



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 PM UTC

PDB ID : 2Q9C / pdb_00002q9c
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

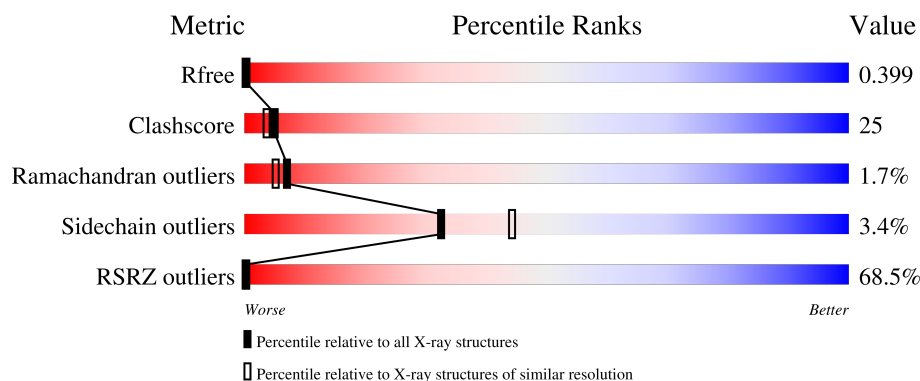
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	72% 61% 35% • •
1	B	304	62% 58% 33% • 5%

2 Entry composition [i](#)

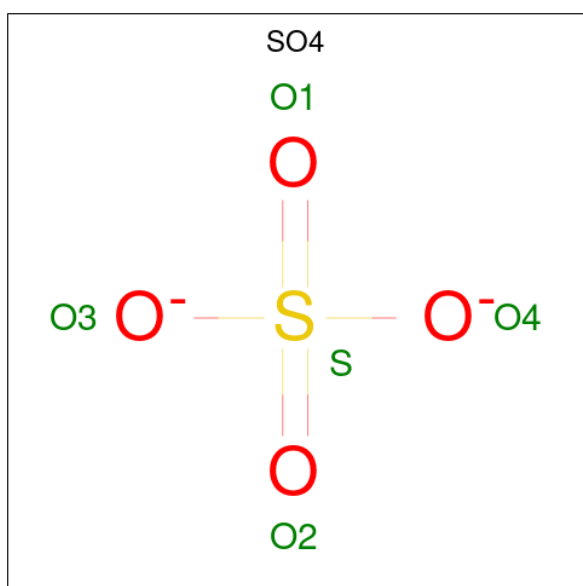
There are 4 unique types of molecules in this entry. The entry contains 4966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cell division protein 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 (CCD ID: SO4) (formula: O₄S).



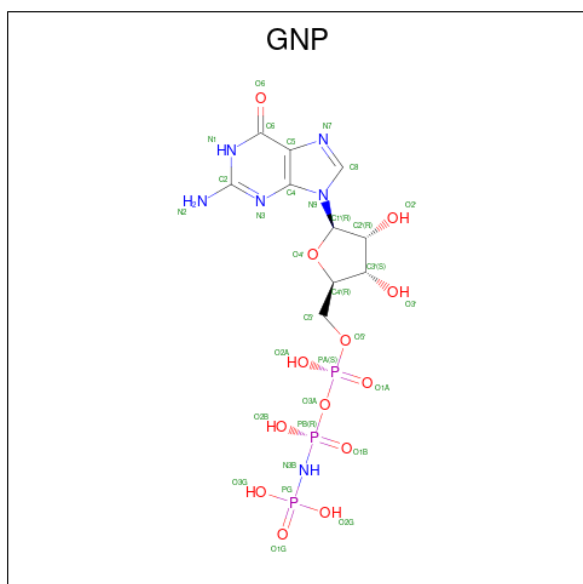
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

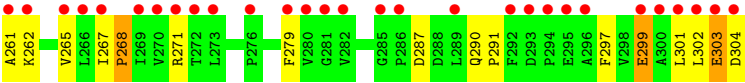
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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		



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) 91.3 (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 0.366 , 0.399	Depositor DCC
R_{free} test set	2892 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	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.

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: SO4, GNP

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	1.30	9/2365 (0.4%)	1.14	7/3189 (0.2%)
1	B	1.26	6/2244 (0.3%)	1.11	0/3026
All	All	1.28	15/4609 (0.3%)	1.12	7/6215 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	MET	SD-CE	-13.63	1.45	1.79
1	A	203	MET	SD-CE	-11.45	1.50	1.79
1	B	37	MET	SD-CE	-8.04	1.59	1.79
1	B	111	ASN	CG-OD1	6.69	1.36	1.23
1	B	220	GLU	C-O	-6.55	1.17	1.24
1	B	268	PRO	C-O	-5.92	1.16	1.24
1	A	158	ILE	CA-C	-5.85	1.47	1.53
1	A	266	LEU	CA-C	5.78	1.60	1.52
1	A	1	MET	SD-CE	5.73	1.93	1.79
1	A	224	VAL	CA-CB	5.68	1.61	1.54
1	A	111	ASN	CG-OD1	5.51	1.34	1.23
1	A	179	ALA	CA-CB	5.47	1.61	1.53
1	A	179	ALA	C-O	-5.26	1.17	1.24
1	B	299	GLU	C-O	-5.17	1.18	1.24
1	A	125	TYR	C-O	-5.10	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ARG	N-CA-C	6.89	118.79	111.28
1	A	3	PHE	N-CA-C	-5.80	104.93	112.23
1	A	217	ASP	O-C-N	5.73	124.71	121.27
1	A	237	LEU	N-CA-C	-5.35	105.11	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	GLU	N-CA-C	-5.31	105.39	111.07
1	A	133	VAL	N-CA-C	5.12	116.33	108.71
1	A	232	THR	OG1-CB-CG2	-5.09	99.12	109.30

