



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:26 pm BST

PDB ID : 2Q9B
Title : Structure of FTSY:GMPPNP Complex
Authors : Reyes, C.L.; Stroud, R.M.
Deposited on : 2007-06-12
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

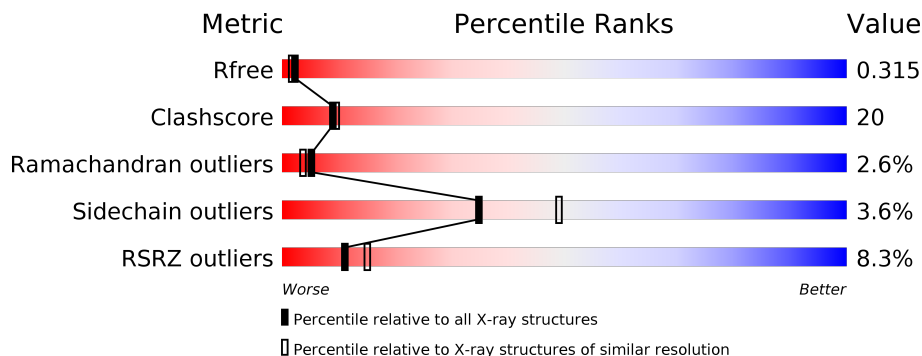
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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	 6% 66% 29% ••
1	B	304	 10% 57% 33% • 6%

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
2	SO4	A	956	-	X	-	X
3	EDO	A	905	-	-	-	X

2 Entry composition [i](#)

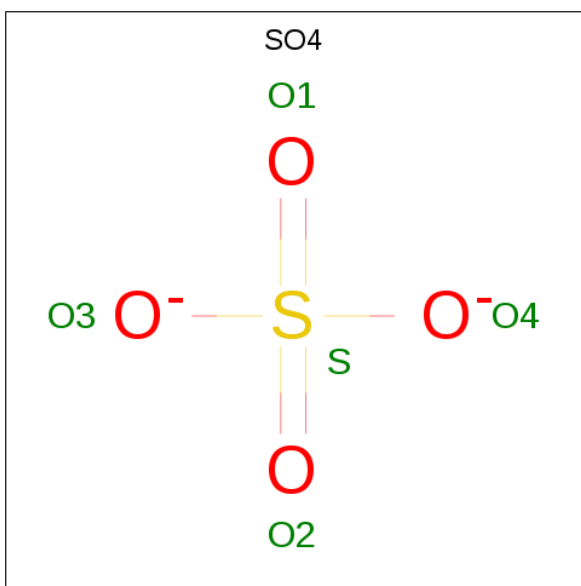
There are 5 unique types of molecules in this entry. The entry contains 4818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	303	Total 2318	C 1481	N 404	O 426	S 7	0	0	0
1	B	287	Total 2181	C 1396	N 372	O 406	S 7	0	0	0

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



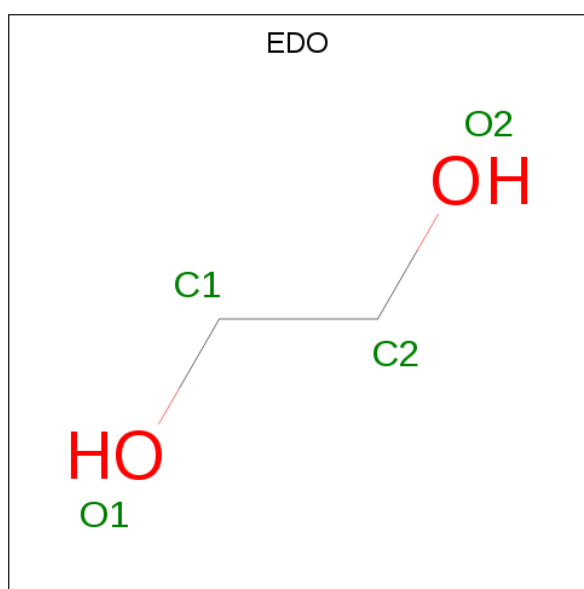
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

Continued on next page...

Continued from previous page...

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	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



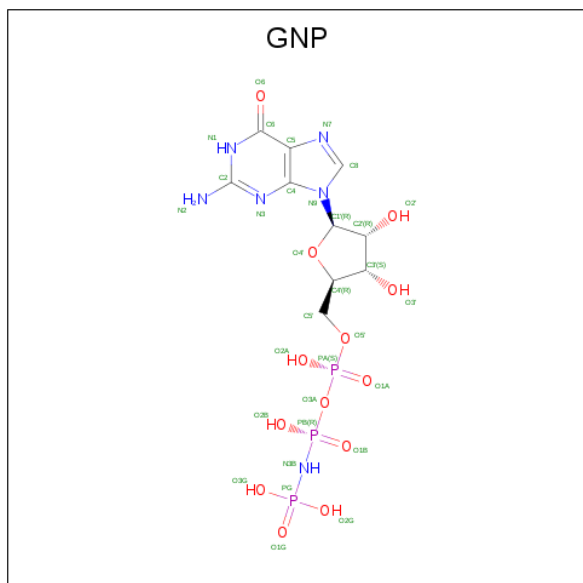
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

