	HIS
1	C	2286	ASN
1	C	2310	GLN
1	C	2318	ASN
1	C	2330	GLN
1	C	2369	GLN
1	C	2381	GLN
1	C	2383	GLN
1	C	2497	GLN
1	C	2584	HIS
2	B	794	ASN
2	B	845	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SFD	A	1000	-	62,62,62	4.82	38 (61%)	95,97,97	2.55	36 (37%)
6	AMP	A	1302	-	25,25,25	3.16	12 (48%)	38,38,38	4.63	19 (50%)
6	AMP	A	1303	-	25,25,25	3.07	13 (52%)	38,38,38	4.37	21 (55%)
5	SF4	B	1100	2	12,12,12	11.25	10 (83%)	0,24,24	0.00	-
5	SF4	B	1110	2	12,12,12	14.96	11 (91%)	0,24,24	0.00	-
6	AMP	C	1301	3	25,25,25	3.18	12 (48%)	38,38,38	4.73	20 (52%)
4	SFD	C	3000	-	62,62,62	4.87	38 (61%)	95,97,97	2.80	35 (36%)
5	SF4	D	3100	2	12,12,12	12.51	11 (91%)	0,24,24	0.00	-
5	SF4	D	3110	2	12,12,12	13.34	12 (100%)	0,24,24	0.00	-

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	SFD	A	1000	-	1/1/16/17	0/38/88/88	0/1/6/6
6	AMP	A	1302	-	1/1/5/5	0/10/26/26	0/1/3/3
6	AMP	A	1303	-	1/1/5/5	0/10/26/26	0/1/3/3
5	SF4	B	1100	2	-	0/0/48/48	0/0/5/5
5	SF4	B	1110	2	-	0/0/48/48	0/0/5/5
6	AMP	C	1301	3	1/1/5/5	0/10/26/26	0/1/3/3
4	SFD	C	3000	-	1/1/16/17	0/38/88/88	0/1/6/6
5	SF4	D	3100	2	-	0/0/48/48	0/0/5/5
5	SF4	D	3110	2	-	0/0/48/48	0/0/5/5

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1110	SF4	S2-FE4	-29.27	2.13	2.33
5	D	3100	SF4	S2-FE4	-24.16	2.17	2.33
5	D	3110	SF4	S2-FE4	-23.32	2.17	2.33
5	D	3110	SF4	S2-FE3	-22.86	2.17	2.33
5	B	1110	SF4	S2-FE3	-21.49	2.18	2.33
5	B	1100	SF4	S2-FE4	-21.47	2.18	2.33
5	B	1110	SF4	S2-FE1	-20.31	2.19	2.33
5	D	3100	SF4	S2-FE3	-20.16	2.19	2.33
5	D	3110	SF4	S4-FE3	-19.98	2.19	2.33
5	B	1110	SF4	S4-FE3	-19.39	2.20	2.33
5	B	1100	SF4	S2-FE3	-17.36	2.21	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3110	SF4	S2-FE1	-17.09	2.21	2.33
5	D	3100	SF4	S4-FE3	-15.68	2.22	2.33
5	B	1110	SF4	S3-FE2	-14.21	2.23	2.33
5	B	1100	SF4	S3-FE2	-13.81	2.24	2.33
5	B	1110	SF4	S4-FE1	-13.70	2.24	2.33
5	B	1100	SF4	S4-FE3	-13.59	2.24	2.33
5	D	3100	SF4	S2-FE1	-12.75	2.24	2.33
5	D	3110	SF4	S3-FE2	-11.80	2.25	2.33
5	D	3110	SF4	S4-FE1	-11.27	2.25	2.33
4	A	1000	SFD	C5R-C4R	10.92	1.69	1.51
4	C	3000	SFD	C1F-C9F	10.81	1.59	1.39
5	D	3100	SF4	S3-FE4	-10.69	2.26	2.33
5	B	1100	SF4	S2-FE1	-10.65	2.26	2.33
4	C	3000	SFD	S-N5F	10.43	2.09	1.65
5	B	1100	SF4	S3-FE4	-10.40	2.26	2.33