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	2327	0	2425	115	1
1	B	2209	0	2299	132	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	11	2
4	B	176	0	0	12	0
All	All	4966	0	4737	234	3

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 25.

All (234) 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:203:MET:HE1	1:A:243:PHE:HA	1.34	1.04
1:B:1:MET:HE2	1:B:3:PHE:H	1.23	1.01
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:36:GLU:CD	1:B:37:MET:HE2	1.92	0.94
1:B:203:MET:HE1	1:B:243:PHE:HA	1.50	0.92
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:36:GLU:CG	1:B:37:MET:HE2	2.17	0.74
1:B:183:ARG:NH1	4:B:1054:HOH:O	2.13	0.74
1:B:28:LEU:H	1:B:28:LEU:HD12	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:CE	1:A:243:PHE:HA	2.17	0.73
1:A:142:ARG:HG2	1:A:195:ARG:NE	2.01	0.73
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:A:203:MET:HE3	1:A:246:ALA:CB	2.23	0.69
1:B:3:PHE:CD1	1:B:95:PRO:HD3	2.28	0.69
1:A:33:GLU:HG2	1:A:37:MET:HE2	1.75	0.68
1:A:141:PHE:HD1	1:A:141:PHE:H	1.41	0.68
1:B:52:ILE:HG13	1:B:75:MET:HE2	1.75	0.68
1:B:271:ARG:HD3	4:B:916:HOH:O	1.92	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	2.04	0.68
1:B:20:LYS:HG3	1:B:304:ASP:O	1.94	0.67
1:A:50:GLU:O	1:A:54:GLN:HG3	1.95	0.67
1:A:82:ARG:HG2	1:A:82:ARG:HH11	1.58	0.67
1:B:137:ALA:HB1	1:B:146:GLY:HA2	1.76	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:A:266:LEU:HD13	1:A:277:ILE:HD13	1.76	0.66
1:B:201:ASN:HD22	1:B:204:GLU:HG2	1.61	0.66
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.61	0.66
1:B:28:LEU:C	1:B:61:ARG:HH22	2.05	0.65
1:A:11:LEU:HD12	1:A:300:ALA:HB3	1.79	0.65
1:B:271:ARG:HG2	1:B:271:ARG:HH21	1.60	0.65
1:B:75:MET:CE	1:B:271:ARG:HE	2.09	0.64
1:A:93:GLN:HG2	1:A:94:LYS:H	1.62	0.64
1:B:131:LYS:NZ	4:B:957:HOH:O	2.30	0.64
1:B:201:ASN:HD21	1:B:203:MET:HB2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:55:GLU:HB3	1:A:71:LYS:HZ2	1.64	0.62
1:B:201:ASN:ND2	1:B:204:GLU:HG2	2.14	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:A:203:MET:HE3	1:A:246:ALA:HB3	1.82	0.61
1:B:303:GLU:C	1:B:303:GLU:OE1	2.43	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: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:303:GLU:O	1:B:304:ASP:HB3	2.01	0.60
1:A:143:ALA:O	1:A:144:ALA:C	2.45	0.60
1:A:192:THR:HG22	4:A:1106:HOH:O	2.00	0.59
1:B:115:LYS:HE2	4:B:952:HOH:O	2.01	0.59
1:B:203:MET:HE3	1:B:246:ALA:HB2	1.84	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: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:A:40:LEU:HD12	1:B:37:MET:HE3	1.85	0.57
1:B:229:ASP:O	1:B:232:THR:HG23	2.04	0.57
1:B:203:MET:HE3	1:B:246:ALA:CB	2.34	0.57
1:A:65:LYS:NZ	1:A:303:GLU:OE2	2.36	0.57
1:B:201:ASN:ND2	1:B:204:GLU:H	2.02	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:6:ARG:HG2	1:B:6:ARG:NH1	2.21	0.56
1:B:27:ASN:HB3	1:B:30:GLU:HB3	1.87	0.56
1:B:1:MET:CG	1:B:2:GLY:H	2.19	0.56
1:A:77:GLU:HG2	1:A:86:ARG:HH12	1.71	0.55
1:B:28:LEU:HB3	1:B:61:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:N	1:B:53:LEU:CD2	2.70	0.55
1:B:203:MET:HE1	1:B:243:PHE:CA	2.31	0.54
1:B:271:ARG:NH1	4:B:1047:HOH:O	2.40	0.54
1:A:285:GLY:HA3	4:A:969:HOH:O	2.06	0.54
1:B:26:GLY:O	1:B:28:LEU:N	2.40	0.54
1:A:37:MET:SD	1:B:36:GLU:CD	2.90	0.54
1:B:208:LYS:HE3	4:B:1038:HOH:O	2.06	0.54
1:A:82:ARG:HG2	1:A:82:ARG:NH1	2.22	0.54
1:A:11:LEU:HD21	1:A:297:PHE:CE1	2.43	0.54
1:B:26:GLY:O	1:B:28:LEU:HD12	2.08	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:B:265:VAL:C	1:B:268:PRO:HD2	2.32	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:A:3:PHE:CD1	1:A:3:PHE:C	2.86	0.53
1:B:53:LEU:N	1:B:53:LEU:HD22	2.24	0.53
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:B:23:PRO:C	1:B:25:GLY:H	2.17	0.52
1:B:32:LEU:HD13	1:B:57:ARG:NE	2.25	0.51
1:A:203:MET:HE2	1:A:242:LYS:C	2.36	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:95:PRO:HB3	1:A:293:ASP:HB2	1.92	0.51
1:A:234:GLN:HE22	1:B:262:LYS:HD2	1.70	0.51
1:A:203:MET:HE3	1:A:246:ALA:HB2	1.93	0.50
1:B:232:THR:HB	4:B:933:HOH:O	2.11	0.50