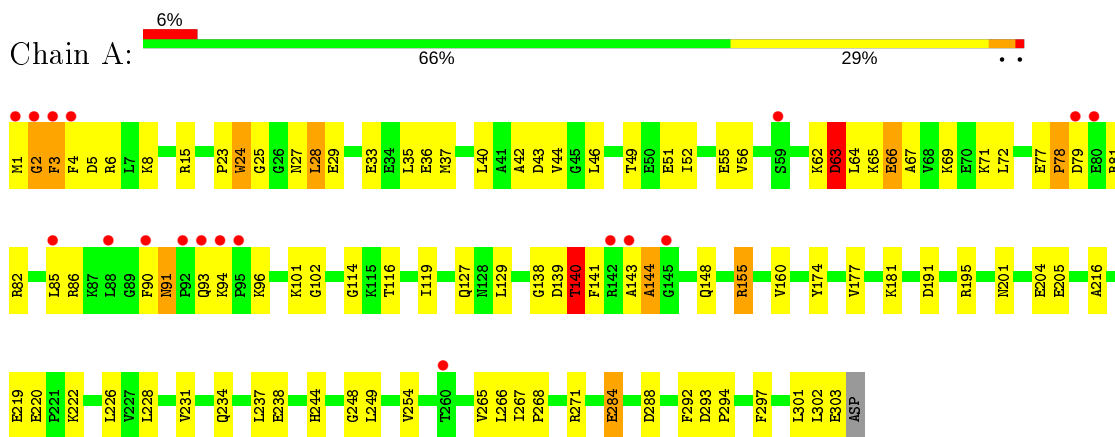
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	101	Total	O	0	0
			101	101		

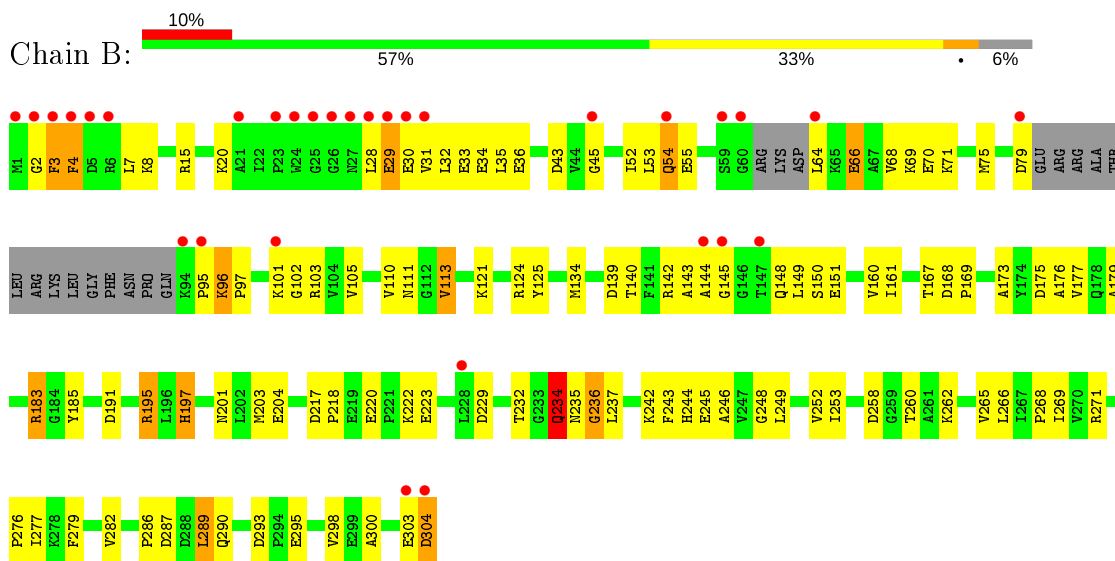
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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	63.84Å 97.30Å 99.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.35 – 2.30 36.35 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.9 (36.35-2.30) 90.0 (36.35-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.269 0.248 , 0.315	Depositor DCC
R_{free} test set	1730 reflections (6.83%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtrriage
Anisotropy	0.329	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for -h,l,k	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4818	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GNP, SO4, EDO

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	1.24	7/2356 (0.3%)	1.04	8/3178 (0.3%)
1	B	1.25	11/2215 (0.5%)	1.05	13/2987 (0.4%)
All	All	1.25	18/4571 (0.4%)	1.04	21/6165 (0.3%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	GLU	CD-OE1	7.35	1.33	1.25
1	A	160	VAL	CB-CG1	6.70	1.67	1.52
1	B	185	TYR	CD2-CE2	6.60	1.49	1.39
1	B	282	VAL	CB-CG2	6.49	1.66	1.52
1	B	183	ARG	CZ-NH1	6.40	1.41	1.33
1	A	284	GLU	CD-OE2	5.92	1.32	1.25
1	A	297	PHE	CE1-CZ	-5.86	1.26	1.37
1	A	220	GLU	CD-OE2	-5.60	1.19	1.25
1	A	205	GLU	CD-OE2	-5.51	1.19	1.25
1	B	110	VAL	CB-CG1	-5.44	1.41	1.52
1	B	295	GLU	CD-OE2	5.44	1.31	1.25
1	A	177	VAL	CB-CG1	5.41	1.64	1.52
1	B	220	GLU	CD-OE1	5.24	1.31	1.25
1	B	113	VAL	CB-CG2	-5.16	1.42	1.52
1	A	66	GLU	CD-OE1	5.12	1.31	1.25
1	B	111	ASN	CG-ND2	-5.08	1.20	1.32
1	B	113	VAL	CB-CG1	5.05	1.63	1.52
1	B	185	TYR	CD1-CE1	5.01	1.46	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ASP	CB-CG-OD2	8.98	126.39	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	ASP	CB-CG-OD2	8.14	125.63	118.30
1	A	293	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	195	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	155	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	304	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	139	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	258	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	103	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	288	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	191	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	5	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	287	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	195	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	183	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	195	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	B	79	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	271	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	181	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	B	175	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	293	ASP	CB-CG-OD2	5.01	122.81	118.30

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	2318	0	2421	94	0
1	B	2181	0	2268	104	0
2	A	30	0	0	1	0
2	B	10	0	0	0	0
3	A	12	0	18	2	0
3	B	24	0	36	5	0
4	A	32	0	13	6	0
5	A	110	0	0	6	0
5	B	101	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4818	0	4756	189	0

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 20.

