



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:41 AM UTC

PDB ID : 4I3Y / pdb_00004i3y
Title : Crystal structure of Staphylococcal inositol monophosphatase-1: 100 mM LiCl soaked inhibitory complex
Authors : Dutta, A.; Bhattacharyya, S.; Dutta, D.; Das, A.K.
Deposited on : 2012-11-26
Resolution : 2.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

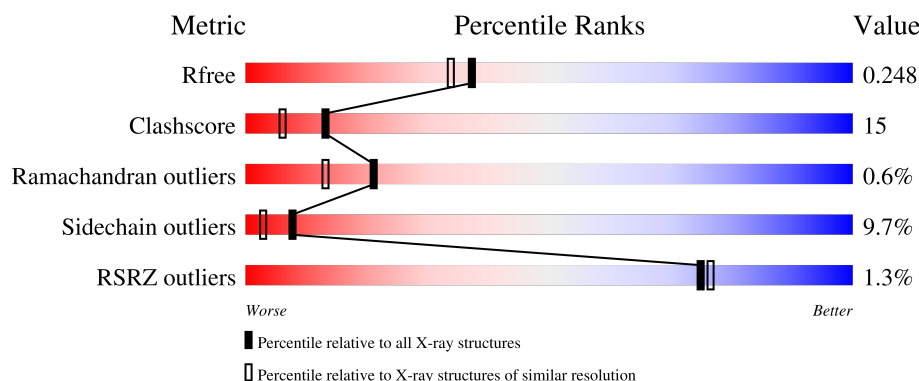
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	271	% 69% 23% ...
1	B	271	2% 69% 21% ...

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4519 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 Inositol monophosphatase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	1	0
			2122	1365	352	391	14			
1	B	262	Total	C	N	O	S	0	2	0
			2114	1361	352	387	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q6G709
A	-4	HIS	-	expression tag	UNP Q6G709
A	-3	HIS	-	expression tag	UNP Q6G709
A	-2	HIS	-	expression tag	UNP Q6G709
A	-1	HIS	-	expression tag	UNP Q6G709
A	0	HIS	-	expression tag	UNP Q6G709
B	-5	HIS	-	expression tag	UNP Q6G709
B	-4	HIS	-	expression tag	UNP Q6G709
B	-3	HIS	-	expression tag	UNP Q6G709
B	-2	HIS	-	expression tag	UNP Q6G709
B	-1	HIS	-	expression tag	UNP Q6G709
B	0	HIS	-	expression tag	UNP Q6G709

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

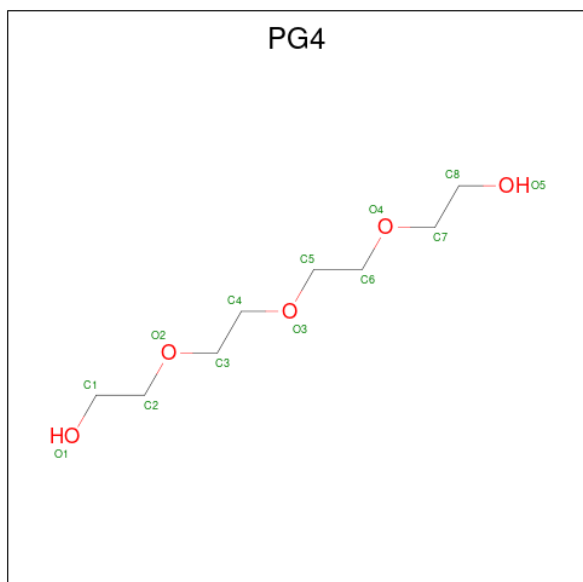
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	105	Total O 105 105	0	0
6	B	113	Total O 113 113	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.14Å 62.82Å 141.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.59 – 2.04 19.59 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.59-2.04) 99.8 (19.59-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.248 0.184 , 0.248	Depositor DCC
R_{free} test set	1753 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4519	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PO4, GOL, MG

