



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:58 AM GMT

PDB ID : 2Q9C
Title : Structure of FTSY:GMPPNP with MGCL Complex
Authors : Reyes, C.L.; Stroud, R.M.
Deposited on : 2007-06-12
Resolution : 2.20 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>

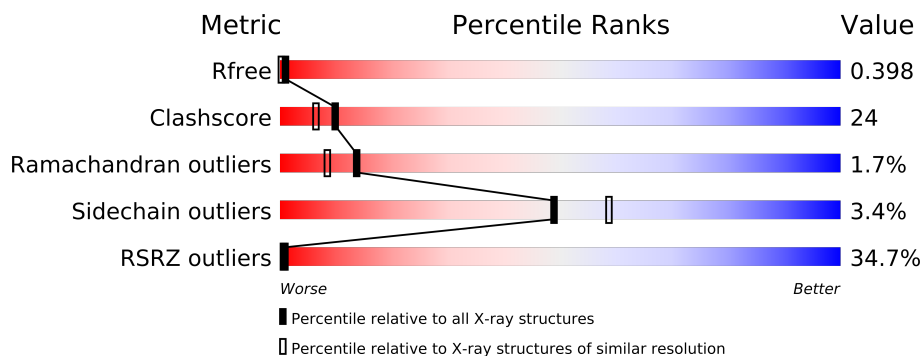
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Mol	Chain	Length	Quality of chain
1	A	304	
1	B	304	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4966 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 Cell division protein ftsY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2327	1485	405	430	7			
1	B	290	Total	C	N	O	S	0	0	0
			2209	1412	379	411	7			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



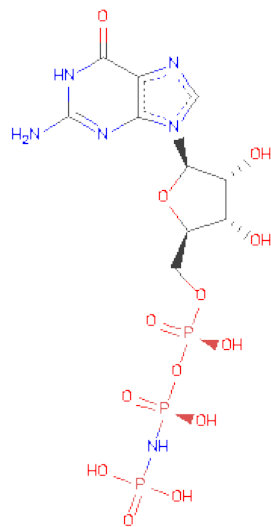
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

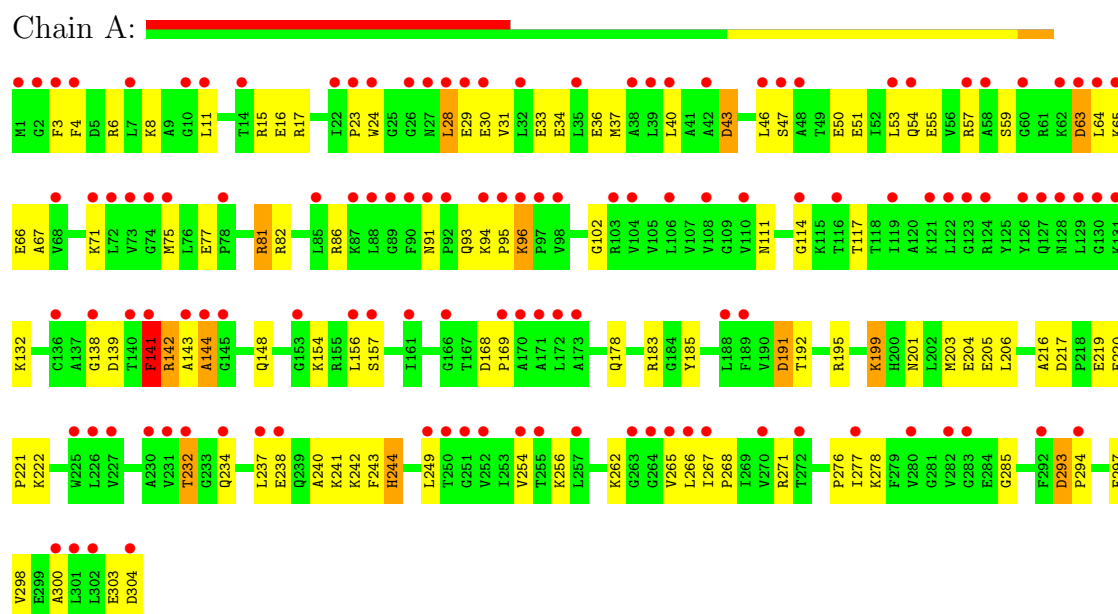
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	182	Total	O	0	0
			182	182		
4	B	176	Total	O	0	0
			176	176		