1:B:303:GLU:OE1	1:B:304:ASP:HB2	2.11	0.50
1:A:254:VAL:HG21	1:A:266:LEU:HD22	1.93	0.50
1:B:63:ASP:CG	1:B:66:GLU:HB2	2.36	0.50
1:A:234:GLN:O	1:A:238:GLU:HG3	2.12	0.50
1:A:36:GLU:HG2	1:B:37:MET:HE2	1.94	0.49
1:A:244:HIS:HA	1:A:249:LEU:HG	1.94	0.49
1:B:65:LYS:HE2	1:B:69:LYS:HE3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:PRO:HG2	1:A:278:LYS:HE2	1.94	0.49
1:B:31:VAL:HG13	1:B:32:LEU:H	1.77	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:A:203:MET:HE1	1:A:243:PHE:CA	2.25	0.48
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:143:ALA:HA	4:A:1069:HOH:O	2.13	0.48
1:A:199:LYS:NZ	1:B:143:ALA:HB2	2.28	0.48
1:B:19:LEU:HD23	1:B:38:ALA:HB1	1.96	0.48
1:A:219:GLU:OE2	1:A:222:LYS:HE2	2.14	0.47
1:B:60:GLY:O	1:B:61:ARG:HD2	2.13	0.47
1:B:290:GLN:O	1:B:291:PRO:C	2.55	0.47
1:A:220:GLU:HB3	1:A:221:PRO:HA	1.96	0.47
1:B:28:LEU:CA	1:B:61:ARG:HH22	2.27	0.47
1:A:265:VAL:C	1:A:268:PRO:HD2	2.39	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:53:LEU:O	1:A:57:ARG:N	2.44	0.46
1:B:201:ASN:HD22	1:B:204:GLU:N	2.08	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:8:LYS:O	1:A:15:ARG:NH2	2.45	0.46
1:A:11:LEU:HD21	1:A:297:PHE:HE1	1.80	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:36:GLU:HG3	1:A:53:LEU:HD11	1.99	0.45
1:B:161:ILE:N	1:B:161:ILE:CD1	2.79	0.45
1:A:30:GLU:O	1:A:34:GLU:HG2	2.17	0.45
1:A:303:GLU:O	1:A:304:ASP:CB	2.64	0.45
1:B:12:ALA:O	1:B:16:GLU:HG3	2.17	0.45
1:B:203:MET:HE2	1:B:242:LYS:C	2.41	0.45
1:A:148:GLN:HB3	4:A:1034:HOH:O	2.16	0.44
1:A:203:MET:HE2	1:A:242:LYS:O	2.17	0.44
1:B:28:LEU:H	1:B:28:LEU:CD1	2.27	0.44
1:B:302:LEU:O	1:B:303:GLU:C	2.58	0.44
1:A:141:PHE:CZ	1:A:205:GLU:OE1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:O	1:A:157:SER:HB2	2.17	0.44
1:B:16:GLU:HG2	1:B:20:LYS:HE3	1.99	0.44
1:A:23:PRO:C	1:A:25:GLY:H	2.26	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:A:3:PHE:HA	1:A:6:ARG:CZ	2.47	0.44
1:B:271:ARG:HH21	1:B:271:ARG:CG	2.26	0.44
1:A:82:ARG:CZ	1:A:96:LYS:HD2	2.48	0.44
1:B:11:LEU:HD11	1:B:297:PHE:CE1	2.52	0.44
1:B:19:LEU:HD13	1:B:301:LEU:HG	1.99	0.44
1:B:303:GLU:OE1	1:B:303:GLU:O	2.36	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:263:GLY:C	1:A:265:VAL:H	2.26	0.43
1:A:43:ASP:HB2	1:A:262:LYS:HB3	2.00	0.43
1:A:102:GLY:CA	1:A:222:LYS:HD2	2.48	0.43
1:A:23:PRO:O	1:A:31:VAL:HG22	2.18	0.43
1:A:138:GLY:HA3	1:A:191:ASP:O	2.18	0.43
1:B:77:GLU:HA	1:B:78:PRO:HD3	1.88	0.43
1:A:2:GLY:C	1:A:6:ARG:NH1	2.76	0.43
1:A:63:ASP:OD2	1:A:66:GLU:HG2	2.18	0.43
1:B:20:LYS:HG2	1:B:20:LYS:O	2.17	0.43
1:A:102:GLY:HA3	1:A:222:LYS:HB2	2.00	0.42
1:B:1:MET:HG2	1:B:2:GLY:N	2.30	0.42
1:B:135:PHE:HB2	1:B:160:VAL:HG22	2.02	0.42
1:A:36:GLU:CG	1:B:37:MET:CE	2.92	0.42
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.86	0.42
1:B:164:PRO:O	1:B:167:THR:OG1	2.32	0.42
1:B:220:GLU:HB3	1:B:221:PRO:HA	2.00	0.42
1:B:267:ILE:HB	1:B:268:PRO:HD3	2.02	0.42
1:A:81:ARG:NH2	4:A:986:HOH:O	2.41	0.42
1:A:93:GLN:HG2	1:A:94:LYS:N	2.31	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:139:ASP:CG	1:B:142:ARG:HD3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LYS:HD3	1:A:304:ASP:CG	2.45	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:27:ASN:O	1:A:28:LEU:C	2.63	0.41
1:A:132:LYS:HG2	1:A:185:TYR:CE2	2.55	0.41
1:A:256:LYS:HG2	3:A:950:GNP:C2	2.51	0.41
1:B:69:LYS:HG2	1:B:302:LEU:HD12	2.02	0.41
1:B:303:GLU:OE1	1:B:304:ASP:CB	2.69	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:B:43:ASP:CG	1:B:262:LYS:HD3	2.46	0.40
1:A:59:SER:O	1:A:60:GLY:C	2.64	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:B:230:ALA:C	1:B:232:THR:H	2.29	0.40
1:A:114:GLY:HA2	3:A:950:GNP:O5'	2.21	0.40
1:A:111:ASN:ND2	3:A:950:GNP:O3G	2.54	0.40
1:A:206:LEU:HD11	1:A:243:PHE:HE1	1.86	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	Interatomic distance (Å)	Clash overlap (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%)	7	5
1	B	286/304 (94%)	267 (93%)	14 (5%)	5 (2%)	7	5
All	All	588/608 (97%)	548 (93%)	30 (5%)	10 (2%)	7	5