All (189) 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:B:28:LEU:HD23	1:B:29:GLU:N	1.71	1.04
1:B:8:LYS:NZ	1:B:303:GLU:HG3	1.84	0.92
1:B:266:LEU:HG	1:B:277:ILE:HD13	1.55	0.89
1:B:28:LEU:CD2	1:B:29:GLU:HG3	2.04	0.87
1:A:86:ARG:HD2	5:A:982:HOH:O	1.75	0.85
1:A:143:ALA:O	1:A:144:ALA:HB2	1.76	0.85
1:A:44:VAL:O	1:A:268:PRO:HG3	1.79	0.82
1:B:28:LEU:HD23	1:B:29:GLU:H	1.47	0.79
1:B:8:LYS:HZ1	1:B:303:GLU:HG3	1.45	0.78
1:B:203:MET:HE1	1:B:243:PHE:HA	1.65	0.77
1:B:279:PHE:HB3	1:B:289:LEU:HD22	1.67	0.76
1:B:148:GLN:HE21	1:B:148:GLN:HA	1.49	0.75
1:A:82:ARG:HH12	1:A:96:LYS:NZ	1.84	0.75
1:B:28:LEU:HD23	1:B:28:LEU:C	2.07	0.74
1:B:161:ILE:HD13	1:B:176:ALA:HA	1.69	0.74
1:B:28:LEU:HD23	1:B:29:GLU:HG3	1.69	0.74
1:B:201:ASN:HD22	1:B:204:GLU:HG2	1.53	0.73
1:A:1:MET:SD	1:A:2:GLY:N	2.63	0.72
1:A:55:GLU:HB3	1:A:71:LYS:NZ	2.05	0.71
1:B:145:GLY:O	5:B:1029:HOH:O	2.10	0.70
1:A:114:GLY:HA2	4:A:950:GNP:O5'	1.93	0.69
1:B:161:ILE:CD1	1:B:176:ALA:HA	2.23	0.69
1:A:143:ALA:O	1:A:144:ALA:CB	2.40	0.69
1:A:101:LYS:HG2	1:A:222:LYS:HD2	1.76	0.67
1:B:3:PHE:CE1	1:B:95:PRO:HD3	2.29	0.67
1:A:143:ALA:HB1	4:A:950:GNP:O3G	1.95	0.66
1:A:234:GLN:HB3	1:B:262:LYS:NZ	2.10	0.66
1:A:129:LEU:HA	3:A:905:EDO:H22	1.77	0.66
1:A:254:VAL:HG21	1:A:266:LEU:HD22	1.77	0.65
1:A:3:PHE:HA	1:A:6:ARG:HH21	1.62	0.65
1:B:69:LYS:HG3	1:B:298:VAL:HG12	1.79	0.65
1:B:201:ASN:ND2	1:B:204:GLU:HG2	2.11	0.65
1:B:266:LEU:HG	1:B:277:ILE:CD1	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:O	1:B:75:MET:HE2	1.97	0.64
1:B:144:ALA:O	1:B:148:GLN:HG2	1.98	0.64
1:B:28:LEU:CD2	1:B:28:LEU:C	2.65	0.64
1:A:265:VAL:O	1:A:268:PRO:HD2	1.98	0.63
1:A:82:ARG:HH12	1:A:96:LYS:HZ2	1.46	0.63
1:B:244:HIS:HA	1:B:249:LEU:HG	1.81	0.62
1:A:55:GLU:HB3	1:A:71:LYS:HZ2	1.64	0.62
1:A:23:PRO:O	1:A:25:GLY:N	2.32	0.62
1:B:234:GLN:CG	1:B:235:ASN:N	2.59	0.62
1:A:3:PHE:HA	1:A:6:ARG:HE	1.65	0.61
1:B:139:ASP:OD2	1:B:142:ARG:HD3	2.00	0.61
1:A:284:GLU:HB2	4:A:950:GNP:N2	2.15	0.61
1:B:15:ARG:HD2	1:B:20:LYS:HE3	1.83	0.61
1:A:8:LYS:O	1:A:15:ARG:NH2	2.30	0.61
1:A:36:GLU:HG3	1:A:49:THR:HG21	1.83	0.61
1:B:4:PHE:O	1:B:8:LYS:HG2	2.00	0.60
1:B:113:VAL:HG23	1:B:229:ASP:HB2	1.84	0.60
1:A:140:THR:HG23	5:A:1046:HOH:O	2.02	0.60
1:A:3:PHE:HB3	1:A:94:LYS:NZ	2.17	0.60
1:B:183:ARG:HH22	3:B:902:EDO:H22	1.67	0.59
1:B:286:PRO:HD2	5:B:1044:HOH:O	2.02	0.59
1:B:96:LYS:HE3	1:B:97:PRO:O	2.02	0.59
1:A:62:LYS:O	1:A:63:ASP:CB	2.51	0.58
1:A:51:GLU:OE1	1:A:271:ARG:NH1	2.36	0.58
1:B:260:THR:HG23	1:B:262:LYS:H	1.67	0.58
1:B:20:LYS:HE2	1:B:304:ASP:HB3	1.85	0.58
1:B:234:GLN:HG2	1:B:235:ASN:N	2.19	0.57
1:B:148:GLN:NE2	1:B:148:GLN:HA	2.19	0.57
1:B:3:PHE:CD1	1:B:95:PRO:HD3	2.40	0.56
1:B:29:GLU:O	1:B:31:VAL:HG12	2.06	0.56
1:A:114:GLY:HA3	4:A:950:GNP:H8	1.87	0.56
1:B:203:MET:CE	1:B:243:PHE:HA	2.33	0.56
1:A:302:LEU:N	1:A:302:LEU:HD12	2.19	0.55