4	A	1000	SFD	C1F-C9F	10.38	1.58	1.39
6	A	1302	AMP	C1'-N9	-10.24	1.16	1.48
4	C	3000	SFD	C5R-C4R	10.22	1.67	1.51
6	C	1301	AMP	C1'-N9	-10.16	1.16	1.48
4	A	1000	SFD	C7R-C6R	10.09	1.67	1.53
4	A	1000	SFD	C9F-C6F	10.06	1.58	1.40
5	B	1100	SF4	S1-FE2	-9.89	2.26	2.33
5	D	3100	SF4	S3-FE2	-9.89	2.26	2.33
5	B	1110	SF4	S3-FE4	-9.81	2.26	2.33
4	C	3000	SFD	C7R-C6R	9.72	1.67	1.53
4	C	3000	SFD	C9F-C6F	9.67	1.57	1.40
5	D	3100	SF4	S4-FE1	-9.59	2.26	2.33
4	C	3000	SFD	C4A-N3A	9.32	1.49	1.35
5	D	3100	SF4	S1-FE2	-9.25	2.27	2.33
4	C	3000	SFD	C7F-C8F	9.24	1.67	1.40
4	C	3000	SFD	C9F-N10	9.22	1.57	1.41
4	A	1000	SFD	C4A-N3A	8.98	1.49	1.35
4	A	1000	SFD	C7F-C8F	8.93	1.66	1.40
4	A	1000	SFD	C9F-N10	8.90	1.57	1.41
4	C	3000	SFD	C1R-N10	-8.17	1.24	1.48
4	C	3000	SFD	C5F-C4F	-8.17	1.45	1.52
4	A	1000	SFD	C1R-N10	-8.00	1.25	1.48
4	A	1000	SFD	CBF-C7F	7.96	1.52	1.39
4	A	1000	SFD	S-N5F	7.66	1.97	1.65
4	A	1000	SFD	C4F-N3F	7.45	1.50	1.37
6	A	1303	AMP	C1'-N9	-7.37	1.25	1.48
5	D	3100	SF4	S1-FE4	7.19	2.38	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	SFD	C0F-N10	7.06	1.51	1.38
4	C	3000	SFD	C0F-N10	6.99	1.51	1.38
4	A	1000	SFD	C5F-C4F	-6.92	1.46	1.52
4	C	3000	SFD	CBF-C7F	6.91	1.50	1.39
4	C	3000	SFD	C4F-N3F	6.85	1.49	1.37
4	A	1000	SFD	C2A-N3A	6.42	1.44	1.32
5	D	3110	SF4	S3-FE4	-6.37	2.29	2.33
4	C	3000	SFD	C2A-N3A	6.23	1.44	1.32
4	A	1000	SFD	C2A-N1A	5.91	1.45	1.33
5	B	1110	SF4	S1-FE2	-5.76	2.29	2.33
4	A	1000	SFD	O7R-C7R	5.62	1.56	1.43
5	D	3100	SF4	S1-FE3	-5.58	2.29	2.33
6	C	1301	AMP	C4-N3	5.50	1.44	1.35
6	A	1302	AMP	C4-N3	5.42	1.43	1.35
5	B	1110	SF4	S4-FE2	-5.30	2.29	2.33
6	A	1303	AMP	C4-N3	5.29	1.43	1.35
4	C	3000	SFD	PA-OP	5.25	1.69	1.59
4	C	3000	SFD	C5M-C4A	5.24	1.52	1.40
4	A	1000	SFD	PA-OP	5.22	1.69	1.59
4	C	3000	SFD	O7R-C7R	5.16	1.55	1.43
5	D	3110	SF4	S1-FE3	-5.14	2.29	2.33
4	C	3000	SFD	C2A-N1A	4.98	1.43	1.33
6	A	1303	AMP	C2'-C1'	4.83	1.60	1.53
5	B	1100	SF4	S4-FE2	-4.75	2.30	2.33
5	B	1100	SF4	S3-FE1	-4.73	2.30	2.33
5	D	3110	SF4	S1-FE2	-4.65	2.30	2.33
4	C	3000	SFD	C2R-C3R	4.56	1.63	1.53
4	A	1000	SFD	C2R-C3R	4.52	1.62	1.53
4	A	1000	SFD	PA-OP3	-4.44	1.35	1.55
4	A	1000	SFD	C8R-C9R	4.38	1.65	1.53
4	A	1000	SFD	O2F-C2F	-4.37	1.16	1.24
4	A	1000	SFD	PF-OP	-4.30	1.52	1.59
