



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:28 AM UTC

PDB ID : 3E9Z / pdb_00003e9z
Title : Crystal structure of purine nucleoside phosphorylase from *Schistosoma mansoni* in complex with 6-chloroguanine
Authors : Pereira, H.M.; Rezende, M.M.; Oliva, G.; Garratt, R.C.
Deposited on : 2008-08-24
Resolution : 2.31 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
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

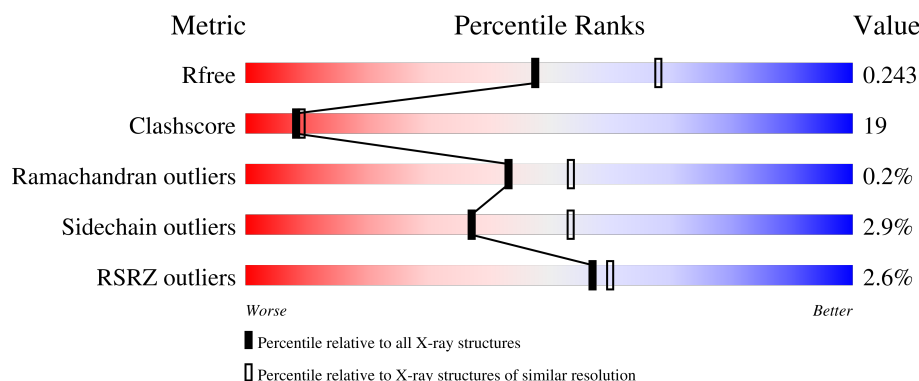
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	287	2% 64% 30% • •
1	B	287	3% 69% 23% • 6%
1	C	287	2% 67% 30% • •

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	6GU	A	704	-	X	X	-
4	6GU	C	704	-	X	X	-

2 Entry composition [i](#)

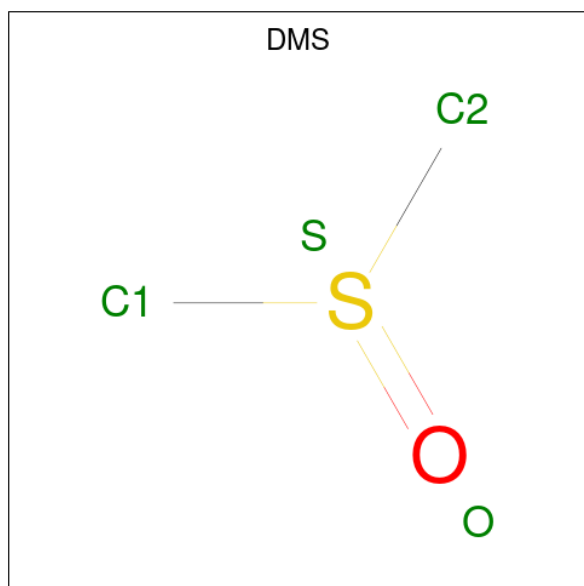
There are 6 unique types of molecules in this entry. The entry contains 7055 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Purine-nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2127	1356	365	392	14			
1	B	270	Total	C	N	O	S	0	0	0
			2049	1309	351	375	14			
1	C	283	Total	C	N	O	S	0	0	0
			2142	1367	370	391	14			

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



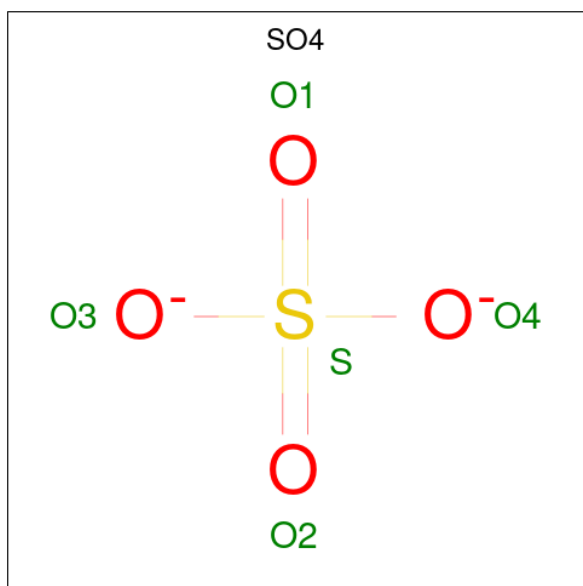
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