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%)	234 (97%)	8 (3%)	33	45
1	B	230/242 (95%)	222 (96%)	8 (4%)	32	43
All	All	472/484 (98%)	456 (97%)	16 (3%)	32	44

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

Mol	Chain	Res	Type
1	A	35	LEU
1	A	43	ASP
1	A	46	LEU
1	A	81	ARG
1	A	116	THR
1	A	117	THR

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Mol	Chain	Res	Type
1	A	141	PHE
1	A	199	LYS
1	B	28	LEU
1	B	54	GLN
1	B	61	ARG
1	B	64	LEU
1	B	110	VAL
1	B	113	VAL
1	B	161	ILE
1	B	303	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	54	GLN
1	A	91	ASN
1	A	111	ASN
1	A	127	GLN
1	A	148	GLN
1	A	178	GLN
1	A	197	HIS
1	A	201	ASN
1	A	235	ASN
1	A	239	GLN
1	B	162	GLN
1	B	201	ASN
1	B	234	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

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	B	907	-	4,4,4	0.77	0	6,6,6	0.33	0
2	SO4	A	905	-	4,4,4	0.59	0	6,6,6	0.48	0
2	SO4	B	904	-	4,4,4	0.41	0	6,6,6	0.46	0
2	SO4	B	901	-	4,4,4	0.33	0	6,6,6	0.54	0
2	SO4	A	903	-	4,4,4	0.34	0	6,6,6	0.65	0
2	SO4	A	908	-	4,4,4	0.51	0	6,6,6	0.53	0
2	SO4	A	902	-	4,4,4	0.38	0	6,6,6	0.90	0
3	GNP	A	950	-	34,34,34	1.60	6 (17%)	47,54,54	1.56	6 (12%)
2	SO4	A	906	-	4,4,4	0.54	0	6,6,6	0.40	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
3	GNP	A	950	-	-	3/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	950	GNP	PG-O1G	5.29	1.54	1.46
3	A	950	GNP	PB-O2B	-3.30	1.48	1.56
3	A	950	GNP	PB-O3A	-3.18	1.55	1.59
3	A	950	GNP	PB-N3B	-2.82	1.56	1.63
3	A	950	GNP	O3'-C3'	2.47	1.49	1.43
3	A	950	GNP	PG-O3G	-2.04	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	950	GNP	O1B-PB-N3B	4.61	118.56	111.77
3	A	950	GNP	O2B-PB-O1B	4.58	119.69	109.87
3	A	950	GNP	O2B-PB-O3A	-3.58	92.70	104.64
3	A	950	GNP	O1G-PG-N3B	-3.55	106.54	111.77
3	A	950	GNP	O3A-PB-N3B	-3.38	97.21	106.59
3	A	950	GNP	O3A-PA-O1A	2.04	116.84	110.70

There are no chirality outliers.