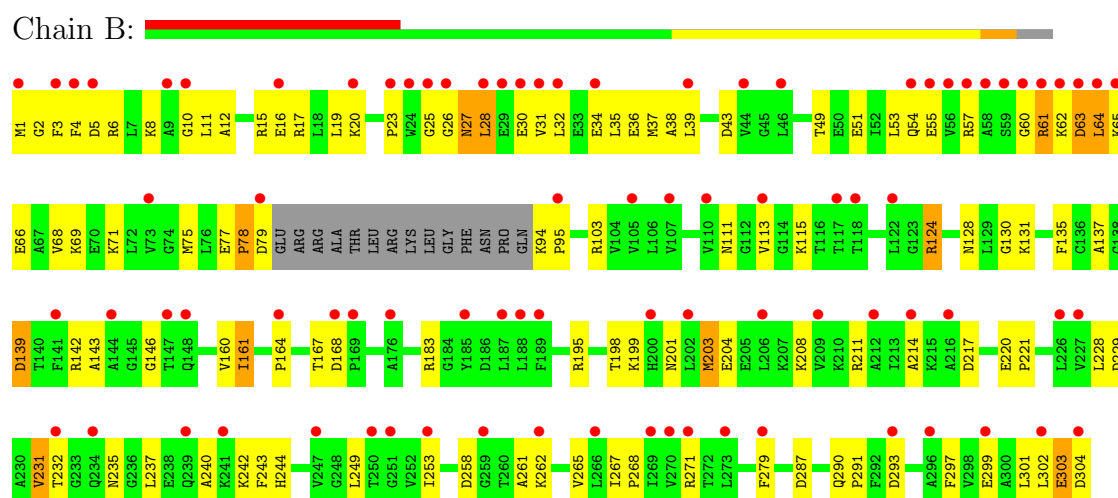
3 Residue-property plots

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: Cell division protein ftsY



• Molecule 1: Cell division protein ftsY



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 97.28Å 99.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.96 – 2.20 35.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.3 (35.96-2.20) 91.4 (35.96-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.203 , 0.274 0.365 , 0.398	Depositor DCC
R_{free} test set	2891 reflections (9.95%)	DCC
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.6	EDS
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29068 reflections	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	4966	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, SO4

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	1.01	0/2365	0.91	6/3189 (0.2%)
1	B	0.96	2/2244 (0.1%)	0.91	9/3026 (0.3%)
All	All	0.98	2/4609 (0.0%)	0.91	15/6215 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	MET	SD-CE	-5.78	1.45	1.77
1	B	111	ASN	CG-OD1	5.59	1.36	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	A	139	ASP	CB-CG-OD2	7.54	125.08	118.30
1	A	63	ASP	CB-CG-OD2	7.14	124.73	118.30
1	B	293	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	124	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	168	ASP	CB-CG-OD2	6.26	123.93	118.30
1	B	79	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	17	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	B	139	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	191	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	43	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	63	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	217	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	103	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	293	ASP	CB-CG-OD2	5.03	122.82	118.30

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	2327	0	2425	110	1
1	B	2209	0	2299	130	3
2	A	25	0	0	1	0
2	B	15	0	0	0	0
3	A	32	0	13	4	0
4	A	182	0	0	12	2
4	B	176	0	0	12	0
All	All	4966	0	4737	225	3

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 24.