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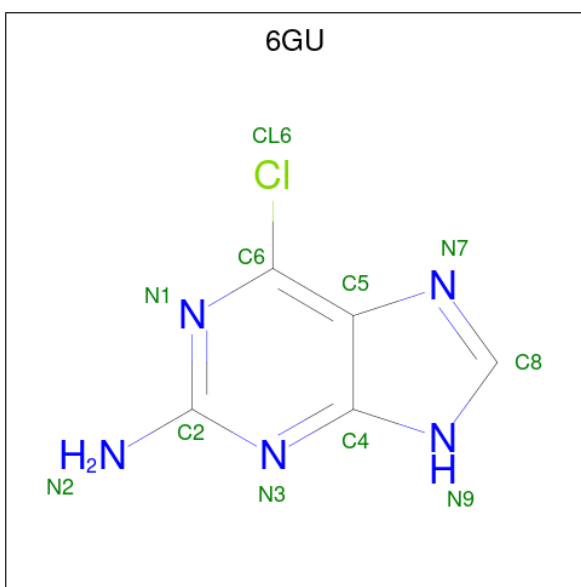
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



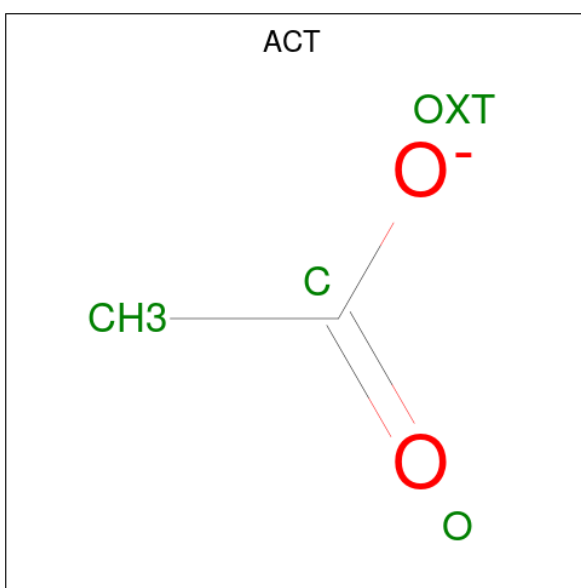
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 6-chloroguanine (CCD ID: 6GU) (formula: C₅H₄ClN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			11	5	1	5		
4	C	1	Total	C	Cl	N	0	0
			11	5	1	5		

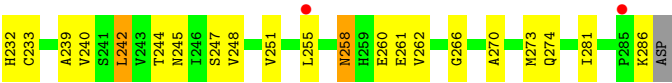
- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total 213	O 213	0	0
6	B	216	Total 216	O 216	0	0
6	C	251	Total 251	O 251	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.82Å 118.12Å 129.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.63 – 2.31 56.63 – 2.31	Depositor EDS
% Data completeness (in resolution range)	91.0 (56.63-2.31) 90.9 (56.63-2.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.177 , 0.249 0.169 , 0.243	Depositor DCC
R_{free} test set	1480 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7055	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, 6GU, SO4, ACT

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	0.58	0/2163	0.90	3/2927 (0.1%)
1	B	0.58	0/2081	0.92	8/2813 (0.3%)
1	C	0.61	0/2180	0.87	4/2954 (0.1%)
All	All	0.59	0/6424	0.89	15/8694 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ARG	NE-CZ-NH2	10.96	129.07	119.20
1	B	269	ARG	NE-CZ-NH1	-9.60	111.90	121.50
1	A	251	VAL	CB-CA-C	-8.11	99.12	112.26
1	B	269	ARG	CD-NE-CZ	7.69	135.17	124.40
1	B	268	GLN	CA-C-N	-7.33	109.16	120.31
1	B	268	GLN	C-N-CA	-7.33	109.16	120.31
1	A	256	LYS	N-CA-C	6.75	114.08	108.07
1	C	224	ILE	N-CA-CB	6.67	114.99	110.52
1	B	224	ILE	CB-CA-C	-6.30	107.72	113.70
1	B	224	ILE	N-CA-CB	5.78	114.39	110.52
1	A	224	ILE	CB-CA-C	-5.54	108.44	113.70
1	C	61	THR	CA-C-N	-5.53	112.07	121.85
1	C	61	THR	C-N-CA	-5.53	112.07	121.85
1	C	224	ILE	CB-CA-C	-5.53	108.45	113.70
1	B	5	VAL	N-CA-CB	5.04	116.02	110.53

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	2127	0	2179	103	1
1	B	2049	0	2092	62	1
1	C	2142	0	2198	88	0
2	A	8	0	12	2	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	11	0	4	10	0
4	C	11	0	4	10	0
5	B	4	0	3	1	0
6	A	213	0	0	15	0
6	B	216	0	0	12	0
6	C	251	0	0	12	0
All	All	7055	0	6504	247	1

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 19.

