



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:20 AM GMT

PDB ID : 3E9Z  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

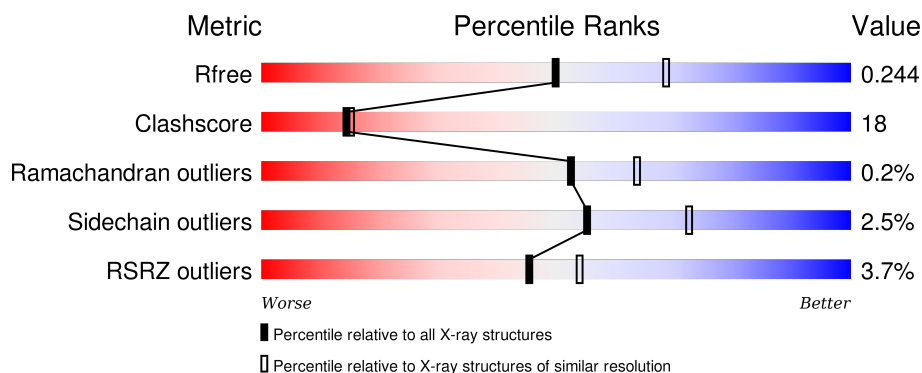
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>66%</div> <div>29%</div> <div>••</div> </div>
1	B	287	<div> <div>6%</div> <div>70%</div> <div>23%</div> <div>• 6%</div> </div>
1	C	287	<div> <div>2%</div> <div>68%</div> <div>30%</div> <div>••</div> </div>

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
3	SO4	A	291	-	-	-	X
3	SO4	B	291	-	-	-	X
4	6GU	A	704	-	X	X	X
4	6GU	C	704	-	-	X	X

## 2 Entry composition [i](#)

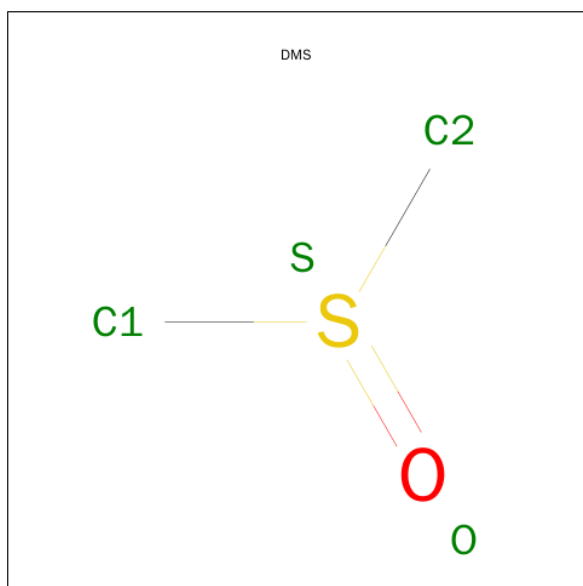
There are 6 unique types of molecules in this entry. The entry contains 7055 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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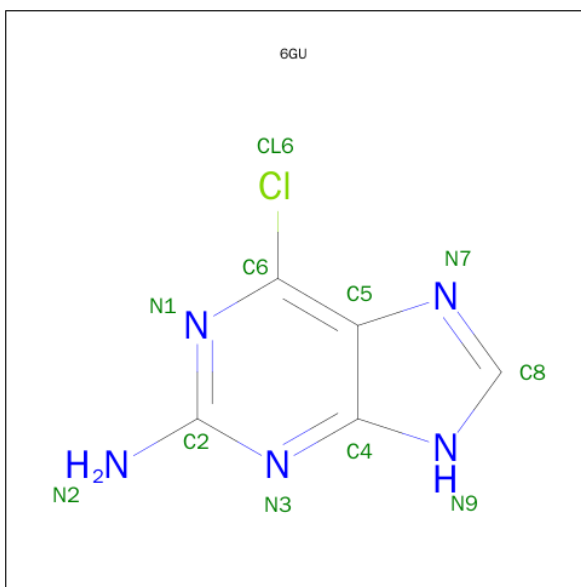
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: 6GU) (formula: C<sub>5</sub>H<sub>4</sub>ClN<sub>5</sub>).