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	1.20	3/2168 (0.1%)	1.24	13/2930 (0.4%)
1	B	1.14	3/2166 (0.1%)	1.31	24/2928 (0.8%)
All	All	1.17	6/4334 (0.1%)	1.27	37/5858 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	ARG	CD-NE	-6.13	1.37	1.46
1	B	180	ARG	CD-NE	-5.95	1.38	1.46
1	B	78	THR	N-CA	5.34	1.53	1.46
1	B	72	LYS	CA-C	-5.16	1.46	1.52
1	A	66	GLN	CA-C	5.04	1.59	1.52
1	A	20	ILE	CA-C	5.02	1.60	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	MET	N-CA-C	-10.81	87.77	110.80
1	A	180	ARG	NE-CZ-NH2	-9.72	110.45	119.20
1	B	180	ARG	NE-CZ-NH2	-8.37	111.66	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	NE-CZ-NH2	-7.92	112.08	119.20
1	B	60	THR	N-CA-C	7.71	119.32	111.07
1	B	133	ARG	NE-CZ-NH2	-7.57	112.39	119.20
1	B	192	VAL	N-CA-C	-7.33	103.64	110.53
1	A	180	ARG	CD-NE-CZ	7.22	134.50	124.40
1	A	60	THR	N-CA-CB	-6.98	100.40	110.65
1	B	133	ARG	NE-CZ-NH1	6.80	128.30	121.50
1	B	180	ARG	NE-CZ-NH1	6.69	128.19	121.50
1	B	24	ILE	N-CA-CB	6.69	114.72	110.50
1	A	180	ARG	NE-CZ-NH1	6.68	128.18	121.50
1	B	78	THR	CA-C-N	6.66	133.68	121.70
1	B	78	THR	C-N-CA	6.66	133.68	121.70
1	A	180	ARG	CG-CD-NE	-6.49	97.71	112.00
1	A	60	THR	CB-CA-C	6.40	120.30	109.55
1	B	81	ILE	CB-CA-C	-6.29	102.11	110.98
1	B	180	ARG	CG-CD-NE	-6.27	98.22	112.00
1	A	133	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	B	5	THR	N-CA-C	5.87	117.76	111.36
1	A	70	GLU	N-CA-C	5.84	118.11	111.11
1	B	142	ILE	N-CA-CB	5.51	116.72	110.72
1	B	260	GLY	N-CA-C	5.49	120.94	112.81
1	B	54	PHE	N-CA-C	-5.49	105.38	111.36
1	A	180	ARG	CB-CG-CD	5.48	123.91	111.30
1	A	133	ARG	CD-NE-CZ	5.46	132.04	124.40
1	B	133	ARG	CD-NE-CZ	5.28	131.79	124.40
1	B	75	ALA	N-CA-C	-5.21	99.70	110.80
1	A	113	GLY	N-CA-C	5.21	122.30	115.47
1	B	236	LYS	CA-C-N	-5.21	111.20	121.41
1	B	236	LYS	C-N-CA	-5.21	111.20	121.41
1	B	180	ARG	CD-NE-CZ	5.18	131.66	124.40
1	A	49	GLN	N-CA-C	5.16	116.59	111.07
1	B	238	ALA	N-CA-C	-5.03	103.69	108.22
1	B	76	MET	CA-C-N	5.01	130.72	121.70
1	B	76	MET	C-N-CA	5.01	130.72	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	GLY	Peptide
1	B	237	GLY	Peptide
1	B	75	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	B	78	THR	Peptide