All (3) torsion outliers are listed below:

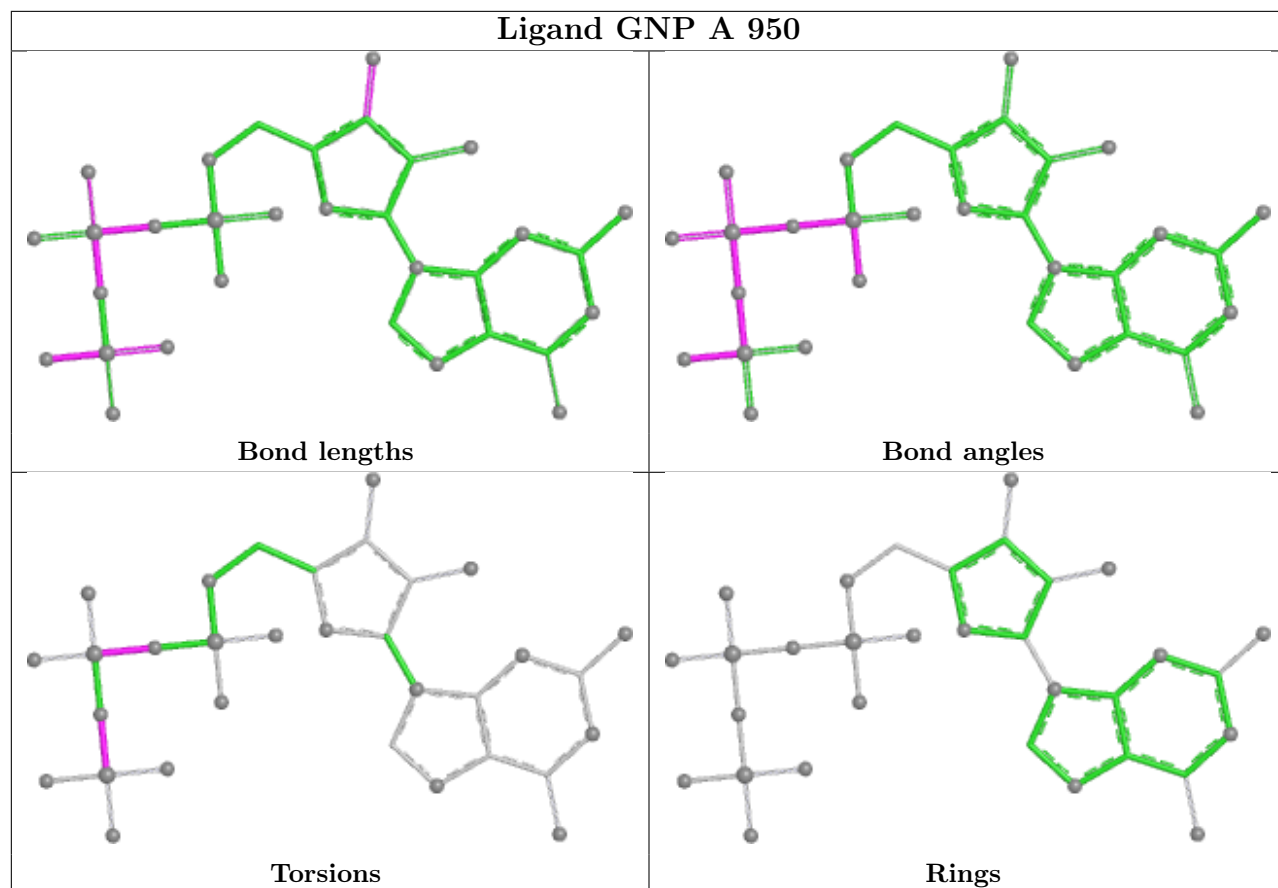
Mol	Chain	Res	Type	Atoms
3	A	950	GNP	PA-O3A-PB-O2B
3	A	950	GNP	PA-O3A-PB-O1B
3	A	950	GNP	PB-N3B-PG-O1G