All (247) 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:61:THR:O	1:A:62:SER:HB2	1.53	1.05
1:C:165:SER:HB2	6:C:804:HOH:O	1.55	1.04
5:B:700:ACT:H1	6:B:1034:HOH:O	1.72	0.89
1:A:245:ASN:ND2	4:A:704:6GU:N7	2.22	0.87
1:A:258:ASN:HD22	1:A:261:GLU:H	1.23	0.87
1:C:48:ILE:HD11	6:C:861:HOH:O	1.75	0.87
1:C:59:PRO:HB3	1:C:97:THR:HG23	1.58	0.86
1:A:59:PRO:HB3	1:A:97:THR:HG23	1.57	0.85
1:B:59:PRO:HB3	1:B:97:THR:HG23	1.58	0.83
1:A:39:LYS:HB2	6:A:794:HOH:O	1.79	0.83
1:C:221:MET:HG2	4:C:704:6GU:HN2A	1.45	0.81
1:B:173:ARG:HE	1:B:191:GLN:NE2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:HE	1:C:191:GLN:NE2	1.78	0.81
1:A:242:LEU:HD13	1:A:266:GLY:HA2	1.61	0.80
1:A:120:GLY:HA3	4:A:704:6GU:CL6	2.19	0.80
1:A:173:ARG:HE	1:A:191:GLN:NE2	1.81	0.79
1:A:173:ARG:HE	1:A:191:GLN:HE22	1.31	0.78
1:A:62:SER:HA	1:A:67:SER:HA	1.64	0.78
1:A:61:THR:O	1:A:62:SER:CB	2.29	0.77
1:A:17:HIS:HB3	6:A:777:HOH:O	1.84	0.76
1:C:173:ARG:HE	1:C:191:GLN:HE22	1.34	0.76
1:C:31:ILE:HG21	1:C:40:LEU:HD23	1.68	0.76
1:A:48:ILE:HD11	6:A:765:HOH:O	1.86	0.75
1:B:31:ILE:HG21	1:B:40:LEU:HD23	1.67	0.75
1:B:173:ARG:HE	1:B:191:GLN:HE22	1.34	0.74
1:A:242:LEU:CD1	1:A:266:GLY:HA2	2.17	0.73
1:B:286:LYS:HG3	6:B:1004:HOH:O	1.90	0.72
4:A:704:6GU:CL6	6:A:739:HOH:O	2.45	0.71
1:C:286:LYS:HB3	6:C:983:HOH:O	1.90	0.71
1:B:59:PRO:HB2	1:B:87:PHE:CZ	2.25	0.71
1:C:59:PRO:HB2	1:C:87:PHE:CE1	2.26	0.70
1:A:62:SER:HA	1:A:67:SER:CA	2.20	0.70
1:C:221:MET:CG	4:C:704:6GU:HN2A	2.04	0.70
1:C:59:PRO:HB2	1:C:87:PHE:CZ	2.27	0.69
1:A:203:GLU:OE2	4:A:704:6GU:N2	2.25	0.69
1:C:35:SER:HB2	6:C:911:HOH:O	1.94	0.68
1:A:258:ASN:HD21	1:A:260:GLU:HB2	1.59	0.67
1:A:258:ASN:ND2	1:A:261:GLU:HG3	2.09	0.67
1:C:258:ASN:ND2	1:C:261:GLU:H	1.90	0.67
1:A:59:PRO:HB2	1:A:87:PHE:CE1	2.30	0.67
1:B:54:LYS:HD2	6:B:986:HOH:O	1.93	0.67
1:B:59:PRO:HB2	1:B:87:PHE:CE1	2.30	0.67
1:A:140:LEU:O	2:A:705:DMS:H22	1.95	0.66
1:A:59:PRO:HB2	1:A:87:PHE:CZ	2.30	0.66
1:C:258:ASN:HD21	1:C:261:GLU:H	1.44	0.65
1:A:258:ASN:ND2	1:A:261:GLU:H	1.93	0.65
1:A:245:ASN:OD1	4:A:704:6GU:CL6	2.52	0.64
1:A:62:SER:HA	1:A:67:SER:N	2.12	0.63
1:A:221:MET:CG	4:A:704:6GU:HN2A	2.12	0.63
1:A:221:MET:HG2	4:A:704:6GU:HN2A	1.64	0.62
1:C:166:ASN:HA	6:C:766:HOH:O	1.98	0.62
1:A:177:VAL:O	1:A:181:GLU:HG2	2.00	0.61
1:B:177:VAL:O	1:B:181:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:VAL:HG21	1:C:255:LEU:O	2.00	0.60
1:C:221:MET:HG2	4:C:704:6GU:N2	2.17	0.59
1:C:41:ALA:HB1	1:C:71:ILE:HD12	1.84	0.59
1:B:195:VAL:HB	1:B:216:CYS:SG	2.42	0.59
1:C:177:VAL:O	1:C:181:GLU:HG2	2.02	0.59
1:B:287:ASP:HB2	6:B:1048:HOH:O	2.02	0.59
1:A:248:VAL:HG22	1:A:255:LEU:HD21	1.85	0.59
1:B:131:PHE:CE2	1:B:273:MET:HE3	2.38	0.58