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1:MET:HE2	1:B:3:PHE:H	1.18	1.02
1:A:142:ARG:HG2	1:A:195:ARG:HE	1.21	1.01
1:B:23:PRO:HD2	1:B:34:GLU:OE1	1.60	0.99
1:A:234:GLN:NE2	1:B:262:LYS:HD2	1.89	0.88
1:B:231:VAL:HG12	1:B:231:VAL:O	1.72	0.86
1:B:75:MET:HE3	1:B:271:ARG:HE	1.37	0.86
1:A:234:GLN:HG2	1:B:231:VAL:HG13	1.59	0.85
1:B:1:MET:O	1:B:5:ASP:HB2	1.78	0.83
1:B:55:GLU:HG2	1:B:71:LYS:HD3	1.62	0.81
1:B:1:MET:SD	1:B:94:LYS:HG2	2.22	0.80
1:A:234:GLN:HG2	1:B:231:VAL:CG1	2.13	0.79
1:B:183:ARG:NH1	4:B:1054:HOH:O	2.13	0.74
1:B:28:LEU:HD12	1:B:28:LEU:H	1.53	0.74
1:B:201:ASN:HD22	1:B:204:GLU:H	1.36	0.74
1:A:55:GLU:HB3	1:A:71:LYS:NZ	2.03	0.73
1:A:203:MET:HE1	1:A:243:PHE:HA	1.69	0.73
1:A:203:MET:CE	1:A:243:PHE:HA	2.17	0.73
1:A:142:ARG:HG2	1:A:195:ARG:NE	2.01	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:ASN:HD22	1:A:204:GLU:H	1.34	0.72
1:A:142:ARG:CG	1:A:195:ARG:HE	2.01	0.71
1:A:47:SER:OG	1:A:271:ARG:NH2	2.24	0.70
1:A:71:LYS:NZ	4:A:1074:HOH:O	2.23	0.70
1:B:3:PHE:CD1	1:B:95:PRO:HD3	2.28	0.69
1:B:271:ARG:HD3	4:B:916:HOH:O	1.92	0.68
1:A:141:PHE:H	1:A:141:PHE:HD1	1.41	0.68
1:A:234:GLN:CG	1:B:231:VAL:HG13	2.23	0.68
1:B:1:MET:HE2	1:B:3:PHE:N	2.03	0.67
1:B:20:LYS:HG3	1:B:304:ASP:O	1.94	0.67
1:A:36:GLU:HB3	1:B:37:MET:HE1	1.76	0.67
1:B:137:ALA:HB1	1:B:146:GLY:HA2	1.76	0.67
1:A:50:GLU:O	1:A:54:GLN:HG3	1.95	0.67
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.58	0.67
1:B:10:GLY:O	1:B:258:ASP:HA	1.94	0.67
1:B:139:ASP:OD2	1:B:142:ARG:HD3	1.96	0.66
1:A:201:ASN:ND2	1:A:204:GLU:HG2	2.10	0.66
1:B:271:ARG:HG2	1:B:271:ARG:NH2	2.09	0.66
1:B:1:MET:HG2	1:B:2:GLY:H	1.60	0.66
1:B:201:ASN:HD22	1:B:204:GLU:HG2	1.61	0.66
1:A:266:LEU:HD13	1:A:277:ILE:HD13	1.76	0.66
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.61	0.66
1:B:271:ARG:HG2	1:B:271:ARG:HH21	1.60	0.65
1:A:11:LEU:HD12	1:A:300:ALA:HB3	1.79	0.65
1:A:93:GLN:HG2	1:A:94:LYS:H	1.62	0.64
1:B:201:ASN:HD21	1:B:203:MET:HB2	1.62	0.64
1:A:29:GLU:HG2	4:A:1018:HOH:O	1.98	0.64
1:A:178:GLN:HE21	1:A:216:ALA:HB1	1.63	0.63
1:A:265:VAL:O	1:A:268:PRO:HD2	1.99	0.63
1:A:222:LYS:HG2	4:A:1097:HOH:O	1.98	0.63
1:B:75:MET:CE	1:B:271:ARG:HE	2.09	0.62
1:B:201:ASN:ND2	1:B:204:GLU:HG2	2.14	0.62
1:A:55:GLU:HB3	1:A:71:LYS:HZ2	1.64	0.62
1:B:131:LYS:NZ	4:B:957:HOH:O	2.30	0.62
1:B:32:LEU:HD13	1:B:57:ARG:HE	1.65	0.61
1:A:168:ASP:OD2	1:A:169:PRO:HD2	2.00	0.61
1:A:55:GLU:OE1	1:A:71:LYS:HB3	2.00	0.61
1:B:303:GLU:O	1:B:304:ASP:HB3	2.01	0.61
1:A:36:GLU:CD	1:B:37:MET:HE2	2.21	0.61
1:B:51:GLU:OE2	1:B:271:ARG:NH1	2.34	0.60
1:B:199:LYS:HG3	4:B:1000:HOH:O	2.01	0.60
1:B:28:LEU:C	1:B:61:ARG:HH22	2.05	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:ASN:ND2	1:A:204:GLU:H	1.99	0.60
1:B:49:THR:O	1:B:53:LEU:HD23	2.02	0.60
1:B:10:GLY:HA2	1:B:258:ASP:HB3	1.84	0.60
1:B:232:THR:CG2	4:B:965:HOH:O	2.50	0.60
1:B:115:LYS:HE2	4:B:952:HOH:O	2.01	0.59
1:A:192:THR:HG22	4:A:1106:HOH:O	2.00	0.59
1:B:208:LYS:HD3	4:B:1052:HOH:O	2.01	0.59
1:B:124:ARG:NH2	1:B:287:ASP:OD1	2.34	0.59
1:B:262:LYS:HE2	4:B:1069:HOH:O	2.03	0.58
1:B:203:MET:HE1	1:B:242:LYS:C	2.22	0.58
1:A:55:GLU:O	1:A:59:SER:HB3	2.03	0.58
1:A:8:LYS:HD3	1:A:304:ASP:CB	2.34	0.58
1:A:8:LYS:HD3	1:A:304:ASP:HB2	1.83	0.58