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	2122	0	2113	70	1
1	B	2114	0	2115	60	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	12	0	16	0	0
4	B	18	0	24	1	0
5	A	21	0	25	11	0
6	A	105	0	0	9	0
6	B	113	0	0	9	0
All	All	4519	0	4293	128	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (128) 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:165:ASN:HD22	1:A:168:THR:HG22	1.23	1.03
1:A:165:ASN:ND2	1:A:168:THR:HG22	1.73	1.02
1:B:32:THR:HG23	6:B:509:HOH:O	1.59	0.99
1:A:60:THR:HG22	1:A:61:TYR:CE2	1.98	0.99
1:B:78:THR:HB	1:B:79:ASN:CB	1.98	0.94
1:B:51:GLN:HE22	1:B:71:GLU:H	1.05	0.93
1:A:5:THR:H	1:A:8:GLN:HE21	1.18	0.92
1:A:165:ASN:HD22	1:A:168:THR:CG2	1.84	0.90
1:A:51:GLN:HE22	1:A:71:GLU:H	1.17	0.90
1:A:72:LYS:HZ3	1:A:76:MET:HE1	1.36	0.89
1:B:133:ARG:NH2	1:B:218:GLU:OE2	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:THR:O	1:B:81:ILE:HD11	1.75	0.86
1:A:125:HIS:HD2	6:A:476:HOH:O	1.60	0.85
1:A:165:ASN:CG	6:A:458:HOH:O	2.20	0.85
1:A:168:THR:HG21	1:A:261:TYR:HA	1.59	0.84
1:A:66:GLN:OE1	1:A:81:ILE:HD13	1.79	0.82
1:A:191:ARG:HH11	1:B:99:GLN:HE22	1.27	0.80
1:A:57:PHE:O	1:A:61:TYR:HD2	1.65	0.78
5:A:308:PG4:H31	1:B:98:LYS:HZ2	1.51	0.75
1:B:206:LYS:HD3	1:B:208:TRP:CZ2	2.21	0.75
1:A:99:GLN:HE22	1:B:191:ARG:HH11	1.33	0.73
1:A:165:ASN:ND2	1:A:168:THR:CG2	2.46	0.73
5:A:308:PG4:H22	6:A:505:HOH:O	1.90	0.72
1:A:60:THR:HG22	1:A:61:TYR:CD2	2.24	0.71
1:A:165:ASN:HB2	6:A:458:HOH:O	1.89	0.71
1:B:45:ASN:H	1:B:45:ASN:HD22	1.37	0.71
1:A:114:LYS:HE3	1:A:116:MET:HE1	1.72	0.71
1:A:5:THR:H	1:A:8:GLN:NE2	1.88	0.71
1:B:148:PRO:HD2	6:B:511:HOH:O	1.90	0.71
1:A:133:ARG:NH2	1:A:218:GLU:OE2	2.26	0.68
1:A:31:MET:HA	1:A:45:ASN:HD21	1.58	0.67
1:A:165:ASN:CB	6:A:458:HOH:O	2.43	0.67
1:B:32:THR:H	1:B:45:ASN:ND2	1.93	0.66
1:B:74:ASN:C	1:B:75:ALA:O	2.36	0.65
1:B:76:MET:CB	1:B:77:ILE:HA	2.26	0.65
1:B:262:GLN:HG2	6:B:473:HOH:O	1.97	0.64
1:A:60:THR:CG2	1:A:61:TYR:CE2	2.79	0.63
1:B:51:GLN:NE2	1:B:71:GLU:H	1.88	0.62
1:B:69:ALA:H	1:B:74:ASN:HD21	1.46	0.62
1:A:57:PHE:O	1:A:61:TYR:CD2	2.51	0.61
1:A:5:THR:N	1:A:8:GLN:HE21	1.94	0.61
1:B:133:ARG:HH22	1:B:218:GLU:CD	2.09	0.60
1:A:66:GLN:OE1	1:A:81:ILE:CD1	2.49	0.60
1:B:76:MET:HB2	1:B:77:ILE:HA	1.83	0.60
1:B:51:GLN:HE22	1:B:71:GLU:N	1.89	0.59
1:A:82:ASN:HD22	1:A:112:GLU:HG2	1.67	0.59
1:A:55:GLN:NE2	6:A:441:HOH:O	2.36	0.59
5:A:308:PG4:H31	1:B:98:LYS:NZ	2.16	0.58
1:B:26[B]:GLN:NE2	1:B:30:GLU:OE1	2.37	0.58
1:B:81:ILE:HD12	1:B:81:ILE:H	1.68	0.58
1:B:16:TRP:O	1:B:19:GLN:HG2	2.05	0.57
1:B:7:GLN:H	1:B:7:GLN:CD	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LYS:HE3	1:A:116:MET:CE	2.35	0.56
1:A:32:THR:HG22	1:A:45:ASN:HB3	1.87	0.55
1:A:260:GLY:HA3	5:A:306:PG4:H52	1.89	0.54
1:A:69:ALA:H	1:A:74:ASN:HD21	1.56	0.53
1:A:60:THR:HG22	1:A:61:TYR:HE2	1.65	0.53
1:A:256:ASN:OD1	5:A:306:PG4:H31	2.08	0.53
1:A:55:GLN:HG2	6:A:467:HOH:O	2.09	0.52
1:B:168:THR:HG21	1:B:261:TYR:HA	1.90	0.52