1:C:162:PRO:HG3	1:C:232:HIS:HD2	1.69	0.58
1:B:162:PRO:HG3	1:B:232:HIS:HD2	1.69	0.57
1:A:131:PHE:CE2	1:A:273:MET:HE3	2.39	0.57
1:A:135:LYS:O	1:C:251:VAL:HG21	2.05	0.57
1:A:253:SER:OG	1:A:255:LEU:HD22	2.05	0.57
1:A:274:GLN:HB2	6:A:794:HOH:O	2.05	0.57
1:A:41:ALA:HB1	1:A:71:ILE:HD12	1.87	0.57
1:A:127:LYS:HE3	6:A:758:HOH:O	2.04	0.56
1:A:248:VAL:HG22	1:A:255:LEU:CD2	2.35	0.56
1:C:131:PHE:CE2	1:C:273:MET:HE3	2.40	0.56
1:B:59:PRO:HD3	1:B:100:LEU:HD22	1.87	0.56
1:B:47:LYS:HA	1:B:72:PHE:O	2.05	0.56
1:C:258:ASN:HD22	1:C:260:GLU:H	1.53	0.56
1:A:271:GLU:HB2	6:A:747:HOH:O	2.05	0.56
1:C:61:THR:HG21	1:C:86:ARG:O	2.05	0.56
1:A:194:TYR:CD1	1:A:224:ILE:HD11	2.40	0.56
1:C:59:PRO:HD3	1:C:100:LEU:HD22	1.87	0.56
1:A:111:LYS:HE2	6:A:812:HOH:O	2.06	0.56
1:A:44:VAL:HG12	1:A:47:LYS:HB3	1.88	0.55
1:B:251:VAL:HG21	1:C:135:LYS:O	2.07	0.55
1:A:59:PRO:HD3	1:A:100:LEU:HD22	1.87	0.55
1:A:135:LYS:HE3	6:A:879:HOH:O	2.05	0.55
1:B:23:THR:CB	1:B:48:ILE:HD12	2.37	0.55
1:B:58:PHE:CD2	1:B:59:PRO:HD2	2.42	0.55
1:C:37:LEU:HD22	1:C:40:LEU:HD22	1.88	0.55
1:A:162:PRO:HG3	1:A:232:HIS:HD2	1.72	0.55
1:A:47:LYS:HA	1:A:72:PHE:O	2.07	0.54
1:A:37:LEU:HD11	1:A:277:PHE:CE2	2.43	0.54
1:B:41:ALA:HB1	1:B:71:ILE:HD12	1.89	0.54
1:A:175:LEU:HD13	1:A:280:ILE:HG23	1.90	0.54
1:C:47:LYS:HA	1:C:72:PHE:O	2.07	0.54
1:B:12:VAL:HG12	1:B:107:LEU:HD12	1.90	0.54
1:B:27:PRO:HD2	1:B:108:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:HD3	1:B:286:LYS:HD2	1.89	0.53
1:B:194:TYR:CD1	1:B:224:ILE:HD11	2.43	0.53
1:B:40:LEU:HD11	1:B:75:LEU:HD21	1.90	0.53
1:C:44:VAL:HG12	1:C:47:LYS:HB3	1.90	0.53
1:A:174:LYS:NZ	6:A:889:HOH:O	2.41	0.52
1:C:194:TYR:CD1	1:C:224:ILE:HD11	2.45	0.52
1:A:251:VAL:HG11	1:B:135:LYS:O	2.09	0.52
1:C:58:PHE:CD2	1:C:59:PRO:HD2	2.45	0.52
1:C:157:PHE:O	1:C:233:CYS:HA	2.09	0.52
1:B:159:THR:HG22	6:B:962:HOH:O	2.10	0.52
1:C:42:ASP:HB2	6:C:948:HOH:O	2.10	0.52
1:A:205:PRO:HG2	1:A:251:VAL:HA	1.92	0.52
1:C:245:ASN:ND2	4:C:704:6GU:N7	2.56	0.52
1:B:285:PRO:HA	6:B:1014:HOH:O	2.10	0.52
1:C:23:THR:CB	1:C:48:ILE:HD12	2.40	0.52
1:C:221:MET:CG	4:C:704:6GU:N2	2.73	0.51
1:C:61:THR:OG1	1:C:87:PHE:CE1	2.60	0.51
1:C:208:CYS:SG	1:C:247:SER:HB3	2.51	0.51
1:C:258:ASN:OD1	1:C:261:GLU:HG3	2.11	0.51
1:B:23:THR:HB	1:B:48:ILE:HD12	1.92	0.51
1:A:23:THR:CB	1:A:48:ILE:HD12	2.41	0.50
1:A:157:PHE:O	1:A:233:CYS:HA	2.12	0.50
1:B:168:TYR:O	1:B:173:ARG:HD3	2.10	0.50
1:C:40:LEU:HD11	1:C:75:LEU:HD21	1.93	0.50
1:B:155:GLU:OE2	6:B:1093:HOH:O	2.20	0.50
1:C:12:VAL:HG12	1:C:107:LEU:HD12	1.94	0.50
1:B:44:VAL:HG12	1:B:47:LYS:HB3	1.92	0.49
1:C:145:LEU:HA	6:C:878:HOH:O	2.11	0.49
1:C:220:GLY:HA2	4:C:704:6GU:N3	2.26	0.49
1:A:31:ILE:HG21	1:A:40:LEU:CD1	2.41	0.49