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 (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

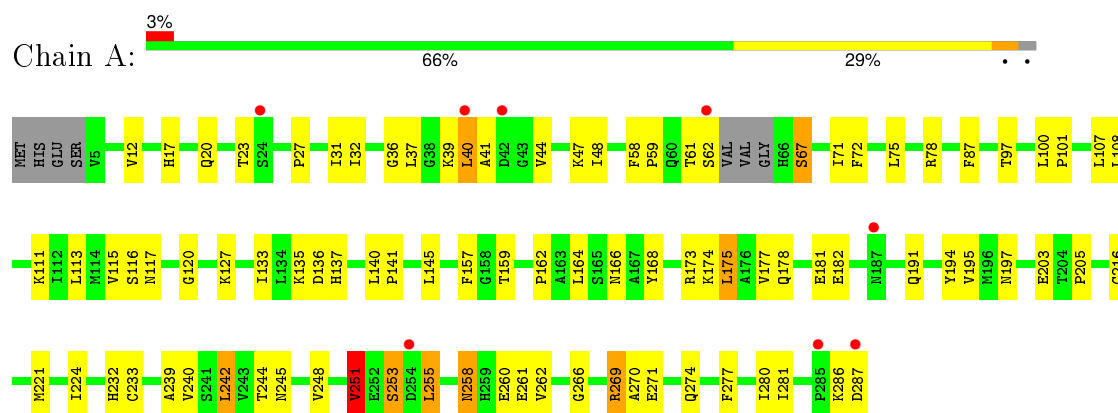
- Molecule 6 is water.

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

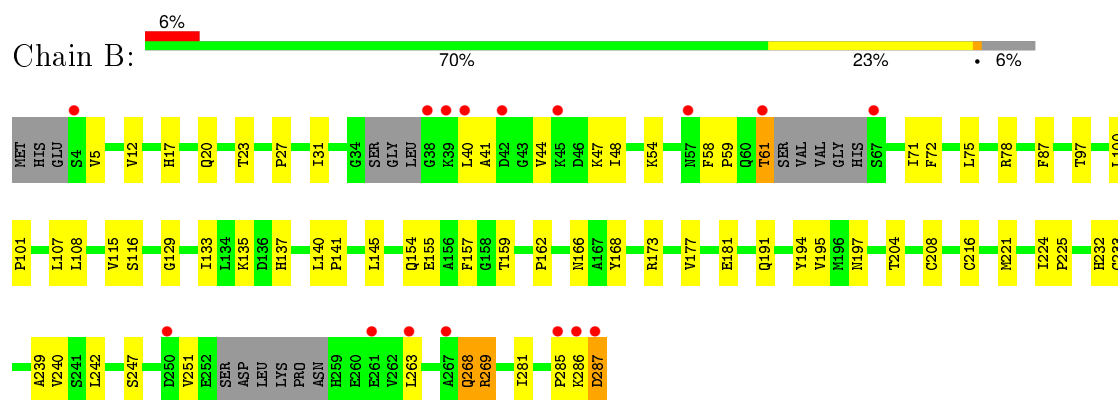
### 3 Residue-property plots

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.

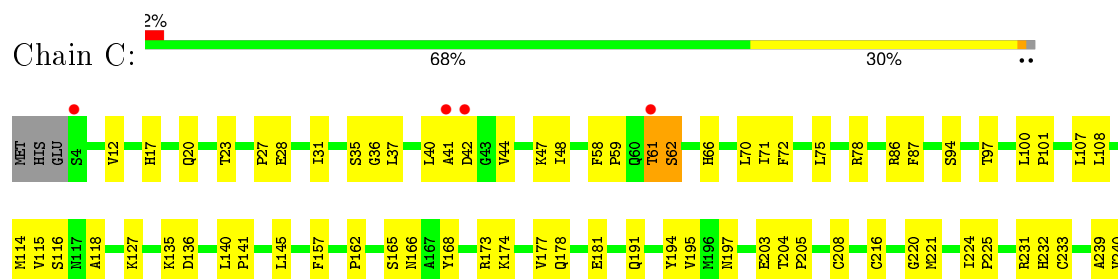
#### • Molecule 1: Purine-nucleoside phosphorylase



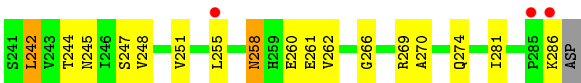
#### • Molecule 1: Purine-nucleoside phosphorylase



#### • Molecule 1: Purine-nucleoside phosphorylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 91.0 (56.63-2.31)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.177 , 0.249 0.176 , 0.244	Depositor DCC
$R_{free}$ test set	1480 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 29343 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 6GU, DMS, 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	0.46	0/2163	0.68	4/2927 (0.1%)
1	B	0.46	0/2081	0.78	4/2813 (0.1%)
1	C	0.47	0/2180	0.63	2/2954 (0.1%)
All	All	0.47	0/6424	0.70	10/8694 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ARG	NE-CZ-NH2	17.53	129.07	120.30
1	B	269	ARG	NE-CZ-NH1	-16.80	111.90	120.30
1	B	269	ARG	CD-NE-CZ	8.26	135.17	123.60
1	C	269	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	269	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	251	VAL	CB-CA-C	-6.46	99.12	111.40
1	C	269	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	269	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	251	VAL	CG1-CB-CG2	5.71	120.04	110.90
1	B	268	GLN	C-N-CA	-5.01	109.16	121.70

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	96	1
1	B	2049	0	2092	59	1
1	C	2142	0	2198	83	0
2	A	8	0	12	0	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	12	0
6	B	216	0	0	12	0
6	C	251	0	0	11	0
All	All	7055	0	6504	232	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 18.