2:A:903:SO4:O4	1:B:195:ARG:HD3	2.04	0.58
1:B:229:ASP:O	1:B:232:THR:HG23	2.04	0.57
1:A:203:MET:HE1	1:A:243:PHE:CA	2.33	0.57
1:A:36:GLU:CB	1:B:37:MET:HE1	2.33	0.57
1:A:40:LEU:HD12	1:B:37:MET:HE3	1.86	0.57
1:B:303:GLU:OE1	1:B:303:GLU:C	2.43	0.57
1:B:201:ASN:ND2	1:B:204:GLU:H	2.02	0.57
1:A:65:LYS:NZ	1:A:303:GLU:OE2	2.36	0.57
1:B:55:GLU:HG2	1:B:71:LYS:CD	2.33	0.56
1:B:30:GLU:O	1:B:34:GLU:HG3	2.06	0.56
1:B:27:ASN:HB3	1:B:30:GLU:HB3	1.87	0.56
1:B:6:ARG:NH1	1:B:6:ARG:HG2	2.21	0.56
1:B:1:MET:CG	1:B:2:GLY:H	2.19	0.56
1:B:28:LEU:HB3	1:B:61:ARG:NH2	2.22	0.55
1:A:77:GLU:HG2	1:A:86:ARG:HH12	1.71	0.55
1:A:143:ALA:O	1:A:144:ALA:C	2.45	0.55
1:B:53:LEU:CD2	1:B:53:LEU:N	2.70	0.55
1:B:271:ARG:NH1	4:B:1047:HOH:O	2.40	0.54
1:B:26:GLY:O	1:B:28:LEU:N	2.40	0.54
1:A:285:GLY:HA3	4:A:969:HOH:O	2.06	0.54
1:B:208:LYS:HE3	4:B:1038:HOH:O	2.06	0.54
1:A:82:ARG:NH1	1:A:82:ARG:HG2	2.22	0.54
1:B:26:GLY:O	1:B:28:LEU:HD12	2.08	0.54
1:A:11:LEU:HD21	1:A:297:PHE:CE1	2.43	0.54
1:B:15:ARG:HD2	1:B:20:LYS:NZ	2.22	0.54
1:B:265:VAL:O	1:B:268:PRO:HD2	2.07	0.54
1:A:11:LEU:HD12	1:A:300:ALA:CB	2.37	0.53
1:A:15:ARG:HD2	1:A:16:GLU:OE2	2.08	0.53
1:B:53:LEU:N	1:B:53:LEU:HD22	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:8:LYS:HD2	1:B:15:ARG:NH2	2.23	0.53
1:B:65:LYS:HG2	1:B:69:LYS:HE3	1.92	0.52
1:B:64:LEU:O	1:B:68:VAL:HG23	2.09	0.52
1:A:267:ILE:HB	1:A:268:PRO:HD3	1.92	0.52
1:A:36:GLU:CG	1:B:37:MET:HE1	2.39	0.52
1:B:32:LEU:HD13	1:B:57:ARG:NE	2.25	0.51
1:A:237:LEU:O	1:A:240:ALA:HB3	2.09	0.51
1:A:55:GLU:HB3	1:A:71:LYS:HZ3	1.75	0.51
1:A:114:GLY:HA2	3:A:950:GNP:PA	2.51	0.51
1:A:142:ARG:HA	4:A:1052:HOH:O	2.10	0.51
1:B:231:VAL:O	1:B:231:VAL:CG1	2.48	0.51
1:B:65:LYS:HE2	1:B:69:LYS:CE	2.41	0.51
1:A:234:GLN:HE22	1:B:262:LYS:HD2	1.70	0.51
1:A:95:PRO:HB3	1:A:293:ASP:HB2	1.92	0.51
1:B:75:MET:HE3	1:B:271:ARG:NE	2.18	0.50
1:B:303:GLU:OE1	1:B:304:ASP:HB2	2.11	0.50
1:B:232:THR:HB	4:B:933:HOH:O	2.11	0.50
1:A:254:VAL:HG21	1:A:266:LEU:HD22	1.93	0.50
1:A:234:GLN:O	1:A:238:GLU:HG3	2.12	0.50
1:A:37:MET:SD	1:B:36:GLU:CD	2.90	0.49
1:B:65:LYS:HE2	1:B:69:LYS:HE3	1.92	0.49
1:A:244:HIS:HA	1:A:249:LEU:HG	1.94	0.49
1:B:203:MET:CE	1:B:243:PHE:HA	2.43	0.49
1:B:31:VAL:HG13	1:B:32:LEU:H	1.77	0.49
1:A:276:PRO:HG2	1:A:278:LYS:HE2	1.94	0.49
1:B:31:VAL:HG13	1:B:32:LEU:N	2.28	0.49
1:A:54:GLN:HB2	4:A:1036:HOH:O	2.13	0.49
1:B:265:VAL:C	1:B:268:PRO:HD2	2.32	0.49
1:A:203:MET:HE3	1:A:243:PHE:HA	1.91	0.49
1:A:67:ALA:O	1:A:71:LYS:HG2	2.13	0.48
1:B:71:LYS:O	1:B:75:MET:HG2	2.12	0.48
1:A:241:LYS:NZ	4:A:1011:HOH:O	2.46	0.48
1:A:143:ALA:HA	4:A:1069:HOH:O	2.13	0.48
1:A:3:PHE:C	1:A:3:PHE:CD1	2.86	0.48
1:B:203:MET:HE1	1:B:243:PHE:N	2.28	0.48
1:A:199:LYS:NZ	1:B:143:ALA:HB2	2.28	0.48
1:B:203:MET:HE3	1:B:243:PHE:HA	1.95	0.48
1:B:19:LEU:HD23	1:B:38:ALA:HB1	1.96	0.48
1:B:23:PRO:C	1:B:25:GLY:H	2.17	0.47
1:B:60:GLY:O	1:B:61:ARG:HD2	2.13	0.47
1:A:219:GLU:OE2	1:A:222:LYS:HE2	2.14	0.47
1:A:220:GLU:HB3	1:A:221:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:28:LEU:CA	1:B:61:ARG:HH22	2.27	0.47
1:A:36:GLU:CG	1:B:37:MET:CE	2.92	0.47
1:B:244:HIS:HA	1:B:249:LEU:HG	1.96	0.47
1:B:32:LEU:HD13	1:B:57:ARG:HD3	1.97	0.47
1:A:141:PHE:HZ	1:A:205:GLU:OE1	1.98	0.46