1:A:31:MET:HA	1:A:45:ASN:ND2	2.24	0.52
1:A:99:GLN:NE2	1:B:191:ARG:HH11	2.05	0.52
1:A:263:LYS:HE3	6:A:487:HOH:O	2.09	0.52
1:A:191:ARG:HH11	1:B:99:GLN:NE2	2.02	0.52
1:B:76:MET:HB2	1:B:77:ILE:CA	2.40	0.52
1:A:38:HIS:CE1	1:A:40:PHE:HB2	2.45	0.51
1:A:196:GLN:HB3	1:B:99:GLN:HE21	1.74	0.51
1:A:227:LEU:HD22	1:A:255:LEU:HD13	1.94	0.50
1:B:75:ALA:O	1:B:76:MET:SD	2.70	0.50
1:A:99:GLN:HE21	1:B:196:GLN:HB3	1.76	0.50
1:A:260:GLY:HA3	5:A:306:PG4:H32	1.94	0.50
1:B:31:MET:HA	1:B:45:ASN:HD21	1.77	0.50
1:A:45:ASN:HD22	1:A:45:ASN:H	1.58	0.49
1:B:45:ASN:H	1:B:45:ASN:ND2	2.08	0.49
1:A:38:HIS:HE1	1:A:40:PHE:HB2	1.78	0.49
1:A:62:PHE:HB3	1:A:65:HIS:CG	2.47	0.49
1:A:133:ARG:HH22	1:A:218:GLU:CD	2.17	0.48
1:A:32:THR:CG2	1:A:45:ASN:HB3	2.43	0.48
1:B:248:HIS:HD2	6:B:447:HOH:O	1.96	0.48
1:A:32:THR:H	1:A:45:ASN:ND2	2.11	0.48
1:B:4:LYS:HE2	1:B:4:LYS:HA	1.95	0.48
1:A:61:TYR:CD2	1:A:61:TYR:N	2.81	0.47
1:A:165:ASN:ND2	1:A:265:ARG:NH2	2.61	0.47
1:B:223:LYS:HE2	6:B:448:HOH:O	2.14	0.47
5:A:305:PG4:H51	6:A:479:HOH:O	2.14	0.47
1:B:164:MET:HE3	6:B:426:HOH:O	2.15	0.47
1:B:4:LYS:NZ	1:B:5:THR:HG23	2.30	0.46
1:B:247:CYS:O	1:B:251:VAL:HG23	2.14	0.46
1:B:59:ALA:O	1:B:63:PRO:HG3	2.14	0.46
1:A:56:GLN:O	1:A:60:THR:HB	2.15	0.46
1:A:150:LEU:HD23	5:A:308:PG4:H21	1.97	0.46
1:A:234:HIS:CD2	1:A:235:LEU:HD13	2.51	0.46
1:B:125:HIS:HE1	6:B:502:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TRP:O	1:A:19:GLN:HG3	2.16	0.45
1:A:236:LYS:O	1:A:237:GLY:C	2.58	0.45
5:A:308:PG4:H42	6:B:467:HOH:O	2.17	0.45
5:A:306:PG4:H52	5:A:306:PG4:H32	1.68	0.45
1:B:45:ASN:HD22	1:B:45:ASN:N	2.10	0.45
1:B:95:ASN:HB3	1:B:101:GLU:O	2.17	0.44
1:B:165:ASN:HD21	1:B:168:THR:CG2	2.29	0.44
1:A:17:LEU:O	1:A:20:ILE:HG22	2.18	0.44
1:A:253:LYS:HG3	1:A:254:ILE:N	2.33	0.44
1:A:28:ILE:HD13	1:A:96:LEU:HD11	1.99	0.44
1:A:107:LEU:HB2	1:A:119:TYR:HB2	2.00	0.43
1:B:7:GLN:CD	1:B:7:GLN:N	2.76	0.43
1:B:78:THR:CB	1:B:79:ASN:CB	2.86	0.43
1:A:2:THR:O	1:A:3:ASP:HB2	2.17	0.43
1:B:100[A]:GLN:CD	4:B:305:GOL:H11	2.43	0.43
1:A:72:LYS:NZ	1:A:74:ASN:ND2	2.68	0.42
1:A:52:GLN:HA	1:A:55:GLN:HE21	1.83	0.42
1:B:45:ASN:ND2	1:B:45:ASN:N	2.65	0.42
1:B:162:GLN:O	1:B:263:LYS:NZ	2.50	0.42
1:B:205:PRO:HD2	1:B:238:ALA:O	2.20	0.42
1:A:157:ILE:HD13	1:A:157:ILE:HG21	1.88	0.41
1:A:168:THR:CG2	1:A:261:TYR:HA	2.42	0.41
1:B:75:ALA:C	1:B:76:MET:O	2.49	0.41
1:B:69:ALA:H	1:B:74:ASN:ND2	2.16	0.41
1:A:262:GLN:CG	5:A:306:PG4:H62	2.51	0.41
1:B:55:GLN:HE22	1:B:72:LYS:HD3	1.86	0.41
1:B:32:THR:CG2	6:B:509:HOH:O	2.38	0.41
1:B:51:GLN:OE1	1:B:72:LYS:HG3	2.21	0.41
1:B:157:ILE:HD12	1:B:159:PHE:CE2	2.56	0.41
1:A:225:THR:OG1	1:A:248:HIS:HE1	2.04	0.41
1:B:11:LYS:HB3	1:B:11:LYS:HE3	1.78	0.41
1:B:72:LYS:HZ2	1:B:74:ASN:ND2	2.19	0.41
1:B:155:ALA:HB1	1:B:198:GLY:HA3	2.02	0.41
1:A:69:ALA:H	1:A:74:ASN:ND2	2.19	0.40
1:A:156:ILE:HG21	1:A:180:ARG:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TYR:OH	1:A:145:GLU:OE2[3_555]	1.95	0.25