All (232) 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:C:48:ILE:HD11	6:C:861:HOH:O	1.75	0.87
1:A:258:ASN:HD22	1:A:261:GLU:H	1.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:PRO:HB2	1:B:87:PHE:CE1	2.30	0.67
1:B:54:LYS:HD2	6:B:986:HOH:O	1.93	0.67
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
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:C:162:PRO:HG3	1:C:232:HIS:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:PRO:HG3	1:B:232:HIS:HD2	1.69	0.57
1:A:135:LYS:O	1:C:251:VAL:HG21	2.05	0.57
1:A:274:GLN:HB2	6:A:794:HOH:O	2.05	0.57
1:A:253:SER:OG	1:A:255:LEU:HD22	2.05	0.57
1:A:41:ALA:HB1	1:A:71:ILE:HD12	1.87	0.57
1:A:248:VAL:HG22	1:A:255:LEU:CD2	2.35	0.56
1:A:127:LYS:HE3	6:A:758:HOH:O	2.04	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:C:59:PRO:HD3	1:C:100:LEU:HD22	1.87	0.56
1:A:194:TYR:CD1	1:A:224:ILE:HD11	2.40	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ASN:ND2	4:C:704:6GU:N7	2.56	0.52
1:C:23:THR:CB	1:C:48:ILE:HD12	2.40	0.52
1:B:285:PRO:HA	6:B:1014:HOH:O	2.10	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:C:220:GLY:HA2	4:C:704:6GU:N3	2.26	0.49
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: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:58:PHE:CD2	1:A:59:PRO:HD2	2.48	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:27:PRO:HD2	1:A:108:LEU:O	2.13	0.49
1:C:195:VAL:HB	1:C:216:CYS:SG	2.53	0.49
1:A:195:VAL:HB	1:A:216:CYS:SG	2.53	0.49
1:B:157:PHE:O	1:B:233:CYS:HA	2.13	0.48
1:C:220:GLY:HA2	4:C:704:6GU:C2	2.43	0.48
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: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:C:127:LYS:HG3	6:C:853:HOH:O	2.13	0.48
1:B:166:ASN:HA	6:B:943:HOH:O	2.14	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:B:141:PRO:HB3	1:C:145:LEU:HB2	1.95	0.48
1:A:78:ARG:HD3	1:A:286:LYS:HD2	1.96	0.48
1:A:12:VAL:HG12	1:A:107:LEU:HD12	1.95	0.48
1:A:40:LEU:CD2	1:A:75:LEU:HD21	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:23:THR:HB	1:C:48:ILE:HD12	1.96	0.47
1:A:194:TYR:HD1	1:A:224:ILE:HD11	1.79	0.47
1:C:94:SER:HB2	6:C:920:HOH:O	2.14	0.47
1:C:168:TYR:O	1:C:173:ARG:HD3	2.15	0.46
1:B:17:HIS:HA	1:B:20:GLN:HE21	1.81	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:203:GLU:OE1	4:A:704:6GU:N1	2.49	0.46
1:A:145:LEU:HB2	1:C:141:PRO:HB3	1.98	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:B:129:GLY:O	1:B:269:ARG:HD2	2.16	0.45
1:A:159:THR:HG22	6:A:737:HOH:O	2.16	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:C:78:ARG:CD	1:C:286:LYS:HD2	2.47	0.45
1:B:115:VAL:O	1:B:239:ALA:HA	2.17	0.45
1:C:274:GLN:NE2	6:C:739:HOH:O	2.40	0.45
1:C:231:ARG:HA	1:C:231:ARG:HD2	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:HA	1:C:70:LEU:HD12	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:C:205:PRO:HG2	1:C:251:VAL:HA	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:41:ALA:HB1	1:B:71:ILE:CD1	2.49	0.42
1:A:174:LYS:O	1:A:178:GLN:HG3	2.19	0.42
1:A:31:ILE:HG21	1:A:40:LEU:HD13	2.01	0.42
1:C:118:ALA:HB1	4:C:704:6GU:H8	2.01	0.42
1:C:31:ILE:HD11	1:C:281:ILE:HD11	2.01	0.42
1:A:36:GLY:O	1:A:270:ALA:HA	2.18	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:A:164:LEU:HA	1:A:164:LEU:HD23	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:B:133:ILE:HG21	1:B:173:ARG:HG2	2.03	0.41
1:A:32:ILE:HG13	1:A:113:LEU:HD11	2.02	0.41
1:A:197:ASN:O	1:A:221:MET:HA	2.21	0.41
1:C:100:LEU:HB3	1:C:101:PRO:HD3	2.01	0.41
1:B:162:PRO:HG3	1:B:232:HIS:CD2	2.53	0.41
1:C:61:THR:O	1:C:62:SER:CB	2.68	0.41
1:C:145:LEU:HD12	1:C:145:LEU:HA	1.89	0.41
1:B:204:THR:HB	1:C:136:ASP:OD1	2.21	0.41
1:A:258:ASN:HD22	1:A:261:GLU:HG3	1.80	0.41
1:A:137:HIS:HA	1:A:194:TYR:O	2.20	0.41
1:A:27:PRO:HG3	1:A:72:PHE:CE2	2.56	0.41
1:B:116:SER:HA	1:B:240:VAL:O	2.21	0.41
1:C:31:ILE:HA	1:C:114:MET:O	2.20	0.40
1:B:197:ASN:O	1:B:221:MET:HA	2.21	0.40
1:A:100:LEU:HB3	1:A:101:PRO:HD3	2.03	0.40
1:C:221:MET:HG3	4:C:704:6GU:N3	2.35	0.40
1:A:133:ILE:HG21	1:A:173:ARG:HG2	2.03	0.40
1:A:41:ALA:HB1	1:A:71:ILE:CD1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:TYR:HD1	1:C:224:ILE:HD11	1.84	0.40
1:A:274:GLN:NE2	6:A:911:HOH:O	2.55	0.40
1:A:17:HIS:HA	1:A:20:GLN:HE21	1.85	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: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%)	26	31
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%)	52	64