5	B	1110	SF4	S1-FE3	-4.24	2.30	2.33
4	C	3000	SFD	C6F-N5F	4.24	1.48	1.44
4	C	3000	SFD	O2F-C2F	-4.22	1.16	1.24
4	C	3000	SFD	PA-OP3	-4.08	1.36	1.55
4	C	3000	SFD	C8R-C9R	4.07	1.64	1.53
4	C	3000	SFD	C1F-C8F	4.06	1.46	1.39
4	A	1000	SFD	C8A-N9A	4.05	1.42	1.36
6	C	1301	AMP	C2-N3	3.96	1.40	1.32
6	A	1303	AMP	O4'-C4'	-3.92	1.35	1.45
6	A	1303	AMP	C2-N1	3.91	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1302	AMP	C2-N3	3.90	1.39	1.32
6	A	1303	AMP	C2-N3	3.88	1.39	1.32
4	A	1000	SFD	C2F-N3F	3.83	1.49	1.39
4	A	1000	SFD	C4R-C3R	-3.81	1.45	1.53
4	C	3000	SFD	O9R-C6R	3.79	1.47	1.41
4	A	1000	SFD	C5M-C4A	3.78	1.49	1.40
4	A	1000	SFD	O9R-C6R	3.78	1.47	1.41
6	A	1302	AMP	P-O2P	-3.74	1.41	1.54
6	C	1301	AMP	P-O2P	-3.73	1.41	1.54
6	A	1303	AMP	P-O2P	-3.67	1.41	1.54
5	B	1100	SF4	S1-FE4	-3.67	2.30	2.33
6	C	1301	AMP	C2'-C1'	3.65	1.58	1.53
6	A	1303	AMP	O5'-C5'	3.63	1.59	1.44
4	C	3000	SFD	C8A-N7A	-3.63	1.27	1.34
4	C	3000	SFD	C4A-N9A	-3.63	1.32	1.37
4	C	3000	SFD	C8A-N9A	3.55	1.41	1.36
4	C	3000	SFD	PF-OP	-3.55	1.53	1.59
4	C	3000	SFD	C0F-N1F	3.52	1.40	1.31
5	D	3110	SF4	S4-FE2	-3.49	2.30	2.33
6	A	1303	AMP	C5-C4	3.38	1.48	1.40
4	A	1000	SFD	C6F-N5F	-3.37	1.40	1.44
6	C	1301	AMP	C2-N1	3.37	1.40	1.33
6	A	1302	AMP	C2'-C1'	3.35	1.58	1.53
6	A	1302	AMP	P-O5'	-3.34	1.48	1.60
6	C	1301	AMP	C5'-C4'	3.30	1.62	1.51
4	A	1000	SFD	C1F-C8F	3.28	1.45	1.39
4	C	3000	SFD	C2F-N3F	3.28	1.47	1.39
4	A	1000	SFD	C0F-N1F	3.27	1.40	1.31
6	C	1301	AMP	P-O5'	-3.23	1.48	1.60
4	A	1000	SFD	O3-S	3.23	1.45	1.42
5	B	1110	SF4	S3-FE1	3.21	2.35	2.33
6	A	1302	AMP	C5'-C4'	3.21	1.62	1.51
6	A	1303	AMP	C5'-C4'	3.19	1.62	1.51
6	A	1302	AMP	C2-N1	3.17	1.40	1.33
6	C	1301	AMP	O4'-C1'	3.17	1.46	1.41
6	A	1302	AMP	O4'-C1'	3.14	1.46	1.41
4	A	1000	SFD	C6R-N9A	-3.12	1.39	1.48
4	A	1000	SFD	CBF-C6F	3.10	1.45	1.39
4	C	3000	SFD	CBF-C6F	2.85	1.44	1.39
6	C	1301	AMP	O5'-C5'	2.83	1.56	1.44
5	D	3100	SF4	S3-FE1	-2.80	2.31	2.33
6	A	1302	AMP	O5'-C5'	2.72	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3000	SFD	C6R-N9A	-2.71	1.40	1.48
5	D	3110	SF4	S1-FE4	-2.71	2.31	2.33
4	A	1000	SFD	PF-OP1	-2.70	1.43	1.55
4	A	1000	SFD	C8A-N7A	-2.62	1.29	1.34
6	C	1301	AMP	C8-N9	2.57	1.40	1.36
4	C	3000	SFD	O2R-C2R	-2.57	1.37	1.43
6	A	1302	AMP	O4'-C4'	-2.57	1.39	1.45