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	263/271 (97%)	257 (98%)	5 (2%)	1 (0%)	30	22
1	B	262/271 (97%)	253 (97%)	7 (3%)	2 (1%)	16	9
All	All	525/542 (97%)	510 (97%)	12 (2%)	3 (1%)	21	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	ASN
1	B	75	ALA
1	A	237	GLY

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	228/238 (96%)	207 (91%)	21 (9%)	8	4
1	B	229/238 (96%)	206 (90%)	23 (10%)	7	3
All	All	457/476 (96%)	413 (90%)	44 (10%)	8	3

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	12	LEU
1	A	17	LEU

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Mol	Chain	Res	Type
1	A	20	ILE
1	A	28	ILE
1	A	42	LEU
1	A	52	GLN
1	A	55	GLN
1	A	60	THR
1	A	149	SER
1	A	163	VAL
1	A	165	ASN
1	A	166	LEU
1	A	168	THR
1	A	180	ARG
1	A	206	LYS
1	A	230	LYS
1	A	235	LEU
1	A	240	PHE
1	A	253	LYS
1	A	265	ARG
1	B	4	LYS
1	B	5	THR
1	B	7	GLN
1	B	12	LEU
1	B	17	LEU
1	B	45	ASN
1	B	52	GLN
1	B	56	GLN
1	B	58	LEU
1	B	68	LEU
1	B	72	LYS
1	B	76	MET
1	B	81	ILE
1	B	126	LYS
1	B	142	ILE
1	B	166	LEU
1	B	168	THR
1	B	180	ARG
1	B	206	LYS
1	B	221	ASN
1	B	235	LEU
1	B	240	PHE
1	B	263	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	45	ASN
1	A	49	GLN
1	A	51	GLN
1	A	52	GLN
1	A	53	GLN
1	A	55	GLN
1	A	74	ASN
1	A	82	ASN
1	A	99	GLN
1	A	125	HIS
1	A	162	GLN
1	A	165	ASN
1	A	204	ASN
1	A	248	HIS
1	B	8	GLN
1	B	45	ASN
1	B	49	GLN
1	B	51	GLN
1	B	53	GLN
1	B	55	GLN
1	B	66	GLN
1	B	74	ASN
1	B	82	ASN
1	B	99	GLN
1	B	125	HIS
1	B	170	GLN
1	B	248	HIS