1:A:219:GLU:O	1:A:222:LYS:HE3	2.06	0.55
1:A:3:PHE:HA	1:A:6:ARG:NH2	2.22	0.55
1:B:124:ARG:HD3	3:B:908:EDO:O2	2.07	0.55
1:A:226:LEU:HD21	1:A:228:LEU:CD2	2.38	0.54
1:A:302:LEU:N	1:A:302:LEU:CD1	2.70	0.54
1:A:36:GLU:HG3	1:A:49:THR:CG2	2.37	0.54
1:B:15:ARG:HD2	1:B:20:LYS:CE	2.37	0.54
2:A:952:SO4:O4	1:B:195:ARG:HD3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG21	1:A:266:LEU:CD2	2.37	0.54
1:B:36:GLU:HG3	1:B:53:LEU:HD11	1.89	0.54
1:A:4:PHE:CE2	1:A:8:LYS:HE3	2.42	0.53
1:B:45:GLY:HA2	3:B:901:EDO:H22	1.91	0.53
1:A:79:ASP:OD2	1:A:82:ARG:HG3	2.08	0.53
1:B:31:VAL:HG13	1:B:32:LEU:H	1.72	0.53
1:A:23:PRO:C	1:A:25:GLY:H	2.13	0.52
1:B:167:THR:HG22	1:B:168:ASP:N	2.24	0.52
1:A:234:GLN:HB3	1:B:262:LYS:HZ1	1.75	0.52
1:B:203:MET:HE1	1:B:243:PHE:CA	2.37	0.52
1:A:138:GLY:HA3	1:A:191:ASP:O	2.10	0.52
1:A:82:ARG:NH1	1:A:96:LYS:NZ	2.55	0.51
1:B:143:ALA:C	1:B:145:GLY:H	2.13	0.51
1:A:55:GLU:HB3	1:A:71:LYS:HZ3	1.76	0.51
1:B:8:LYS:HZ2	1:B:303:GLU:HG3	1.73	0.51
1:A:52:ILE:HD13	1:A:72:LEU:HD21	1.92	0.50
1:B:29:GLU:O	1:B:31:VAL:N	2.39	0.50
1:B:102:GLY:HA3	1:B:222:LYS:HD2	1.94	0.50
1:A:284:GLU:HG2	1:A:284:GLU:O	2.12	0.50
1:A:3:PHE:HA	1:A:6:ARG:NE	2.26	0.50
1:B:144:ALA:HB1	1:B:148:GLN:HG2	1.93	0.50
1:A:301:LEU:C	1:A:302:LEU:HD12	2.32	0.50
1:A:3:PHE:HB3	1:A:94:LYS:HZ2	1.76	0.50
1:B:148:GLN:CA	1:B:148:GLN:HE21	2.17	0.50
1:A:102:GLY:HA3	1:A:222:LYS:HG3	1.94	0.49
1:B:54:GLN:HE21	1:B:55:GLU:N	2.10	0.49
1:B:303:GLU:O	1:B:304:ASP:OXT	2.30	0.49
1:A:148:GLN:HB3	5:A:1045:HOH:O	2.10	0.49
1:B:237:LEU:HD21	1:B:269:ILE:HA	1.93	0.49
1:A:244:HIS:HA	1:A:249:LEU:HG	1.95	0.49
1:A:292:PHE:CE2	1:A:294:PRO:HG3	2.48	0.49
1:A:116:THR:HB	4:A:950:GNP:O1A	2.13	0.48
1:B:125:TYR:HB2	3:B:908:EDO:H22	1.94	0.48
1:A:81:ARG:HA	5:A:1022:HOH:O	2.13	0.48
1:A:267:ILE:HB	1:A:268:PRO:HD3	1.94	0.48
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.77	0.48
1:B:101:LYS:HG2	1:B:222:LYS:HD3	1.95	0.48
1:A:37:MET:CE	1:B:36:GLU:OE1	2.62	0.47
1:B:149:LEU:HB2	5:B:1029:HOH:O	2.13	0.47
1:A:85:LEU:O	1:A:90:PHE:HB3	2.14	0.47
1:B:140:THR:OG1	1:B:169:PRO:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ALA:HB1	1:B:148:GLN:CG	2.44	0.47
1:B:30:GLU:O	1:B:34:GLU:HG3	2.15	0.47
1:B:31:VAL:HG13	1:B:32:LEU:N	2.29	0.47
1:B:121:LYS:O	3:B:908:EDO:H22	2.15	0.47
1:B:235:ASN:O	1:B:237:LEU:N	2.49	0.46
1:B:265:VAL:O	1:B:268:PRO:HD2	2.16	0.46
1:A:8:LYS:NZ	1:A:303:GLU:HB2	2.31	0.46
1:A:33:GLU:CD	1:B:33:GLU:HG3	2.35	0.46
1:A:174:TYR:CD2	1:A:216:ALA:HB2	2.51	0.46
1:A:219:GLU:HB3	1:A:222:LYS:HE3	1.98	0.46
1:A:42:ALA:O	1:A:43:ASP:HB2	2.16	0.46
1:A:63:ASP:HB3	1:A:66:GLU:HB2	1.97	0.46
1:B:69:LYS:HG3	1:B:298:VAL:CG1	2.45	0.46
1:B:232:THR:HG22	1:B:236:GLY:H	1.82	0.45
1:B:252:VAL:HG12	1:B:253:ILE:N	2.30	0.45
1:A:40:LEU:HD21	1:A:46:LEU:HA	1.98	0.45
1:B:148:GLN:CA	1:B:148:GLN:NE2	2.79	0.45