4	C	3000	SFD	PF-OP1	-2.51	1.43	1.55
6	A	1302	AMP	C8-N9	2.47	1.40	1.36
4	C	3000	SFD	C4R-C3R	-2.44	1.48	1.53
4	A	1000	SFD	C6A-N1A	2.34	1.48	1.37
6	C	1301	AMP	O4'-C4'	-2.32	1.39	1.45
6	A	1303	AMP	P-O5'	-2.32	1.52	1.60
5	D	3110	SF4	S3-FE1	2.20	2.34	2.33
4	A	1000	SFD	C0R-C9R	2.20	1.58	1.51
6	A	1303	AMP	O4'-C1'	2.18	1.44	1.41
4	C	3000	SFD	C5M-N7A	-2.16	1.32	1.40
6	A	1303	AMP	C4-N9	-2.11	1.34	1.37
4	A	1000	SFD	C5F-N5F	-2.03	1.46	1.49
4	C	3000	SFD	C0R-C9R	2.02	1.58	1.51

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1301	AMP	O4'-C1'-N9	19.16	126.26	108.44
6	A	1302	AMP	O4'-C1'-N9	18.26	125.43	108.44
6	A	1303	AMP	O4'-C1'-N9	14.72	122.13	108.44
6	A	1302	AMP	N3-C2-N1	-12.23	118.49	128.71
4	C	3000	SFD	C5F-N5F-S	-12.21	97.23	117.39
6	C	1301	AMP	N3-C2-N1	-12.09	118.60	128.71
6	A	1303	AMP	C8-N9-C4	-10.66	98.76	106.90
6	A	1303	AMP	C1'-N9-C4	9.62	143.25	126.64
6	A	1303	AMP	N3-C2-N1	-8.93	121.24	128.71
4	A	1000	SFD	N3A-C2A-N1A	-8.68	121.45	128.71
6	C	1301	AMP	C1'-N9-C4	7.97	140.41	126.64
6	A	1302	AMP	C2'-C1'-N9	7.91	133.56	113.27
6	C	1301	AMP	C2'-C1'-N9	7.70	133.04	113.27
4	C	3000	SFD	N3A-C2A-N1A	-7.61	122.35	128.71
6	A	1302	AMP	C1'-N9-C4	7.44	139.49	126.64
4	A	1000	SFD	C5F-N5F-S	-6.92	105.97	117.39
4	C	3000	SFD	O9R-C6R-C7R	-6.74	96.44	106.77
4	C	3000	SFD	C6F-N5F-S	-6.68	97.80	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1303	AMP	O4'-C1'-C2'	-6.67	96.55	106.77
4	C	3000	SFD	CBF-C6F-N5F	-6.27	113.19	121.62
4	C	3000	SFD	C0F-C5F-N5F	6.16	122.63	108.57
4	A	1000	SFD	O9R-C6R-C7R	-5.90	97.72	106.77
6	C	1301	AMP	C8-N9-C4	-5.76	102.50	106.90
6	A	1302	AMP	C4'-O4'-C1'	5.72	115.96	109.75
6	A	1302	AMP	C8-N9-C4	-5.50	102.70	106.90
4	A	1000	SFD	O9R-C9R-C8R	5.26	115.84	105.17
4	A	1000	SFD	C0F-C5F-N5F	5.25	120.53	108.57
4	C	3000	SFD	C7R-C8R-C9R	-5.16	92.38	102.65
4	A	1000	SFD	C7R-C6R-N9A	5.14	126.47	113.27
6	A	1302	AMP	O3'-C3'-C4'	-5.12	95.99	111.08
4	A	1000	SFD	CBF-C6F-N5F	-5.12	114.73	121.62
4	A	1000	SFD	C7R-C8R-C9R	-5.11	92.47	102.65
6	C	1301	AMP	O3'-C3'-C4'	-5.08	96.12	111.08
4	C	3000	SFD	O9R-C9R-C8R	5.06	115.43	105.17
6	C	1301	AMP	C4'-O4'-C1'	4.96	115.14	109.75
6	A	1303	AMP	O3'-C3'-C4'	-4.92	96.58	111.08
6	A	1303	AMP	C4'-O4'-C1'	4.88	115.05	109.75