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%)	227 (97%)	7 (3%)	48	65
1	B	222/242 (92%)	217 (98%)	5 (2%)	58	75
1	C	235/242 (97%)	230 (98%)	5 (2%)	61	78
All	All	691/726 (95%)	674 (98%)	17 (2%)	55	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	175	LEU
1	A	242	LEU
1	A	251	VAL
1	A	255	LEU
1	A	258	ASN
1	A	287	ASP
1	B	5	VAL
1	B	61	THR
1	B	242	LEU
1	B	268	GLN
1	B	287	ASP
1	C	61	THR
1	C	62	SER
1	C	66	HIS
1	C	242	LEU
1	C	258	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	20	GLN
1	A	183	ASN
1	A	191	GLN

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Mol	Chain	Res	Type
1	A	245	ASN
1	A	258	ASN
1	A	268	GLN
1	A	274	GLN
1	B	17	HIS
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	245	ASN
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 carbohydrates 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	A	291	-	4,4,4	0.20	0	6,6,6	0.19	0
2	DMS	A	703	-	3,3,3	1.48	1 (33%)	3,3,3	0.87	0
4	6GU	A	704	-	9,12,12	4.87	7 (77%)	8,17,17	2.98	6 (75%)
2	DMS	A	705	-	3,3,3	1.55	1 (33%)	3,3,3	0.97	0
3	SO4	B	291	-	4,4,4	0.21	0	6,6,6	0.16	0
5	ACT	B	700	-	1,3,3	0.96	0	0,3,3	0.00	-
2	DMS	B	703	-	3,3,3	1.46	1 (33%)	3,3,3	1.68	1 (33%)
3	SO4	C	291	-	4,4,4	0.21	0	6,6,6	0.25	0
2	DMS	C	703	-	3,3,3	1.54	1 (33%)	3,3,3	1.14	0
4	6GU	C	704	-	9,12,12	4.49	7 (77%)	8,17,17	2.38	4 (50%)