1:B:135:LYS:HE3	6:B:1088:HOH:O	2.11	0.49
1:A:23:THR:HB	1:A:48:ILE:HD12	1.93	0.49
1:A:89:MET:HE3	6:A:745:HOH:O	2.12	0.49
1:A:58:PHE:CD2	1:A:59:PRO:HD2	2.48	0.49
1:A:14:LYS:NZ	6:A:839:HOH:O	2.46	0.49
1:A:27:PRO:HD2	1:A:108:LEU:O	2.13	0.49
1:A:31:ILE:HD13	1:A:40:LEU:CD1	2.43	0.49
1:B:78:ARG:CD	1:B:286:LYS:HD2	2.43	0.49
1:A:195:VAL:HB	1:A:216:CYS:SG	2.53	0.49
1:C:195:VAL:HB	1:C:216:CYS:SG	2.53	0.49
1:B:157:PHE:O	1:B:233:CYS:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:OD1	1:C:204:THR:HB	2.12	0.48
1:A:166:ASN:HA	6:A:730:HOH:O	2.13	0.48
1:C:220:GLY:HA2	4:C:704:6GU:C2	2.43	0.48
1:A:168:TYR:O	1:A:173:ARG:HD3	2.12	0.48
1:B:140:LEU:HB2	1:B:141:PRO:HD3	1.96	0.48
1:B:166:ASN:HA	6:B:943:HOH:O	2.14	0.48
1:C:127:LYS:HG3	6:C:853:HOH:O	2.13	0.48
1:C:27:PRO:HD2	1:C:108:LEU:O	2.13	0.48
1:A:117:ASN:HA	3:A:291:SO4:O4	2.14	0.48
1:A:40:LEU:HD23	1:A:274:GLN:HG3	1.94	0.48
1:A:12:VAL:HG12	1:A:107:LEU:HD12	1.95	0.48
1:A:78:ARG:HD3	1:A:286:LYS:HD2	1.96	0.48
1:B:141:PRO:HB3	1:C:145:LEU:HB2	1.95	0.48
1:A:40:LEU:CD2	1:A:75:LEU:HD21	2.43	0.47
1:C:17:HIS:HA	1:C:20:GLN:HE21	1.79	0.47
1:C:61:THR:OG1	1:C:87:PHE:CZ	2.67	0.47
1:A:31:ILE:HD13	1:A:40:LEU:HD13	1.96	0.47
1:C:36:GLY:O	1:C:270:ALA:HA	2.14	0.47
1:B:31:ILE:HD13	1:B:40:LEU:HD21	1.96	0.47
1:C:78:ARG:HD3	1:C:286:LYS:HD2	1.96	0.47
1:A:194:TYR:HD1	1:A:224:ILE:HD11	1.79	0.47
1:C:23:THR:HB	1:C:48:ILE:HD12	1.96	0.47
1:C:94:SER:HB2	6:C:920:HOH:O	2.14	0.47
1:B:17:HIS:HA	1:B:20:GLN:HE21	1.81	0.46
1:C:168:TYR:O	1:C:173:ARG:HD3	2.15	0.46
1:A:141:PRO:HB3	1:B:145:LEU:HB2	1.97	0.46
1:B:154:GLN:HB3	6:B:977:HOH:O	2.15	0.46
1:A:145:LEU:HB2	1:C:141:PRO:HB3	1.98	0.46
1:A:203:GLU:OE1	4:A:704:6GU:N1	2.49	0.46
1:B:31:ILE:HD11	1:B:281:ILE:HD11	1.98	0.46
1:C:28:GLU:HG3	6:C:807:HOH:O	2.15	0.46
1:B:208:CYS:SG	1:B:247:SER:HB3	2.56	0.46
1:B:287:ASP:OD2	1:B:287:ASP:N	2.50	0.45
1:A:31:ILE:HD11	1:A:281:ILE:HD11	1.99	0.45
1:A:159:THR:HG22	6:A:737:HOH:O	2.16	0.45
1:B:129:GLY:O	1:B:269:ARG:HD2	2.16	0.45
1:A:99:ALA:CB	2:A:703:DMS:H13	2.47	0.45
1:A:244:THR:OG1	4:A:704:6GU:H8	2.15	0.45
1:A:37:LEU:HD22	1:A:40:LEU:HG	1.98	0.45
1:B:115:VAL:O	1:B:239:ALA:HA	2.17	0.45
1:C:78:ARG:CD	1:C:286:LYS:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:GLN:NE2	6:C:739:HOH:O	2.40	0.45
1:C:231:ARG:HD2	1:C:231:ARG:HA	1.75	0.45
1:B:100:LEU:HB3	1:B:101:PRO:HD3	1.98	0.44
1:C:140:LEU:HB2	1:C:141:PRO:HD3	1.99	0.44
1:A:40:LEU:HD22	1:A:75:LEU:HD21	2.00	0.44
1:C:70:LEU:HD12	1:C:70:LEU:HA	1.91	0.44
1:C:197:ASN:O	1:C:221:MET:HA	2.18	0.44
1:C:31:ILE:HD13	1:C:40:LEU:HD21	1.99	0.43
1:A:115:VAL:O	1:A:239:ALA:HA	2.19	0.43
1:C:116:SER:HA	1:C:240:VAL:O	2.18	0.43