6	C	1301	AMP	C8-N9-C1'	-4.72	117.09	126.38
4	A	1000	SFD	O7R-C7R-C6R	-4.63	97.22	111.23
4	C	3000	SFD	O7R-C7R-C6R	-4.46	97.75	111.23
4	C	3000	SFD	C8R-C7R-C6R	4.44	107.86	100.91
6	A	1302	AMP	C8-N9-C1'	-4.35	117.81	126.38
4	A	1000	SFD	C8R-C7R-C6R	4.31	107.66	100.91
6	A	1303	AMP	C8-N9-C1'	-4.26	117.98	126.38
4	A	1000	SFD	O3-S-O1	-4.23	106.57	118.27
4	C	3000	SFD	C7R-C6R-N9A	4.05	123.66	113.27
4	A	1000	SFD	C6F-N5F-S	-4.05	106.53	119.96
6	C	1301	AMP	O4'-C1'-C2'	-3.97	100.68	106.77
4	A	1000	SFD	O4R-C4R-C3R	3.92	118.80	109.05
6	A	1302	AMP	O4'-C1'-C2'	-3.87	100.84	106.77
4	C	3000	SFD	C1F-C9F-C6F	-3.86	114.02	119.83
4	C	3000	SFD	CBF-C6F-C9F	3.84	125.61	119.83
4	A	1000	SFD	C6F-N5F-C5F	3.81	122.82	115.76
6	A	1303	AMP	O4'-C4'-C3'	-3.66	97.75	105.17
4	C	3000	SFD	C4A-C5M-N7A	-3.57	106.46	109.52
4	C	3000	SFD	O4R-C4R-C3R	3.57	117.94	109.05
4	C	3000	SFD	O3-S-O1	-3.52	108.52	118.27
6	C	1301	AMP	C2-N1-C6	3.46	125.02	118.77
4	A	1000	SFD	O1-S-N5F	3.41	116.21	109.41
4	A	1000	SFD	C1F-C9F-C6F	-3.39	114.72	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1302	AMP	C2-N1-C6	3.39	124.89	118.77
4	A	1000	SFD	CBF-C6F-C9F	3.37	124.91	119.83
6	A	1303	AMP	N7-C8-N9	3.33	123.79	114.36
4	C	3000	SFD	C6A-C5M-C4A	-3.05	111.65	117.25
4	A	1000	SFD	OP1-PF-OP	3.01	119.42	105.14
6	C	1301	AMP	C4-C5-N7	2.97	112.06	109.52
4	C	3000	SFD	C1F-C9F-N10	2.96	126.19	121.96
4	C	3000	SFD	O2R-C2R-C3R	2.95	116.40	109.05
6	A	1303	AMP	C4-C5-N7	2.94	112.04	109.52
4	C	3000	SFD	C5M-C6A-N9	-2.95	114.06	120.72
4	A	1000	SFD	O2R-C2R-C3R	2.93	116.34	109.05
4	A	1000	SFD	PA-OP-PF	-2.92	123.13	131.68
6	A	1303	AMP	C2-N1-C6	2.90	124.00	118.77
4	A	1000	SFD	O2F-C2F-N3F	2.89	124.21	118.39
6	A	1302	AMP	C4-C5-N7	2.86	111.97	109.52
4	A	1000	SFD	C1F-C9F-N10	2.75	125.90	121.96
6	A	1303	AMP	C2'-C3'-C4'	2.75	108.13	102.65
4	A	1000	SFD	O3-S-N5F	-2.74	103.95	109.41
4	C	3000	SFD	C8A-N9A-C4A	-2.74	104.81	106.90
6	A	1303	AMP	O5'-P-O1P	2.68	114.55	106.71
4	A	1000	SFD	C2F-N1F-C0F	2.67	125.80	115.78
6	A	1303	AMP	O3P-P-O1P	-2.67	101.72	110.44
4	A	1000	SFD	N3A-C4A-N9A	2.67	130.25	125.43
4	C	3000	SFD	PA-OP-PF	-2.66	123.87	131.68
4	C	3000	SFD	OP1-PF-OP	2.66	117.74	105.14
6	A	1303	AMP	O2P-P-O5'	-2.61	99.45	106.65