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

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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
4	GOL	A	307	-	5,5,5	0.27	0	5,5,5	0.52	0
4	GOL	A	303	-	5,5,5	0.18	0	5,5,5	1.32	0
5	PG4	A	305	-	6,6,12	0.79	0	5,5,11	0.78	0
4	GOL	B	305	-	5,5,5	0.47	0	5,5,5	0.53	0
2	PO4	B	302	3	4,4,4	1.39	1 (25%)	6,6,6	1.02	0
5	PG4	A	306	-	6,6,12	0.64	0	5,5,11	0.51	0
5	PG4	A	308	-	6,6,12	1.33	0	5,5,11	1.63	1 (20%)
4	GOL	B	306	-	5,5,5	0.84	0	5,5,5	0.77	0
4	GOL	B	303	-	5,5,5	0.42	0	5,5,5	1.84	2 (40%)
2	PO4	A	301	3	4,4,4	0.96	0	6,6,6	1.48	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	307	-	-	4/4/4/4	-
4	GOL	A	303	-	-	2/4/4/4	-
5	PG4	A	305	-	-	2/4/4/10	-
4	GOL	B	305	-	-	4/4/4/4	-
5	PG4	A	306	-	-	3/4/4/10	-
5	PG4	A	308	-	-	4/4/4/10	-
4	GOL	B	306	-	-	4/4/4/4	-
4	GOL	B	303	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	PO4	P-O4	2.33	1.61	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	GOL	C3-C2-C1	-3.53	98.86	111.80
2	A	301	PO4	O4-P-O3	2.75	116.47	107.91
5	A	308	PG4	O2-C3-C4	2.21	119.87	110.11
4	B	303	GOL	O3-C3-C2	-2.08	101.03	110.38

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	307	GOL	O1-C1-C2-C3
4	A	307	GOL	C1-C2-C3-O3
4	B	303	GOL	O1-C1-C2-C3
4	B	306	GOL	C1-C2-C3-O3
5	A	306	PG4	C3-C4-O3-C5
4	A	307	GOL	O1-C1-C2-O2
4	A	307	GOL	O2-C2-C3-O3
4	B	303	GOL	O1-C1-C2-O2
5	A	308	PG4	O1-C1-C2-O2
5	A	308	PG4	O2-C3-C4-O3
4	A	303	GOL	C1-C2-C3-O3
4	B	305	GOL	C1-C2-C3-O3
4	B	306	GOL	O1-C1-C2-C3
5	A	305	PG4	O3-C5-C6-O4
4	B	306	GOL	O1-C1-C2-O2
4	B	306	GOL	O2-C2-C3-O3
5	A	305	PG4	C6-C5-O3-C4
4	B	305	GOL	O1-C1-C2-C3
4	B	305	GOL	O1-C1-C2-O2
5	A	306	PG4	O2-C3-C4-O3
5	A	308	PG4	C4-C3-O2-C2
5	A	308	PG4	C1-C2-O2-C3
4	A	303	GOL	O2-C2-C3-O3
4	B	305	GOL	O2-C2-C3-O3
5	A	306	PG4	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	305	PG4	1	0
4	B	305	GOL	1	0
5	A	306	PG4	5	0
5	A	308	PG4	5	0

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 [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	264/271 (97%)	-0.51	2 (0%) 82 84	6, 19, 37, 57	1 (0%)
1	B	262/271 (96%)	-0.45	5 (1%) 66 68	9, 20, 38, 73	2 (0%)
All	All	526/542 (97%)	-0.48	7 (1%) 75 76	6, 19, 38, 73	3 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	ILE	3.2
1	A	40	PHE	3.0
1	B	79	ASN	2.6
1	B	75	ALA	2.6
1	A	2	THR	2.5
1	B	78	THR	2.4
1	B	237	GLY	2.1

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
5	PG4	A	305	7/13	0.80	0.14	38,40,47,49	0
5	PG4	A	306	7/13	0.82	0.15	35,43,56,59	0
4	GOL	B	305	6/6	0.85	0.15	39,46,48,48	0
5	PG4	A	308	7/13	0.86	0.16	23,28,34,37	0
4	GOL	B	306	6/6	0.89	0.09	28,32,35,37	0
4	GOL	B	303	6/6	0.90	0.10	24,26,29,30	0
4	GOL	A	307	6/6	0.91	0.10	36,46,49,51	0
4	GOL	A	303	6/6	0.93	0.07	24,28,31,31	0
2	PO4	A	301	5/5	0.98	0.04	17,17,20,21	0
2	PO4	B	302	5/5	0.98	0.05	14,15,16,17	0
3	MG	A	304	1/1	0.98	0.02	20,20,20,20	0
3	MG	B	301	1/1	0.98	0.03	12,12,12,12	0
3	MG	A	302	1/1	0.99	0.03	20,20,20,20	0
3	MG	B	304	1/1	0.99	0.02	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.