1:B:17:ARG:NE	1:B:261:ALA:HB1	2.30	0.46
1:B:299:GLU:O	1:B:303:GLU:HB3	2.15	0.46
1:A:33:GLU:OE2	1:A:37:MET:HE1	2.15	0.46
1:B:201:ASN:HD22	1:B:204:GLU:N	2.08	0.46
1:A:53:LEU:O	1:A:57:ARG:N	2.44	0.46
1:A:294:PRO:O	1:A:298:VAL:HG23	2.16	0.46
1:B:53:LEU:O	1:B:57:ARG:HG2	2.16	0.46
1:A:141:PHE:CD1	1:A:141:PHE:N	2.81	0.46
1:A:11:LEU:HD21	1:A:297:PHE:HE1	1.80	0.46
1:A:8:LYS:O	1:A:15:ARG:NH2	2.45	0.46
1:B:195:ARG:HG2	1:B:198:THR:CG2	2.46	0.46
1:A:303:GLU:O	1:A:304:ASP:HB3	2.16	0.45
1:A:203:MET:HE1	1:A:243:PHE:N	2.31	0.45
1:A:36:GLU:HG3	1:A:53:LEU:HD11	1.99	0.45
1:A:303:GLU:O	1:A:304:ASP:CB	2.64	0.45
1:B:63:ASP:CG	1:B:66:GLU:HB2	2.36	0.45
1:B:161:ILE:N	1:B:161:ILE:CD1	2.79	0.45
1:B:12:ALA:O	1:B:16:GLU:HG3	2.17	0.45
1:A:30:GLU:O	1:A:34:GLU:HG2	2.17	0.45
1:B:28:LEU:CD1	1:B:28:LEU:H	2.27	0.44
1:A:148:GLN:HB3	4:A:1034:HOH:O	2.16	0.44
1:A:141:PHE:CZ	1:A:205:GLU:OE1	2.70	0.44
1:B:16:GLU:HG2	1:B:20:LYS:HE3	1.99	0.44
1:A:156:LEU:O	1:A:157:SER:HB2	2.17	0.44
1:A:51:GLU:OE1	1:A:271:ARG:NH1	2.51	0.44
1:A:154:LYS:NZ	4:A:1084:HOH:O	2.50	0.44
1:B:35:LEU:O	1:B:39:LEU:HG	2.18	0.44
1:B:271:ARG:HH21	1:B:271:ARG:CG	2.26	0.44
1:A:3:PHE:HA	1:A:6:ARG:CZ	2.47	0.44
1:B:303:GLU:OE1	1:B:303:GLU:O	2.36	0.44
1:A:82:ARG:CZ	1:A:96:LYS:HD2	2.48	0.44
1:B:19:LEU:HD13	1:B:301:LEU:HG	1.99	0.44
1:B:11:LEU:HD11	1:B:297:PHE:CE1	2.52	0.44
1:B:228:LEU:HD22	1:B:232:THR:HG21	2.00	0.43
1:B:237:LEU:O	1:B:240:ALA:HB3	2.18	0.43
1:A:102:GLY:CA	1:A:222:LYS:HD2	2.48	0.43
1:A:43:ASP:HB2	1:A:262:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:GLY:HA3	1:A:191:ASP:O	2.18	0.43
1:A:23:PRO:O	1:A:31:VAL:HG22	2.18	0.43
1:B:77:GLU:HA	1:B:78:PRO:HD3	1.88	0.43
1:A:36:GLU:CD	1:B:37:MET:CE	2.87	0.43
1:A:63:ASP:OD2	1:A:66:GLU:HG2	2.18	0.43
1:B:20:LYS:O	1:B:20:LYS:HG2	2.17	0.43
1:B:1:MET:HG2	1:B:2:GLY:N	2.30	0.42
1:A:102:GLY:HA3	1:A:222:LYS:HB2	2.00	0.42
1:B:290:GLN:O	1:B:291:PRO:C	2.55	0.42
1:B:135:PHE:HB2	1:B:160:VAL:HG22	2.02	0.42
1:A:265:VAL:C	1:A:268:PRO:HD2	2.39	0.42
1:B:164:PRO:O	1:B:167:THR:OG1	2.32	0.42
1:B:267:ILE:HB	1:B:268:PRO:HD3	2.02	0.42
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.86	0.42
1:B:220:GLU:HB3	1:B:221:PRO:HA	2.00	0.42
1:A:93:GLN:HG2	1:A:94:LYS:N	2.31	0.42
1:A:81:ARG:NH2	4:A:986:HOH:O	2.41	0.42
1:A:71:LYS:O	1:A:75:MET:HG3	2.19	0.42
1:B:214:ALA:HA	1:B:217:ASP:O	2.20	0.42
1:B:3:PHE:CG	1:B:95:PRO:HD3	2.55	0.42
1:B:253:ILE:HG12	1:B:279:PHE:HB2	2.02	0.42
1:A:28:LEU:CD2	1:A:64:LEU:HD22	2.50	0.41
1:B:3:PHE:CD1	1:B:4:PHE:N	2.88	0.41
1:B:201:ASN:ND2	1:B:203:MET:HB2	2.30	0.41
1:A:232:THR:HA	1:B:235:ASN:HB2	2.01	0.41
1:B:303:GLU:O	1:B:304:ASP:CB	2.69	0.41
1:A:11:LEU:HD11	1:A:297:PHE:CD1	2.56	0.41
1:A:256:LYS:HG2	3:A:950:GNP:C2	2.51	0.41
1:A:132:LYS:HG2	1:A:185:TYR:CE2	2.55	0.41
1:B:303:GLU:OE1	1:B:304:ASP:CB	2.69	0.41
1:B:69:LYS:HG2	1:B:302:LEU:HD12	2.02	0.41
1:B:211:ARG:HD2	4:B:1058:HOH:O	2.20	0.41
1:B:32:LEU:HD13	1:B:57:ARG:CD	2.51	0.40
1:A:203:MET:HE1	1:A:242:LYS:C	2.41	0.40
1:A:65:LYS:CE	1:A:303:GLU:OE2	2.69	0.40
1:A:4:PHE:CE2	1:A:8:LYS:HE3	2.56	0.40
1:A:114:GLY:HA2	3:A:950:GNP:O5'	2.21	0.40
1:A:206:LEU:HD11	1:A:243:PHE:HE1	1.86	0.40
1:A:111:ASN:ND2	3:A:950:GNP:O3G	2.54	0.40