4	A	1000	SFD	C3F-C8F-C7F	2.60	126.74	120.74
4	A	1000	SFD	C5M-C4A-N9A	-2.60	103.41	107.16
4	C	3000	SFD	C3F-C8F-C7F	2.59	126.72	120.74
6	A	1302	AMP	O3P-P-O1P	-2.58	102.01	110.44
4	C	3000	SFD	C2F-N1F-C0F	2.54	125.30	115.78
6	C	1301	AMP	O3P-P-O1P	-2.53	102.17	110.44
6	A	1303	AMP	O3P-P-O2P	2.53	117.46	107.61
6	A	1302	AMP	C3'-C2'-C1'	2.52	104.86	100.91
4	C	3000	SFD	O4R-C4R-C5R	-2.51	104.97	110.12
6	C	1301	AMP	C3'-C2'-C1'	2.51	104.83	100.91
6	A	1303	AMP	N6-C6-N1	2.50	124.28	119.36
6	A	1302	AMP	O2P-P-O5'	-2.46	99.87	106.65
6	A	1302	AMP	C6-C5-C4	-2.46	112.73	117.25
4	A	1000	SFD	C5R-C4R-C3R	-2.45	107.43	112.06
6	C	1301	AMP	O2P-P-O5'	-2.39	100.04	106.65
4	C	3000	SFD	C6F-N5F-C5F	2.38	120.18	115.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1000	SFD	O3R-C3R-C4R	2.31	114.57	108.74
6	C	1301	AMP	N6-C6-N1	2.30	123.89	119.36
4	C	3000	SFD	O2F-C2F-N3F	2.30	123.02	118.39
6	A	1303	AMP	O2'-C2'-C1'	2.29	118.16	111.23
6	C	1301	AMP	O3P-P-O5'	2.28	112.95	106.65
4	C	3000	SFD	C2R-C1R-N10	2.28	120.15	110.54
6	A	1302	AMP	O3P-P-O5'	2.28	112.95	106.65
6	C	1301	AMP	C6-C5-C4	-2.28	113.07	117.25
6	A	1303	AMP	O3P-P-O5'	2.27	112.91	106.65
4	C	3000	SFD	C0R-C9R-C8R	-2.26	106.16	115.21
6	C	1301	AMP	O2'-C2'-C1'	2.25	118.03	111.23
4	C	3000	SFD	C1F-C8F-C7F	-2.18	115.94	119.59
6	A	1302	AMP	C2'-C3'-C4'	2.14	106.93	102.65
6	A	1302	AMP	O2'-C2'-C1'	2.13	117.66	111.23
4	A	1000	SFD	C2R-C1R-N10	2.11	119.44	110.54
4	C	3000	SFD	C9F-C1F-C8F	2.11	124.50	119.37
4	A	1000	SFD	C0R-C9R-C8R	-2.11	106.78	115.21
4	A	1000	SFD	O7R-C7R-C8R	2.10	118.68	111.83
4	C	3000	SFD	C1R-N10-C9F	-2.09	116.74	120.46
4	A	1000	SFD	C9F-C1F-C8F	2.09	124.45	119.37
4	A	1000	SFD	O2-S-O3	-2.08	106.62	114.56
6	A	1302	AMP	O3P-P-O2P	2.06	115.64	107.61
4	C	3000	SFD	C5R-C4R-C3R	-2.05	108.19	112.06
4	A	1000	SFD	O4R-C4R-C5R	-2.04	105.93	110.12
6	A	1303	AMP	C2'-C1'-N9	2.03	118.47	113.27
4	C	3000	SFD	N3A-C4A-N9A	2.03	129.09	125.43
6	C	1301	AMP	C2'-C3'-C4'	2.02	106.68	102.65
6	C	1301	AMP	O3P-P-O2P	2.02	115.46	107.61
4	A	1000	SFD	OP3-PA-OP	2.01	114.67	105.14

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1303	AMP	C1'
6	C	1301	AMP	C1'
4	C	3000	SFD	C5F
6	A	1302	AMP	C1'
4	A	1000	SFD	C5F

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.