1:B:101:LYS:HB3	1:B:222:LYS:HB3	1.99	0.45
1:B:52:ILE:HG12	1:B:75:MET:HE1	1.98	0.45
1:A:141:PHE:CD1	1:A:141:PHE:N	2.85	0.45
1:A:226:LEU:CD2	1:A:228:LEU:HG	2.47	0.45
1:A:3:PHE:HB2	1:A:6:ARG:HH21	1.82	0.45
1:B:64:LEU:O	1:B:68:VAL:HG23	2.16	0.44
1:A:24:TRP:CD1	1:A:65:LYS:HE2	2.52	0.44
1:B:203:MET:HE1	1:B:242:LYS:C	2.37	0.44
1:B:234:GLN:HB3	1:B:234:GLN:HE21	1.62	0.44
1:A:28:LEU:O	1:A:29:GLU:C	2.55	0.44
1:B:105:VAL:HG22	1:B:223:GLU:HB2	2.00	0.44
1:A:155:ARG:HB3	5:A:1026:HOH:O	2.18	0.43
1:B:237:LEU:HA	1:B:237:LEU:HD23	1.83	0.43
1:B:134:MET:SD	1:B:161:ILE:HD11	2.58	0.43
1:B:30:GLU:HA	1:B:33:GLU:HB3	1.99	0.43
1:B:4:PHE:HE2	1:B:300:ALA:HB2	1.83	0.43
1:A:37:MET:SD	1:B:36:GLU:OE1	2.77	0.43
1:A:101:LYS:HE3	1:A:222:LYS:HD2	2.01	0.43
1:A:29:GLU:O	1:A:33:GLU:HG3	2.18	0.43
1:A:33:GLU:OE1	1:B:33:GLU:HG3	2.19	0.43
1:A:62:LYS:O	1:A:63:ASP:HB2	2.19	0.43
1:B:3:PHE:H	1:B:3:PHE:HD1	1.66	0.42
1:B:32:LEU:O	1:B:35:LEU:HB3	2.19	0.42
1:A:237:LEU:O	1:A:238:GLU:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:HD22	1:A:91:ASN:C	2.22	0.42
1:B:150:SER:HA	1:B:160:VAL:HG21	2.01	0.42
1:B:265:VAL:C	1:B:268:PRO:HD2	2.39	0.42
1:B:203:MET:HE1	1:B:242:LYS:O	2.19	0.42
5:A:1048:HOH:O	1:B:234:GLN:CD	2.56	0.42
1:A:28:LEU:HD23	1:A:64:LEU:HD22	2.00	0.42
1:B:7:LEU:HD13	1:B:290:GLN:NE2	2.34	0.42
1:A:67:ALA:O	1:A:71:LYS:HG2	2.20	0.42
1:B:197:HIS:N	1:B:197:HIS:CD2	2.88	0.42
1:B:161:ILE:HD11	1:B:179:ALA:HB3	2.02	0.42
1:A:144:ALA:HB3	1:A:148:GLN:NE2	2.35	0.42
1:A:226:LEU:C	1:A:226:LEU:HD23	2.40	0.42
1:B:203:MET:HE3	1:B:246:ALA:HB3	2.02	0.42
1:A:140:THR:HG22	1:A:140:THR:O	2.20	0.41
1:A:234:GLN:OE1	1:B:234:GLN:HB3	2.19	0.41
1:A:69:LYS:HB2	1:A:69:LYS:HE3	1.74	0.41
1:B:203:MET:CE	1:B:246:ALA:HB3	2.50	0.41
1:B:303:GLU:O	1:B:304:ASP:HB3	2.20	0.41
1:A:119:ILE:CD1	1:A:191:ASP:HB2	2.50	0.41
1:A:52:ILE:O	1:A:56:VAL:HG23	2.20	0.41
1:A:231:VAL:HG12	1:B:235:ASN:OD1	2.20	0.41
1:B:66:GLU:O	1:B:70:GLU:HB2	2.20	0.41
1:A:129:LEU:CD2	3:A:905:EDO:H22	2.51	0.41
1:A:114:GLY:HA2	4:A:950:GNP:PA	2.61	0.41
1:A:201:ASN:HD22	1:A:204:GLU:H	1.68	0.41
1:A:101:LYS:HB3	1:A:222:LYS:HB3	2.02	0.41
1:A:234:GLN:HG2	5:B:1042:HOH:O	2.21	0.41
1:B:8:LYS:CE	1:B:303:GLU:HG3	2.50	0.41
1:A:219:GLU:HB3	1:A:222:LYS:CE	2.51	0.41
1:B:173:ALA:O	1:B:177:VAL:HG23	2.21	0.41
1:B:279:PHE:HB3	1:B:289:LEU:CD2	2.45	0.41
1:A:234:GLN:OE1	1:B:234:GLN:NE2	2.46	0.40
1:A:77:GLU:HA	1:A:78:PRO:HD3	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	301/304 (99%)	274 (91%)	18 (6%)	9 (3%)	4	2
1	B	281/304 (92%)	257 (92%)	18 (6%)	6 (2%)	7	5
All	All	582/608 (96%)	531 (91%)	36 (6%)	15 (3%)	5	4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	63	ASP
1	A	2	GLY
1	A	28	LEU
1	A	93	GLN
1	A	144	ALA
1	B	2	GLY
1	B	29	GLU
1	A	140	THR
1	B	234	GLN
1	B	248	GLY
1	A	248	GLY
1	B	218	PRO
1	B	236	GLY
1	A	78	PRO