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	SO4	1	0
3	A	950	GNP	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	304/304 (100%)	2.78	220 (72%) 0 0	19, 26, 34, 41	0
1	B	290/304 (95%)	2.46	187 (64%) 0 0	20, 26, 33, 39	0
All	All	594/608 (97%)	2.62	407 (68%) 0 0	19, 26, 34, 41	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	GLY	7.6
1	A	171	ALA	6.8
1	B	24	TRP	6.4
1	A	302	LEU	5.9
1	A	24	TRP	5.9
1	A	283	GLY	5.9
1	A	32	LEU	5.8
1	B	144	ALA	5.7
1	B	58	ALA	5.6
1	B	28	LEU	5.5
1	B	31	VAL	5.3
1	A	141	PHE	5.2
1	A	22	ILE	5.2
1	B	56	VAL	5.0
1	B	251	GLY	5.0
1	B	266	LEU	5.0
1	B	304	ASP	5.0
1	A	126	TYR	4.9
1	A	2	GLY	4.9
1	A	300	ALA	4.8
1	A	280	VAL	4.8
1	B	26	GLY	4.8
1	A	68	VAL	4.8
1	A	110	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	232	THR	4.8
1	B	107	VAL	4.8
1	B	209	VAL	4.7
1	A	304	ASP	4.7
1	B	3	PHE	4.7
1	A	128	ASN	4.6
1	A	1	MET	4.6
1	A	92	PRO	4.6
1	A	104	VAL	4.6
1	A	257	LEU	4.6
1	A	4	PHE	4.5
1	A	72	LEU	4.5
1	A	11	LEU	4.5
1	A	301	LEU	4.4
1	B	62	LYS	4.4
1	B	206	LEU	4.4
1	B	212	ALA	4.4
1	A	95	PRO	4.4
1	A	64	LEU	4.3
1	A	251	GLY	4.3
1	A	124	ARG	4.3
1	B	61	ARG	4.3
1	A	292	PHE	4.3
1	B	214	ALA	4.3
1	B	59	SER	4.2
1	A	143	ALA	4.2
1	A	161	ILE	4.1
1	A	185	TYR	4.1
1	B	22	ILE	4.1
1	A	127	GLN	4.1
1	A	237	LEU	4.1
1	B	9	ALA	4.1
1	A	28	LEU	4.1
1	A	129	LEU	4.1
1	A	130	GLY	4.1
1	B	168	ASP	4.1
1	B	169	PRO	4.1
1	A	263	GLY	4.0
1	B	25	GLY	4.0
1	A	225	TRP	4.0
1	A	173	ALA	4.0
1	B	95	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	265	VAL	3.9
1	A	74	GLY	3.9
1	A	108	VAL	3.9
1	A	138	GLY	3.9
1	A	144	ALA	3.9
1	B	141	PHE	3.9
1	B	269	ILE	3.9
1	A	153	GLY	3.9
1	B	281	GLY	3.8
1	A	109	GLY	3.8
1	B	200	HIS	3.8
1	B	216	ALA	3.8
1	B	262	LYS	3.8
1	A	123	GLY	3.8
1	B	73	VAL	3.8
1	A	12	ALA	3.7
1	B	5	ASP	3.7
1	B	110	VAL	3.7
1	A	94	LYS	3.7
1	A	27	ASN	3.7
1	A	63	ASP	3.7
1	A	3	PHE	3.7
1	B	16	GLU	3.7
1	B	106	LEU	3.7
1	A	227	VAL	3.7
1	A	252	VAL	3.7
1	A	23	PRO	3.7
1	A	107	VAL	3.6
1	B	201	ASN	3.6
1	A	47	SER	3.6
1	A	40	LEU	3.6
1	A	157	SER	3.6
1	A	60	GLY	3.6
1	A	233	GLY	3.6
1	A	62	LYS	3.6
1	B	296	ALA	3.6
1	A	279	PHE	3.6
1	A	7	LEU	3.6
1	A	156	LEU	3.6
1	A	131	LYS	3.6
1	A	38	ALA	3.6
1	B	148	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	90	PHE	3.5
1	A	213	ILE	3.5
1	A	46	LEU	3.5
1	A	172	LEU	3.5
1	A	200	HIS	3.5
1	A	277	ILE	3.5
1	A	88	LEU	3.5
1	B	39	LEU	3.5
1	B	271	ARG	3.5
1	A	270	VAL	3.4
1	B	117	THR	3.4
1	B	219	GLU	3.4
1	A	76	LEU	3.4
1	A	152	TRP	3.4
1	B	239	GLN	3.4
1	B	253	ILE	3.4
1	A	125	TYR	3.4
1	A	54	GLN	3.4
1	A	189	PHE	3.4
1	B	135	PHE	3.4
1	B	213	ILE	3.3
1	A	248	GLY	3.3
1	A	136	CYS	3.3
1	A	250	THR	3.3
1	B	15	ARG	3.3
1	A	73	VAL	3.3
1	A	113	VAL	3.3
1	A	282	VAL	3.3
1	A	25	GLY	3.3
1	A	226	LEU	3.3
1	A	158	ILE	3.3
1	A	116	THR	3.3
1	B	113	VAL	3.3
1	B	265	VAL	3.3
1	A	281	GLY	3.3
1	A	91	ASN	3.3
1	B	302	LEU	3.3
1	B	30	GLU	3.3
1	A	255	THR	3.3
1	B	232	THR	3.3
1	A	41	ALA	3.2
1	A	243	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	186	ASP	3.2
1	B	243	PHE	3.2
1	B	279	PHE	3.2
1	A	177	VAL	3.2
1	A	149	LEU	3.2
1	A	67	ALA	3.2
1	A	188	LEU	3.2
1	B	226	LEU	3.2
1	A	103	ARG	3.1
1	B	4	PHE	3.1
1	A	296	ALA	3.1
1	B	261	ALA	3.1
1	A	35	LEU	3.1
1	B	152	TRP	3.1
1	B	299	GLU	3.1
1	A	170	ALA	3.1
1	A	212	ALA	3.1
1	B	270	VAL	3.1
1	B	241	LYS	3.1
1	A	21	ALA	3.1
1	B	105	VAL	3.1
1	B	1	MET	3.1
1	A	16	GLU	3.1
1	A	102	GLY	3.1
1	A	240	ALA	3.1
1	A	75	MET	3.1
1	A	26	GLY	3.0
1	B	68	VAL	3.0
1	B	104	VAL	3.0
1	B	147	THR	3.0
1	A	234	GLN	3.0
1	B	109	GLY	3.0
1	B	293	ASP	3.0
1	B	32	LEU	3.0
1	B	69	LYS	3.0
1	A	30	GLU	3.0
1	A	105	VAL	3.0
1	A	133	VAL	3.0
1	A	14	THR	3.0
1	A	118	THR	3.0
1	B	255	THR	3.0
1	A	168	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	3.0
1	B	300	ALA	2.9