1:C:205:PRO:HG2	1:C:251:VAL:HA	2.01	0.43
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.81	0.43
1:C:115:VAL:O	1:C:239:ALA:HA	2.19	0.43
1:C:242:LEU:CD1	1:C:266:GLY:HA2	2.48	0.43
1:A:244:THR:HB	1:A:262:VAL:HA	2.00	0.43
1:B:137:HIS:HA	1:B:194:TYR:O	2.19	0.43
1:A:140:LEU:HB2	1:A:141:PRO:HD3	2.00	0.43
1:C:203:GLU:OE2	4:C:704:6GU:N2	2.47	0.43
1:A:36:GLY:HA2	1:A:270:ALA:HA	2.01	0.43
1:A:116:SER:HA	1:A:240:VAL:O	2.19	0.42
1:A:174:LYS:O	1:A:178:GLN:HG3	2.19	0.42
1:B:41:ALA:HB1	1:B:71:ILE:CD1	2.49	0.42
1:A:31:ILE:HG21	1:A:40:LEU:HD13	2.01	0.42
1:A:36:GLY:O	1:A:270:ALA:HA	2.18	0.42
1:C:31:ILE:HD11	1:C:281:ILE:HD11	2.01	0.42
1:C:118:ALA:HB1	4:C:704:6GU:H8	2.01	0.42
1:A:133:ILE:CG2	1:A:173:ARG:HG2	2.49	0.42
1:B:61:THR:O	6:B:1098:HOH:O	2.22	0.42
1:B:27:PRO:HG3	1:B:72:PHE:CE2	2.55	0.42
1:A:120:GLY:CA	4:A:704:6GU:CL6	2.98	0.42
1:B:78:ARG:HD3	1:B:286:LYS:CD	2.50	0.42
1:C:27:PRO:HG3	1:C:72:PHE:CE2	2.55	0.42
1:B:27:PRO:HG3	1:B:72:PHE:HE2	1.85	0.41
1:C:37:LEU:O	1:C:38:GLY:C	2.62	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.85	0.41
1:A:37:LEU:HD22	1:A:40:LEU:HD12	2.03	0.41
1:A:242:LEU:HD11	1:A:269:ARG:HB2	2.03	0.41
1:C:174:LYS:O	1:C:178:GLN:HG3	2.20	0.41
1:A:78:ARG:CD	1:A:286:LYS:HD2	2.50	0.41
1:A:32:ILE:HG13	1:A:113:LEU:HD11	2.02	0.41
1:B:133:ILE:HG21	1:B:173:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:MET:HE3	6:C:745:HOH:O	2.20	0.41
1:C:168:TYR:O	1:C:169:ASP:C	2.64	0.41
1:A:197:ASN:O	1:A:221:MET:HA	2.21	0.41
1:B:39:LYS:O	1:B:40:LEU:C	2.63	0.41
1:B:162:PRO:HG3	1:B:232:HIS:CD2	2.53	0.41
1:C:100:LEU:HB3	1:C:101:PRO:HD3	2.01	0.41
1:B:204:THR:HB	1:C:136:ASP:OD1	2.21	0.41
1:B:266:GLY:C	1:B:268:GLN:H	2.29	0.41
1:C:61:THR:O	1:C:62:SER:CB	2.68	0.41
1:C:145:LEU:HA	1:C:145:LEU:HD12	1.89	0.41
1:A:27:PRO:HG3	1:A:72:PHE:CE2	2.56	0.41
1:A:137:HIS:HA	1:A:194:TYR:O	2.20	0.41
1:A:258:ASN:HD22	1:A:261:GLU:HG3	1.80	0.41
1:B:116:SER:HA	1:B:240:VAL:O	2.21	0.41
1:B:197:ASN:O	1:B:221:MET:HA	2.21	0.40
1:C:31:ILE:HA	1:C:114:MET:O	2.20	0.40
1:A:41:ALA:HB1	1:A:71:ILE:CD1	2.50	0.40
1:A:100:LEU:HB3	1:A:101:PRO:HD3	2.03	0.40
1:A:133:ILE:HG21	1:A:173:ARG:HG2	2.03	0.40
1:C:194:TYR:HD1	1:C:224:ILE:HD11	1.84	0.40
1:C:203:GLU:CD	1:C:203:GLU:H	2.29	0.40
1:C:221:MET:HG3	4:C:704:6GU:N3	2.35	0.40
1:A:17:HIS:HA	1:A:20:GLN:HE21	1.85	0.40
1:A:274:GLN:NE2	6:A:911:HOH:O	2.55	0.40
1:B:263:LEU:HG	6:B:918:HOH:O	2.21	0.40
1:B:224:ILE:N	1:B:225:PRO:CD	2.85	0.40
1:C:244:THR:HB	1:C:262:VAL:HA	2.04	0.40
1:A:39:LYS:O	1:A:40:LEU:C	2.64	0.40
1:C:27:PRO:HG3	1:C:72:PHE:HE2	1.85	0.40
1:C:224:ILE:N	1:C:225:PRO:CD	2.85	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLU:OE2	1:B:286:LYS:NZ[2_455]	2.18	0.02