5.3.2 Protein sidechains [i](#)

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	241/242 (100%)	235 (98%)	6 (2%)	47	65
1	B	227/242 (94%)	216 (95%)	11 (5%)	25	36
All	All	468/484 (97%)	451 (96%)	17 (4%)	35	49

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

Mol	Chain	Res	Type
1	A	3	PHE
1	A	27	ASN
1	A	35	LEU
1	A	91	ASN
1	A	127	GLN
1	A	140	THR
1	B	3	PHE
1	B	4	PHE
1	B	43	ASP
1	B	54	GLN
1	B	66	GLU
1	B	96	LYS
1	B	151	GLU
1	B	197	HIS
1	B	234	GLN
1	B	276	PRO
1	B	289	LEU

Some 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	93	GLN
1	A	111	ASN
1	A	148	GLN
1	A	178	GLN
1	A	197	HIS
1	A	201	ASN
1	B	27	ASN
1	B	54	GLN
1	B	111	ASN
1	B	148	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	201	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 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	957	-	4,4,4	0.33	0	6,6,6	1.08	0
3	EDO	A	904	-	3,3,3	0.34	0	2,2,2	0.08	0
3	EDO	B	902	-	3,3,3	0.31	0	2,2,2	0.13	0
2	SO4	A	956	-	4,4,4	0.74	0	6,6,6	5.19	6 (100%)
3	EDO	A	907	-	3,3,3	0.50	0	2,2,2	0.19	0
2	SO4	A	952	-	4,4,4	0.36	0	6,6,6	0.75	0
3	EDO	B	901	-	3,3,3	0.56	0	2,2,2	0.83	0
3	EDO	B	903	-	3,3,3	0.41	0	2,2,2	0.09	0
2	SO4	B	955	-	4,4,4	0.34	0	6,6,6	0.86	0
2	SO4	A	958	-	4,4,4	0.32	0	6,6,6	0.57	0
2	SO4	A	953	-	4,4,4	0.04	0	6,6,6	0.67	0
3	EDO	A	905	-	3,3,3	0.52	0	2,2,2	0.55	0
2	SO4	A	959	-	4,4,4	0.24	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	954	-	4,4,4	0.41	0	6,6,6	0.86	0
3	EDO	B	900	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	B	908	-	3,3,3	0.38	0	2,2,2	0.63	0
3	EDO	B	906	-	3,3,3	0.70	0	2,2,2	0.39	0
4	GNP	A	950	-	28,34,34	2.45	12 (42%)	30,54,54	3.22	12 (40%)

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	EDO	A	904	-	-	0/1/1/1	-
3	EDO	B	902	-	-	1/1/1/1	-
3	EDO	A	907	-	-	1/1/1/1	-
3	EDO	B	903	-	-	0/1/1/1	-
3	EDO	B	900	-	-	1/1/1/1	-
3	EDO	A	905	-	-	1/1/1/1	-
3	EDO	B	901	-	-	0/1/1/1	-
3	EDO	B	908	-	-	0/1/1/1	-
3	EDO	B	906	-	-	0/1/1/1	-
4	GNP	A	950	-	-	6/17/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	950	GNP	PG-O1G	6.02	1.55	1.46
4	A	950	GNP	C4-N9	-4.65	1.41	1.47
4	A	950	GNP	PB-O2B	-4.53	1.44	1.56
4	A	950	GNP	PB-O3A	-4.48	1.53	1.59
4	A	950	GNP	C6-N1	4.35	1.40	1.33
4	A	950	GNP	O3'-C3'	2.95	1.49	1.43
4	A	950	GNP	PB-N3B	-2.59	1.56	1.63
4	A	950	GNP	PB-O1B	-2.44	1.42	1.46
4	A	950	GNP	C8-N9	-2.41	1.37	1.45
4	A	950	GNP	C5-C6	-2.35	1.48	1.52
4	A	950	GNP	PG-O3G	-2.11	1.51	1.56
4	A	950	GNP	C5-C4	-2.05	1.40	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	950	GNP	O6-C6-N1	-7.86	112.13	122.69
4	A	950	GNP	O6-C6-C5	7.28	134.70	119.86
2	A	956	SO4	O4-S-O3	-6.54	81.16	109.06
4	A	950	GNP	O3A-PB-N3B	-6.07	89.75	106.59
2	A	956	SO4	O4-S-O1	5.76	139.35	109.31
2	A	956	SO4	O4-S-O2	-5.20	82.18	109.31
4	A	950	GNP	O1B-PB-N3B	5.05	119.21	111.77
4	A	950	GNP	O2B-PB-O1B	4.81	120.01	109.92
4	A	950	GNP	O2B-PB-O3A	-4.73	88.87	104.64
2	A	956	SO4	O3-S-O1	-4.69	84.83	109.31
4	A	950	GNP	O1G-PG-N3B	-4.56	105.06	111.77
2	A	956	SO4	O3-S-O2	4.55	133.04	109.31
4	A	950	GNP	C4-C5-N7	4.32	108.18	102.46
4	A	950	GNP	C5-C6-N1	-4.08	113.15	118.19
2	A	956	SO4	O2-S-O1	-3.98	80.05	109.43
4	A	950	GNP	O2'-C2'-C1'	-2.77	100.75	110.02
4	A	950	GNP	O5'-PA-O1A	-2.55	99.09	109.07
4	A	950	GNP	O2G-PG-O1G	-2.15	108.05	113.45