1	A	53	LEU	2.9
1	A	121	LYS	2.9
1	B	167	THR	2.9
1	B	12	ALA	2.9
1	B	301	LEU	2.9
1	A	253	ILE	2.9
1	A	89	GLY	2.9
1	B	27	ASN	2.9
1	A	294	PRO	2.9
1	B	286	PRO	2.9
1	A	20	LYS	2.9
1	A	98	VAL	2.9
1	A	254	VAL	2.9
1	A	238	GLU	2.9
1	B	10	GLY	2.9
1	B	145	GLY	2.9
1	A	15	ARG	2.9
1	A	85	LEU	2.9
1	A	122	LEU	2.9
1	A	209	VAL	2.9
1	B	295	GLU	2.9
1	B	184	GLY	2.8
1	A	291	PRO	2.8
1	B	53	LEU	2.8
1	A	48	ALA	2.8
1	A	33	GLU	2.8
1	A	77	GLU	2.8
1	A	288	ASP	2.8
1	B	79	ASP	2.8
1	A	166	GLY	2.8
1	A	106	LEU	2.8
1	A	266	LEU	2.8
1	A	135	PHE	2.8
1	A	66	GLU	2.8
1	A	284	GLU	2.8
1	A	190	VAL	2.8
1	A	247	VAL	2.8
1	A	298	VAL	2.8
1	A	97	PRO	2.8
1	A	249	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	2.8
1	B	242	LYS	2.8
1	B	108	VAL	2.8
1	A	159	PRO	2.7
1	B	273	LEU	2.7
1	A	174	TYR	2.7
1	B	41	ALA	2.7
1	B	240	ALA	2.7
1	B	231	VAL	2.7
1	A	119	ILE	2.7
1	A	145	GLY	2.7
1	A	165	GLU	2.7
1	B	51	GLU	2.7
1	B	187	LEU	2.7
1	B	197	HIS	2.7
1	A	231	VAL	2.7
1	B	250	THR	2.7
1	A	10	GLY	2.7
1	B	6	ARG	2.7
1	A	230	ALA	2.7
1	B	280	VAL	2.7
1	A	55	GLU	2.7
1	A	151	GLU	2.7
1	A	303	GLU	2.7
1	B	33	GLU	2.7
1	A	45	GLY	2.7
1	B	164	PRO	2.7
1	A	183	ARG	2.7
1	A	19	LEU	2.7
1	B	122	LEU	2.7
1	B	198	THR	2.6
1	B	236	GLY	2.6
1	A	289	LEU	2.6
1	B	115	LYS	2.6
1	B	215	LYS	2.6
1	B	254	VAL	2.6
1	A	264	GLY	2.6
1	A	276	PRO	2.6
1	B	52	ILE	2.6
1	B	159	PRO	2.6
1	B	203	MET	2.6
1	A	290	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	221	PRO	2.6
1	B	202	LEU	2.6
1	B	237	LEU	2.6
1	B	257	LEU	2.6
1	A	191	ASP	2.6
1	A	134	MET	2.6
1	A	198	THR	2.6
1	A	286	PRO	2.6
1	A	297	PHE	2.6
1	B	259	GLY	2.6
1	A	267	ILE	2.6
1	B	54	GLN	2.5
1	B	17	ARG	2.5
1	A	285	GLY	2.5
1	B	272	THR	2.5
1	A	6	ARG	2.5
1	A	142	ARG	2.5
1	B	156	LEU	2.5
1	B	123	GLY	2.5
1	B	189	PHE	2.5
1	B	227	VAL	2.5
1	A	271	ARG	2.5
1	B	142	ARG	2.5
1	A	214	ALA	2.5
1	B	43	ASP	2.5
1	B	65	LYS	2.5
1	B	276	PRO	2.5
1	A	93	GLN	2.5
1	A	187	LEU	2.5
1	B	72	LEU	2.5
1	A	13	LYS	2.5
1	A	96	LYS	2.5
1	A	195	ARG	2.4
1	B	11	LEU	2.4
1	B	185	TYR	2.4
1	A	99	GLU	2.4
1	B	47	SER	2.4
1	B	172	LEU	2.4
1	B	36	GLU	2.4
1	B	50	GLU	2.4
1	B	21	ALA	2.4
1	B	48	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	272	THR	2.4
1	A	222	LYS	2.4
1	A	56	VAL	2.4
1	B	161	ILE	2.4
1	B	249	LEU	2.4
1	B	155	ARG	2.4
1	B	55	GLU	2.4
1	A	246	ALA	2.4
1	B	38	ALA	2.4
1	A	274	LYS	2.4
1	A	275	VAL	2.4
1	B	119	ILE	2.4
1	A	51	GLU	2.4
1	A	71	LYS	2.3
1	A	216	ALA	2.3
1	A	261	ALA	2.3
1	B	176	ALA	2.3
1	B	252	VAL	2.3
1	B	99	GLU	2.3
1	A	37	MET	2.3
1	A	147	THR	2.3
1	B	57	ARG	2.3
1	B	44	VAL	2.3
1	B	292	PHE	2.3
1	B	94	LYS	2.3
1	B	218	PRO	2.3
1	A	146	GLY	2.3
1	A	59	SER	2.3
1	B	70	GLU	2.3
1	B	247	VAL	2.3
1	A	207	LYS	2.3
1	B	76	LEU	2.3
1	B	134	MET	2.3
1	A	82	ARG	2.3
1	B	125	TYR	2.3
1	A	34	GLU	2.3
1	B	244	HIS	2.3
1	A	206	LEU	2.2
1	B	100	PRO	2.2
1	B	63	ASP	2.2
1	A	86	ARG	2.2
1	B	112	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	2.2
1	A	65	LYS	2.2
1	A	39	LEU	2.2
1	B	191	ASP	2.2
1	B	75	MET	2.2
1	B	294	PRO	2.2
1	A	29	GLU	2.2
1	B	256	LYS	2.2
1	B	118	THR	2.2
1	B	267	ILE	2.2
1	A	155	ARG	2.2
1	B	282	VAL	2.2
1	B	130	GLY	2.2
1	B	260	THR	2.2
1	A	5	ASP	2.1
1	A	287	ASP	2.1
1	B	210	LYS	2.1
1	B	23	PRO	2.1
1	B	29	GLU	2.1
1	B	285	GLY	2.1
1	B	150	SER	2.1
1	B	173	ALA	2.1
1	B	40	LEU	2.1
1	B	228	LEU	2.1
1	B	245	GLU	2.1
1	A	31	VAL	2.1
1	A	44	VAL	2.1
1	A	218	PRO	2.1
1	B	78	PRO	2.1
1	B	177	VAL	2.1
1	B	166	GLY	2.1
1	B	66	GLU	2.1
1	B	225	TRP	2.1
1	B	153	GLY	2.1
1	B	101	LYS	2.1
1	A	273	LEU	2.1
1	A	269	ILE	2.1
1	B	111	ASN	2.1
1	A	192	THR	2.0
1	B	192	THR	2.0
1	B	303	GLU	2.0
1	B	258	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	34	GLU	2.0
1	A	42	ALA	2.0
1	B	289	LEU	2.0
1	B	195	ARG	2.0
1	A	241	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](#)