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	SO4	A	291	-	-	0/0/0/0	0/0/0/0
2	DMS	A	703	-	-	0/0/0/0	0/0/0/0
4	6GU	A	704	-	-	0/0/0/0	0/2/2/2
2	DMS	A	705	-	-	0/0/0/0	0/0/0/0
3	SO4	B	291	-	-	0/0/0/0	0/0/0/0
5	ACT	B	700	-	-	0/0/0/0	0/0/0/0
2	DMS	B	703	-	-	0/0/0/0	0/0/0/0
3	SO4	C	291	-	-	0/0/0/0	0/0/0/0
2	DMS	C	703	-	-	0/0/0/0	0/0/0/0
4	6GU	C	704	-	-	0/0/0/0	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	703	DMS	O-S	2.23	1.65	1.50
2	B	703	DMS	O-S	2.24	1.65	1.50
4	A	704	6GU	C2-N3	2.31	1.47	1.35
2	C	703	DMS	O-S	2.33	1.66	1.50
4	C	704	6GU	C2-N3	2.34	1.47	1.35
2	A	705	DMS	O-S	2.36	1.66	1.50
4	C	704	6GU	C5-C4	3.08	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	704	6GU	C5-C4	3.54	1.48	1.40
4	C	704	6GU	C6-N1	4.05	1.43	1.30
4	A	704	6GU	C6-N1	4.81	1.45	1.30
4	A	704	6GU	C4-N3	5.26	1.46	1.36
4	C	704	6GU	C2-N2	5.43	1.45	1.34
4	C	704	6GU	C4-N3	5.44	1.46	1.36
4	A	704	6GU	C2-N2	5.54	1.45	1.34
4	C	704	6GU	C4-N9	5.83	1.45	1.34
4	A	704	6GU	C4-N9	5.94	1.46	1.34
4	C	704	6GU	C2-N1	7.38	1.48	1.35
4	A	704	6GU	C2-N1	8.68	1.50	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	6GU	N3-C2-N1	-4.35	120.81	127.44
4	C	704	6GU	N3-C2-N1	-4.15	121.13	127.44
4	A	704	6GU	C5-C6-N1	-3.61	118.83	125.03
4	A	704	6GU	C4-C5-N7	-2.75	106.95	109.48
4	C	704	6GU	C5-C6-N1	-2.51	120.71	125.03
4	C	704	6GU	C6-N1-C2	2.49	119.09	115.40
4	C	704	6GU	C5-C6-CL6	2.71	121.69	117.74
4	A	704	6GU	N2-C2-N1	2.72	121.70	117.20
2	B	703	DMS	C2-S-C1	2.83	113.08	98.46
4	A	704	6GU	C6-N1-C2	3.00	119.83	115.40
4	A	704	6GU	CL6-C6-N1	3.51	121.03	114.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 22 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	280/287 (97%)	-0.15	8 (2%) 55 64	14, 22, 48, 75	0
1	B	270/287 (94%)	0.08	16 (5%) 26 34	14, 23, 52, 76	0
1	C	283/287 (98%)	-0.13	7 (2%) 61 69	14, 22, 44, 70	0
All	All	833/861 (96%)	-0.07	31 (3%) 45 54	14, 22, 49, 76	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	LYS	6.3
1	B	42	ASP	5.9
1	A	287	ASP	5.9
1	A	24	SER	4.5
1	B	39	LYS	4.3
1	A	42	ASP	3.9
1	B	57	ASN	3.7
1	A	62	SER	3.5
1	B	250	ASP	3.5
1	B	287	ASP	3.3
1	A	254	ASP	3.2
1	B	285	PRO	3.0
1	C	285	PRO	2.9
1	B	67	SER	2.9
1	C	42	ASP	2.9
1	B	261	GLU	2.8
1	B	263	LEU	2.8
1	B	267	ALA	2.8
1	C	286	LYS	2.7
1	C	41	ALA	2.6
1	B	61	THR	2.4
1	A	40	LEU	2.4
1	A	187	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	4	SER	2.3
1	B	4	SER	2.3
1	B	40	LEU	2.2
1	C	255	LEU	2.2
1	C	61	THR	2.2
1	B	45	LYS	2.1
1	A	285	PRO	2.0
1	B	38	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	6GU	A	704	11/11	0.91	0.25	10.25	25,31,40,179	0
4	6GU	C	704	11/11	0.94	0.21	4.98	22,26,46,49	0
3	SO4	A	291	5/5	0.96	0.20	2.95	42,42,55,61	0
3	SO4	B	291	5/5	0.98	0.21	2.42	33,34,37,37	0
2	DMS	A	703	4/4	0.99	0.12	1.29	10,15,16,28	0
2	DMS	B	703	4/4	0.99	0.12	0.95	8,10,17,19	0
5	ACT	B	700	4/4	0.95	0.10	-0.25	21,22,22,31	0
2	DMS	A	705	4/4	0.95	0.11	-0.39	21,26,30,46	0
3	SO4	C	291	5/5	0.99	0.11	-0.39	32,36,44,54	0
2	DMS	C	703	4/4	0.99	0.10	-1.43	12,12,18,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.