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	950	GNP	O4'-C1'-N9-C4
4	A	950	GNP	C2'-C1'-N9-C8
4	A	950	GNP	C2'-C1'-N9-C4
4	A	950	GNP	O4'-C4'-C5'-O5'
3	A	907	EDO	O1-C1-C2-O2
3	B	900	EDO	O1-C1-C2-O2
4	A	950	GNP	C3'-C4'-C5'-O5'
3	A	905	EDO	O1-C1-C2-O2
4	A	950	GNP	PA-O3A-PB-O2B
3	B	902	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

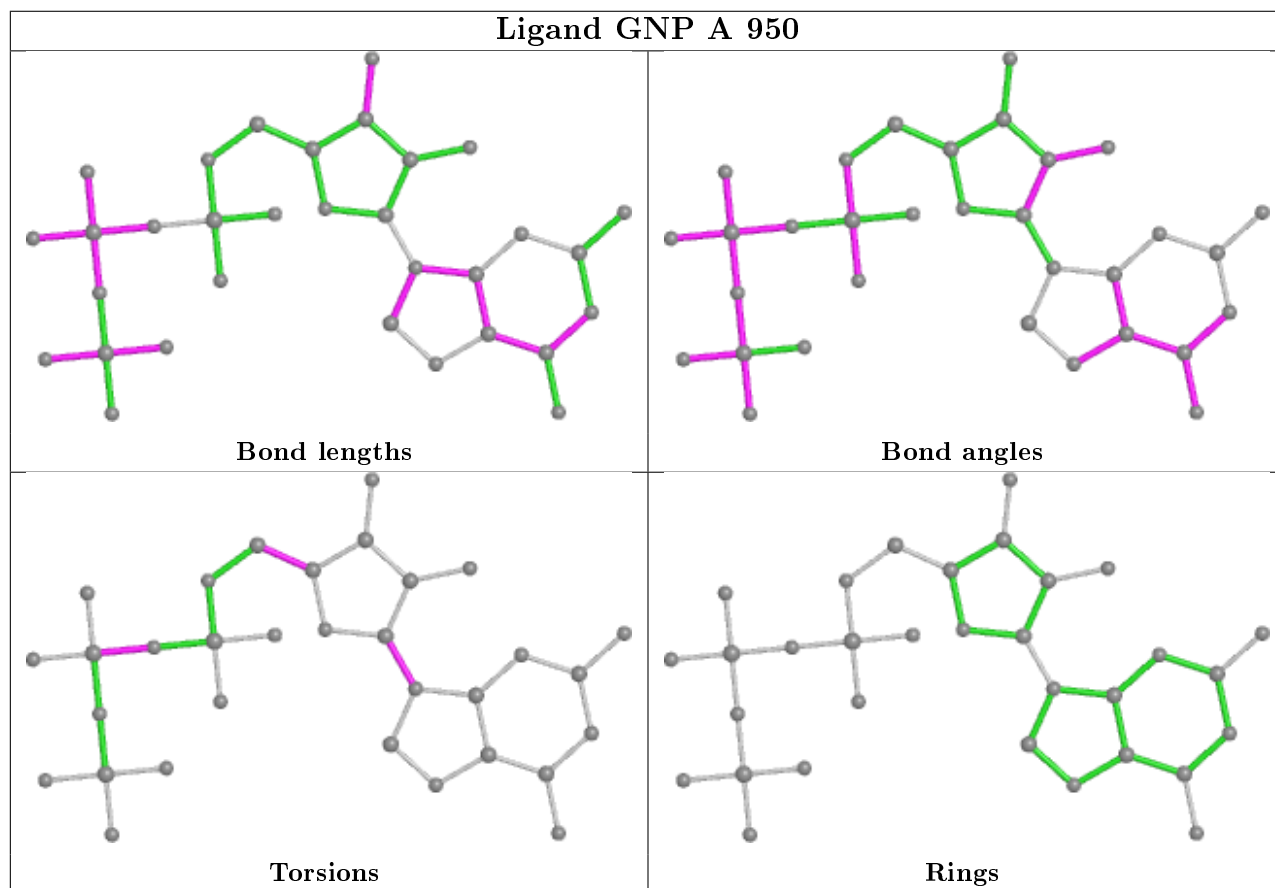
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	EDO	1	0
2	A	952	SO4	1	0
3	B	901	EDO	1	0
3	A	905	EDO	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	908	EDO	3	0
4	A	950	GNP	6	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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	303/304 (99%)	0.33	18 (5%) 22 28	22, 33, 42, 54	0
1	B	287/304 (94%)	0.43	31 (10%) 5 8	22, 34, 41, 51	0
All	All	590/608 (97%)	0.38	49 (8%) 11 15	22, 34, 42, 54	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	LEU	7.9
1	A	1	MET	6.2
1	B	1	MET	6.2
1	A	143	ALA	5.2
1	B	145	GLY	4.9
1	B	25	GLY	4.8
1	A	93	GLN	4.2
1	B	23	PRO	4.0
1	A	2	GLY	3.9
1	B	144	ALA	3.7
1	B	24	TRP	3.4
1	B	29	GLU	3.4
1	B	79	ASP	3.3
1	B	59	SER	3.3
1	B	26	GLY	3.3
1	B	31	VAL	3.3
1	B	147	THR	3.1
1	A	85	LEU	3.1
1	A	145	GLY	3.1
1	B	27	ASN	3.0
1	A	142	ARG	3.0
1	B	64	LEU	2.9
1	B	2	GLY	2.8
1	A	4	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	94	LYS	2.8
1	A	95	PRO	2.7
1	B	6	ARG	2.7
1	B	95	PRO	2.7
1	B	4	PHE	2.7
1	A	3	PHE	2.6
1	B	30	GLU	2.6
1	A	79	ASP	2.4
1	B	101	LYS	2.2
1	B	21	ALA	2.2
1	B	45	GLY	2.2
1	A	92	PRO	2.2
1	B	303	GLU	2.2
1	B	304	ASP	2.2
1	A	90	PHE	2.1
1	B	3	PHE	2.1
1	B	5	ASP	2.1
1	B	228	LEU	2.1
1	A	80	GLU	2.1
1	A	59	SER	2.1
1	B	54	GLN	2.0
1	A	88	LEU	2.0
1	A	260	THR	2.0
1	B	60	GLY	2.0
1	B	94	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](#)