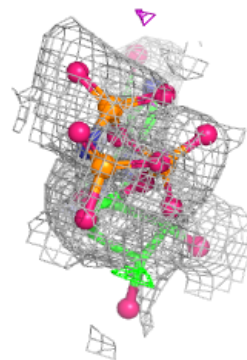
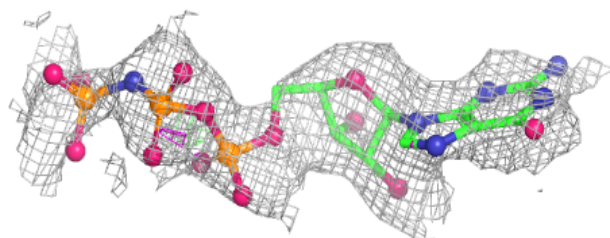
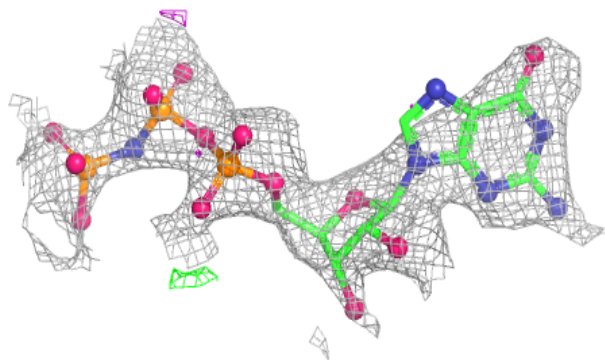
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	SO4	A	905	5/5	0.68	0.19	39,39,45,46	0
2	SO4	A	906	5/5	0.70	0.18	45,46,51,53	0
3	GNP	A	950	32/32	0.72	0.20	43,48,60,62	0
2	SO4	B	907	5/5	0.77	0.17	43,49,52,53	0
2	SO4	B	904	5/5	0.81	0.17	39,41,44,45	0
2	SO4	A	903	5/5	0.81	0.21	35,40,42,44	0
2	SO4	A	908	5/5	0.81	0.19	49,50,52,54	0
2	SO4	A	902	5/5	0.85	0.16	42,42,44,49	0
2	SO4	B	901	5/5	0.92	0.14	32,33,37,37	0

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

Electron density around GNP A 950:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.