All (3) 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:B:287:ASP:OD2	4:A:1095:HOH:O[2.665]	1.58	0.62
1:A:183:ARG:NH1	1:B:130:GLY:O[2.664]	2.16	0.04
1:B:128:ASN:OD1	4:A:1037:HOH:O[2.665]	2.17	0.03

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	302/304 (99%)	281 (93%)	16 (5%)	5 (2%)	14	8
1	B	286/304 (94%)	267 (93%)	14 (5%)	5 (2%)	14	8
All	All	588/608 (97%)	548 (93%)	30 (5%)	10 (2%)	14	8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	PHE
1	B	62	LYS
1	A	24	TRP
1	A	28	LEU
1	A	144	ALA
1	A	232	THR
1	B	28	LEU
1	B	27	ASN
1	B	231	VAL
1	B	78	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/242 (100%)	232 (96%)	10 (4%)	41	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	230/242 (95%)	224 (97%)	6 (3%)	59	70
All	All	472/484 (98%)	456 (97%)	16 (3%)	49	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	46	LEU
1	A	81	ARG
1	A	91	ASN
1	A	96	LYS
1	A	117	THR
1	A	141	PHE
1	A	142	ARG
1	A	199	LYS
1	A	244	HIS
1	B	54	GLN
1	B	61	ARG
1	B	64	LEU
1	B	113	VAL
1	B	161	ILE
1	B	303	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	91	ASN
1	A	111	ASN
1	A	127	GLN
1	A	178	GLN
1	A	197	HIS
1	A	201	ASN
1	A	239	GLN
1	B	111	ASN
1	B	148	GLN
1	B	162	GLN
1	B	201	ASN
1	B	234	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 ⓘ