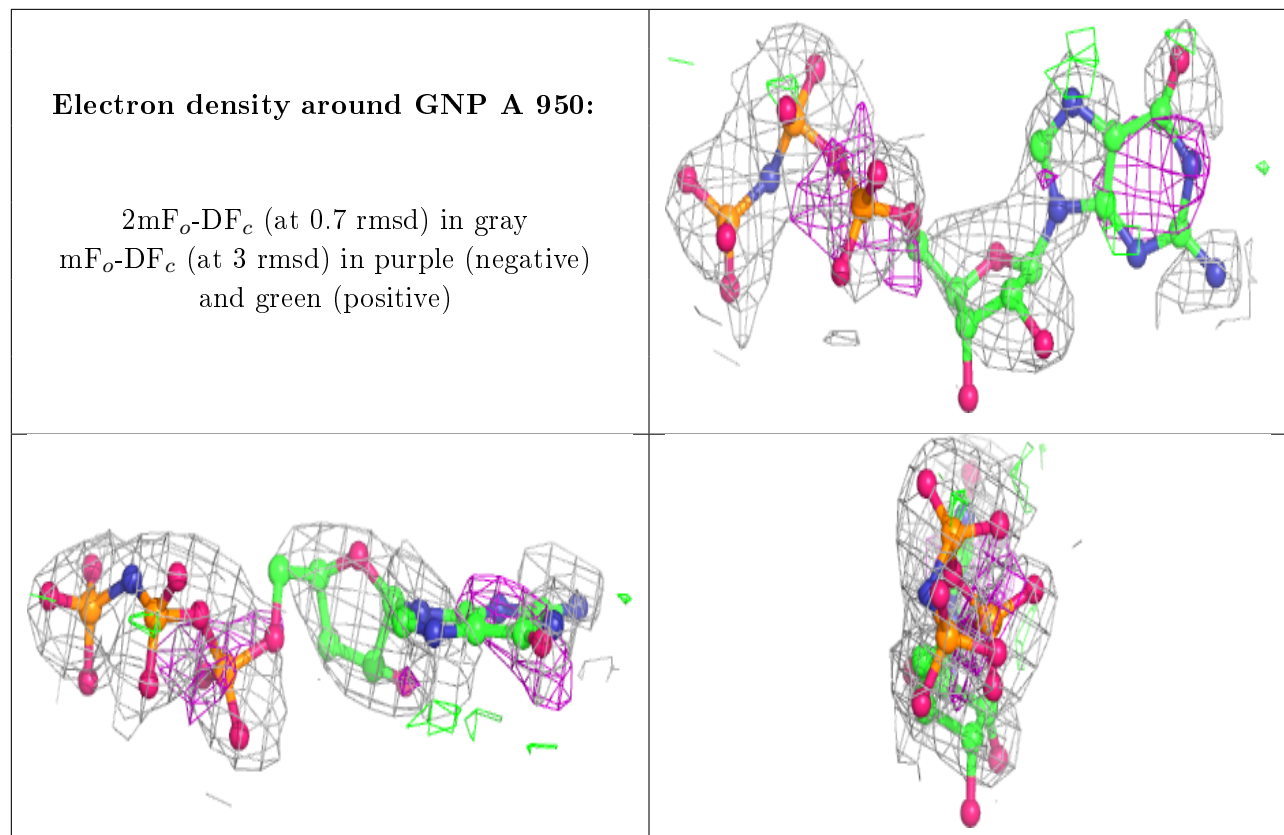
There are no carbohydrates in this entry.

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. 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(\AA^2)	Q<0.9
3	EDO	B	906	4/4	0.55	0.25	65,68,70,72	0
3	EDO	A	905	4/4	0.57	0.43	68,69,72,73	0
3	EDO	B	903	4/4	0.69	0.36	70,70,72,73	0
3	EDO	B	900	4/4	0.70	0.21	57,58,58,60	0
2	SO4	A	956	5/5	0.75	0.41	74,78,78,83	0
3	EDO	A	907	4/4	0.81	0.17	72,72,73,75	0
4	GNP	A	950	32/32	0.81	0.29	54,72,78,80	0
3	EDO	B	902	4/4	0.82	0.28	49,56,59,68	0
3	EDO	B	901	4/4	0.83	0.40	47,54,59,59	0
3	EDO	A	904	4/4	0.85	0.13	57,62,63,66	0
2	SO4	A	958	5/5	0.88	0.19	73,76,76,78	0
3	EDO	B	908	4/4	0.90	0.24	52,53,54,54	0
2	SO4	A	953	5/5	0.96	0.15	53,55,59,59	0
2	SO4	A	954	5/5	0.96	0.11	50,57,62,62	0
2	SO4	A	959	5/5	0.97	0.12	57,59,61,61	0
2	SO4	B	955	5/5	0.97	0.18	47,53,54,56	0
2	SO4	B	957	5/5	0.97	0.16	46,47,49,50	0
2	SO4	A	952	5/5	0.98	0.18	49,50,52,54	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.