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	276/287 (96%)	269 (98%)	5 (2%)	2 (1%)	18	22
1	B	262/287 (91%)	255 (97%)	7 (3%)	0	100	100
1	C	281/287 (98%)	273 (97%)	8 (3%)	0	100	100
All	All	819/861 (95%)	797 (97%)	20 (2%)	2 (0%)	43	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	253	SER

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	234/242 (97%)	226 (97%)	8 (3%)	32	47
1	B	222/242 (92%)	215 (97%)	7 (3%)	34	50
1	C	235/242 (97%)	230 (98%)	5 (2%)	47	65
All	All	691/726 (95%)	671 (97%)	20 (3%)	37	53

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU

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Mol	Chain	Res	Type
1	A	48	ILE
1	A	115	VAL
1	A	175	LEU
1	A	242	LEU
1	A	251	VAL
1	A	255	LEU
1	A	258	ASN
1	B	5	VAL
1	B	48	ILE
1	B	61	THR
1	B	115	VAL
1	B	242	LEU
1	B	268	GLN
1	B	287	ASP
1	C	61	THR
1	C	62	SER
1	C	115	VAL
1	C	242	LEU
1	C	258	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	183	ASN
1	A	191	GLN
1	A	245	ASN
1	A	258	ASN
1	A	274	GLN
1	B	20	GLN
1	B	183	ASN
1	B	191	GLN
1	B	245	ASN
1	B	268	GLN
1	B	274	GLN
1	C	17	HIS
1	C	20	GLN
1	C	183	ASN
1	C	187	ASN
1	C	191	GLN
1	C	258	ASN
1	C	274	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 ⓘ