9 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	$\# Z > 2$
2	SO4	A	902	-	4,4,4	0.71	0	6,6,6	0.56	0
2	SO4	A	903	-	4,4,4	0.73	0	6,6,6	0.69	0
2	SO4	A	905	-	4,4,4	0.78	0	6,6,6	0.71	0
2	SO4	A	906	-	4,4,4	0.72	0	6,6,6	0.29	0
2	SO4	A	908	-	4,4,4	0.48	0	6,6,6	0.67	0
3	GNP	A	950	-	34,34,34	2.45	10 (29%)	50,54,54	3.75	13 (26%)
2	SO4	B	901	-	4,4,4	0.84	0	6,6,6	0.52	0
2	SO4	B	904	-	4,4,4	0.73	0	6,6,6	0.46	0
2	SO4	B	907	-	4,4,4	0.98	0	6,6,6	0.27	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
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	903	-	-	0/0/0/0	0/0/0/0
2	SO4	A	905	-	-	0/0/0/0	0/0/0/0
2	SO4	A	906	-	-	0/0/0/0	0/0/0/0
2	SO4	A	908	-	-	0/0/0/0	0/0/0/0
3	GNP	A	950	-	-	0/18/38/38	0/1/3/3
2	SO4	B	901	-	-	0/0/0/0	0/0/0/0
2	SO4	B	904	-	-	0/0/0/0	0/0/0/0
2	SO4	B	907	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	950	GNP	PB-N3B	-9.54	1.56	1.64
3	A	950	GNP	PG-O1G	6.48	1.54	1.46
3	A	950	GNP	C2-N1	2.97	1.41	1.36
3	A	950	GNP	PB-O3A	-2.84	1.55	1.59
3	A	950	GNP	O3'-C3'	2.53	1.49	1.43
3	A	950	GNP	PB-O1B	2.47	1.49	1.46
3	A	950	GNP	PB-O2B	-2.45	1.48	1.55
3	A	950	GNP	C2-N2	2.40	1.36	1.32
3	A	950	GNP	PG-N3B	-2.33	1.62	1.64
3	A	950	GNP	C6-C5	2.24	1.44	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	950	GNP	C6-C5-N7	-23.04	131.04	134.14
3	A	950	GNP	O4'-C1'-N9	4.56	112.68	108.44
3	A	950	GNP	O1B-PB-N3B	4.45	118.56	111.83
3	A	950	GNP	O2B-PB-O1B	4.25	119.69	109.89
3	A	950	GNP	O2B-PB-N3B	4.23	118.09	106.61
3	A	950	GNP	O1G-PG-N3B	-3.50	106.54	111.83
3	A	950	GNP	O3A-PB-N3B	-3.38	97.21	106.59
3	A	950	GNP	O2G-PG-N3B	3.04	114.86	106.61
3	A	950	GNP	C8-N9-C4	-2.76	104.79	106.90
3	A	950	GNP	N2-C2-N3	-2.66	116.69	120.30
3	A	950	GNP	O2B-PB-O3A	-2.62	92.70	105.14
3	A	950	GNP	C6-N1-C2	2.55	123.97	119.51
3	A	950	GNP	O5'-PA-O1A	-2.13	101.03	109.37