10 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$
3	SO4	C	291	-	4,4,4	0.25	0	6,6,6	0.19	0
2	DMS	A	705	-	3,3,3	1.61	1 (33%)	3,3,3	1.01	0
5	ACT	B	700	-	3,3,3	0.73	0	3,3,3	1.14	0
3	SO4	A	291	-	4,4,4	0.24	0	6,6,6	0.18	0
3	SO4	B	291	-	4,4,4	0.31	0	6,6,6	0.12	0
2	DMS	C	703	-	3,3,3	1.59	1 (33%)	3,3,3	1.18	0
2	DMS	B	703	-	3,3,3	1.52	1 (33%)	3,3,3	1.72	1 (33%)
4	6GU	A	704	-	12,12,12	6.93	12 (100%)	17,17,17	3.76	14 (82%)
4	6GU	C	704	-	12,12,12	6.46	11 (91%)	17,17,17	3.40	12 (70%)
2	DMS	A	703	-	3,3,3	1.53	1 (33%)	3,3,3	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6GU	A	704	-	-	-	0/2/2/2
4	6GU	C	704	-	-	-	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	704	6GU	C6-C5	11.09	1.51	1.38
4	C	704	6GU	C6-C5	10.31	1.50	1.38
4	A	704	6GU	C2-N1	8.92	1.50	1.35
4	A	704	6GU	C6-N1	8.72	1.45	1.32
4	A	704	6GU	C8-N7	7.97	1.48	1.32
4	C	704	6GU	C8-N7	7.83	1.48	1.32
4	C	704	6GU	C2-N1	7.58	1.48	1.35
4	C	704	6GU	C2-N3	7.22	1.47	1.35
4	A	704	6GU	C2-N3	7.13	1.47	1.35
4	C	704	6GU	C6-N1	7.09	1.43	1.32
4	C	704	6GU	C4-N3	6.65	1.46	1.34
4	A	704	6GU	C4-N3	6.46	1.46	1.34
4	A	704	6GU	C4-N9	6.23	1.46	1.36
4	C	704	6GU	C4-N9	6.11	1.45	1.36
4	A	704	6GU	C5-C4	5.90	1.48	1.39
4	A	704	6GU	C2-N2	5.78	1.45	1.33
4	C	704	6GU	C2-N2	5.67	1.45	1.33
4	C	704	6GU	C5-C4	5.23	1.47	1.39
4	C	704	6GU	C8-N9	4.72	1.46	1.35
4	A	704	6GU	C8-N9	4.52	1.46	1.35
4	A	704	6GU	C5-N7	2.79	1.44	1.39
4	C	704	6GU	C5-N7	2.66	1.43	1.39
2	A	705	DMS	O-S	2.44	1.66	1.50
2	C	703	DMS	O-S	2.42	1.66	1.50
4	A	704	6GU	C6-CL6	2.39	1.78	1.74
2	B	703	DMS	O-S	2.32	1.65	1.50
2	A	703	DMS	O-S	2.31	1.65	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	6GU	C6-C5-C4	9.16	120.86	114.75
4	C	704	6GU	C6-C5-C4	7.85	119.99	114.75
4	C	704	6GU	C5-C4-N3	-7.24	119.45	126.55
4	A	704	6GU	C5-C4-N3	-6.75	119.93	126.55
4	A	704	6GU	C5-N7-C8	4.57	108.64	103.48
4	C	704	6GU	C5-N7-C8	4.23	108.26	103.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	704	6GU	N9-C8-N7	-3.96	107.84	113.87
4	A	704	6GU	N9-C8-N7	-3.75	108.16	113.87
4	A	704	6GU	CL6-C6-N1	3.40	121.03	115.57
4	A	704	6GU	C5-C6-N1	-3.35	118.83	122.14
4	A	704	6GU	N3-C2-N1	-3.04	120.81	125.48
4	A	704	6GU	N2-C2-N1	2.99	121.70	117.22
2	B	703	DMS	C2-S-C1	2.86	113.08	98.42
4	C	704	6GU	N3-C2-N1	-2.84	121.13	125.48
4	C	704	6GU	N9-C4-N3	2.80	131.95	127.45
4	A	704	6GU	C4-C5-N7	-2.68	106.95	110.67
4	A	704	6GU	C5-C4-N9	2.63	109.18	105.67
4	A	704	6GU	C6-N1-C2	2.53	119.83	116.14
4	C	704	6GU	C5-C4-N9	2.19	108.60	105.67
4	A	704	6GU	C2-N3-C4	2.17	119.74	114.59
4	A	704	6GU	N9-C4-N3	2.14	130.89	127.45
4	C	704	6GU	C6-C5-N7	-2.12	132.12	134.45
4	C	704	6GU	N2-C2-N3	2.12	120.41	117.22
4	C	704	6GU	C2-N3-C4	2.12	119.63	114.59
4	A	704	6GU	C6-C5-N7	-2.06	132.19	134.45
4	C	704	6GU	C6-N1-C2	2.02	119.09	116.14
4	C	704	6GU	C4-C5-N7	-2.00	107.89	110.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	705	DMS	1	0
5	B	700	ACT	1	0
3	A	291	SO4	1	0
4	A	704	6GU	10	0
4	C	704	6GU	10	0
2	A	703	DMS	1	0

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	280/287 (97%)	-0.31	6 (2%) 63 66	14, 22, 48, 75	0
1	B	270/287 (94%)	-0.13	9 (3%) 49 52	14, 23, 52, 76	0
1	C	283/287 (98%)	-0.27	7 (2%) 58 61	14, 22, 44, 70	0
All	All	833/861 (96%)	-0.24	22 (2%) 57 60	14, 22, 49, 76	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	LYS	3.5
1	B	287	ASP	3.3
1	A	66	HIS	2.9
1	C	41	ALA	2.8
1	B	38	GLY	2.8
1	B	61	THR	2.7
1	B	267	ALA	2.7
1	B	285	PRO	2.6
1	A	286	LYS	2.6
1	C	34	GLY	2.6
1	A	287	ASP	2.4
1	A	285	PRO	2.4
1	C	285	PRO	2.4
1	C	61	THR	2.4
1	A	62	SER	2.4
1	C	255	LEU	2.4
1	C	42	ASP	2.3
1	C	4	SER	2.3
1	B	42	ASP	2.2
1	A	24	SER	2.1
1	B	48	ILE	2.0
1	B	39	LYS	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
4	6GU	A	704	11/11	0.91	0.14	25,31,40,179	0
2	DMS	A	705	4/4	0.92	0.10	21,26,30,46	0
4	6GU	C	704	11/11	0.93	0.10	22,26,46,49	0
5	ACT	B	700	4/4	0.94	0.07	21,22,22,31	0
3	SO4	A	291	5/5	0.96	0.09	42,42,55,61	0
3	SO4	C	291	5/5	0.97	0.07	32,36,44,54	0
3	SO4	B	291	5/5	0.97	0.12	33,34,37,37	0
2	DMS	A	703	4/4	0.99	0.04	10,15,16,28	0
2	DMS	B	703	4/4	0.99	0.04	8,10,17,19	0
2	DMS	C	703	4/4	0.99	0.04	12,12,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.