There are no chirality outliers.

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 ⓘ

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	304/304 (100%)	1.95	123 (40%) 1 0	19, 26, 34, 41	0
1	B	290/304 (95%)	1.72	85 (29%) 1 1	20, 26, 33, 39	0
All	All	594/608 (97%)	1.84	208 (35%) 1 0	19, 26, 34, 41	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	GLY	7.6
1	B	24	TRP	7.5
1	B	28	LEU	7.5
1	A	1	MET	6.6
1	A	24	TRP	6.3
1	A	141	PHE	6.1
1	B	56	VAL	5.8
1	A	95	PRO	5.8
1	A	171	ALA	5.5
1	B	144	ALA	5.3
1	A	32	LEU	5.1
1	B	61	ARG	5.0
1	A	302	LEU	4.9
1	A	60	GLY	4.8
1	A	144	ALA	4.8
1	A	304	ASP	4.7
1	B	59	SER	4.7
1	A	143	ALA	4.6
1	B	147	THR	4.6
1	A	4	PHE	4.6
1	B	25	GLY	4.5
1	B	58	ALA	4.4
1	B	62	LYS	4.4
1	A	28	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	64	LEU	4.4
1	B	266	LEU	4.2
1	B	79	ASP	4.2
1	B	304	ASP	4.1
1	A	63	ASP	4.1
1	A	3	PHE	4.1
1	A	23	PRO	4.0
1	A	283	GLY	4.0
1	A	58	ALA	4.0
1	B	26	GLY	3.9
1	A	145	GLY	3.6
1	A	22	ILE	3.6
1	A	7	LEU	3.5
1	A	68	VAL	3.5
1	A	124	ARG	3.4
1	A	92	PRO	3.4
1	B	16	GLU	3.4
1	B	63	ASP	3.4
1	B	9	ALA	3.4
1	A	42	ALA	3.3
1	B	31	VAL	3.3
1	B	209	VAL	3.3
1	A	161	ILE	3.3
1	A	292	PHE	3.3
1	A	280	VAL	3.3
1	B	3	PHE	3.3
1	B	271	ARG	3.3
1	A	72	LEU	3.2
1	B	251	GLY	3.2
1	A	257	LEU	3.2
1	B	5	ASP	3.1
1	B	4	PHE	3.1
1	A	232	THR	3.1
1	A	90	PHE	3.1
1	B	200	HIS	3.1
1	A	11	LEU	3.1
1	B	259	GLY	3.1
1	A	128	ASN	3.1
1	A	108	VAL	3.1
1	A	116	THR	3.1
1	B	122	LEU	3.0
1	A	73	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	226	LEU	3.0
1	B	23	PRO	3.0
1	A	254	VAL	3.0
1	A	27	ASN	3.0
1	A	252	VAL	3.0
1	A	47	SER	3.0
1	A	265	VAL	2.9
1	A	14	THR	2.9
1	B	212	ALA	2.9
1	A	2	GLY	2.9
1	A	87	LYS	2.9
1	B	107	VAL	2.9
1	A	127	GLN	2.9
1	A	26	GLY	2.9
1	A	74	GLY	2.9
1	A	234	GLN	2.9
1	A	251	GLY	2.9
1	A	294	PRO	2.9
1	A	230	ALA	2.9
1	A	126	TYR	2.9
1	A	35	LEU	2.8
1	A	156	LEU	2.8
1	A	97	PRO	2.8
1	B	65	LYS	2.8
1	B	10	GLY	2.8
1	B	302	LEU	2.8
1	B	95	PRO	2.8
1	B	118	THR	2.8
1	A	94	LYS	2.8
1	A	110	VAL	2.8
1	A	277	ILE	2.8
1	B	279	PHE	2.8
1	A	96	LYS	2.7
1	B	44	VAL	2.7
1	B	39	LEU	2.7
1	B	64	LEU	2.7
1	B	216	ALA	2.7
1	A	103	ARG	2.7
1	B	164	PRO	2.7
1	A	270	VAL	2.7
1	B	105	VAL	2.7
1	B	253	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	269	ILE	2.7
1	A	170	ALA	2.7
1	A	30	GLU	2.7
1	A	40	LEU	2.7
1	A	266	LEU	2.7
1	A	138	GLY	2.7
1	A	300	ALA	2.7
1	A	136	CYS	2.7
1	A	62	LYS	2.6
1	B	296	ALA	2.6
1	A	227	VAL	2.6
1	A	301	LEU	2.6
1	B	206	LEU	2.6
1	A	123	GLY	2.6
1	B	20	LYS	2.6
1	B	46	LEU	2.6
1	A	225	TRP	2.6
1	B	148	GLN	2.6
1	A	46	LEU	2.6
1	B	202	LEU	2.6
1	A	119	ILE	2.5
1	A	98	VAL	2.5
1	A	129	LEU	2.5
1	A	75	MET	2.5
1	A	89	GLY	2.5
1	A	250	THR	2.5
1	A	122	LEU	2.5
1	A	104	VAL	2.5
1	A	237	LEU	2.5
1	A	238	GLU	2.5
1	A	39	LEU	2.5
1	B	32	LEU	2.5
1	A	85	LEU	2.4
1	A	88	LEU	2.4
1	A	188	LEU	2.4
1	A	78	PRO	2.4
1	A	263	GLY	2.4
1	A	157	SER	2.4
1	A	53	LEU	2.4
1	A	71	LYS	2.4
1	A	153	GLY	2.4
1	A	267	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	141	PHE	2.4
1	A	130	GLY	2.4
1	A	264	GLY	2.4
1	A	131	LYS	2.3
1	A	173	ALA	2.3
1	B	262	LYS	2.3
1	B	247	VAL	2.3
1	B	117	THR	2.3
1	B	176	ALA	2.3
1	B	185	TYR	2.3
1	B	214	ALA	2.3
1	A	29	GLU	2.3
1	B	188	LEU	2.3
1	B	189	PHE	2.3
1	A	48	ALA	2.3
1	A	54	GLN	2.3
1	B	110	VAL	2.2
1	B	187	LEU	2.2
1	B	30	GLU	2.2
1	A	65	LYS	2.2
1	A	272	THR	2.2
1	A	166	GLY	2.2
1	B	226	LEU	2.2
1	B	273	LEU	2.2
1	B	1	MET	2.2
1	B	34	GLU	2.2
1	B	57	ARG	2.2
1	B	293	ASP	2.2
1	B	241	LYS	2.2
1	B	73	VAL	2.2
1	B	250	THR	2.2
1	B	113	VAL	2.2
1	A	91	ASN	2.2
1	A	57	ARG	2.1
1	B	239	GLN	2.1
1	A	169	PRO	2.1
1	B	168	ASP	2.1
1	B	232	THR	2.1
1	B	29	GLU	2.1
1	A	231	VAL	2.1
1	B	55	GLU	2.1
1	A	189	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	114	GLY	2.1
1	B	54	GLN	2.1
1	A	255	THR	2.1
1	A	249	LEU	2.1
1	B	227	VAL	2.1
1	A	10	GLY	2.0
1	B	234	GLN	2.0
1	B	299	GLU	2.0
1	A	38	ALA	2.0
1	B	169	PRO	2.0
1	A	140	THR	2.0
1	A	121	LYS	2.0
1	A	106	LEU	2.0
1	A	172	LEU	2.0
1	A	282	VAL	2.0
1	B	270	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	903	5/5	0.23	0.20	35,40,42,44	0
3	GNP	A	950	32/32	0.25	0.07	43,48,60,62	0
2	SO4	B	904	5/5	0.23	-0.16	39,41,44,45	0
2	SO4	B	901	5/5	0.20	-0.60	32,33,37,37	0
2	SO4	A	906	5/5	0.21	-1.19	45,46,51,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	905	5/5	0.20	-1.57	39,39,45,46	0
2	SO4	B	907	5/5	0.15	-1.79	43,49,52,53	0
2	SO4	A	902	5/5	0.13	-1.98	42,42,44,49	0
2	SO4	A	908	5/5	0.15	-2.43	49,50,52,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.