



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:51 am BST

PDB ID : 2I54
Title : Phosphomannomutase from Leishmania mexicana
Authors : Smith, B.J.
Deposited on : 2006-08-24
Resolution : 2.10 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
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

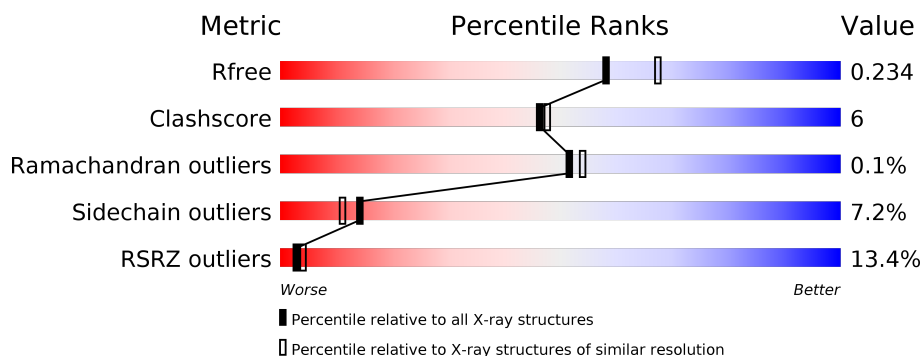
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	247	<div> <div>13%</div> <div>81%</div> <div>13%</div> <div>..</div> </div>
1	B	247	<div> <div>9%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>
1	C	247	<div> <div>17%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	C	3003[A]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6201 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 Phosphomannomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1951	1244	329	373	5			
1	B	242	Total	C	N	O	S	0	3	0
			1954	1247	328	374	5			
1	C	242	Total	C	N	O	S	0	0	0
			1946	1240	328	373	5			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	1
			26	12	14		
4	C	1	Total	C	O	0	1
			26	12	14		

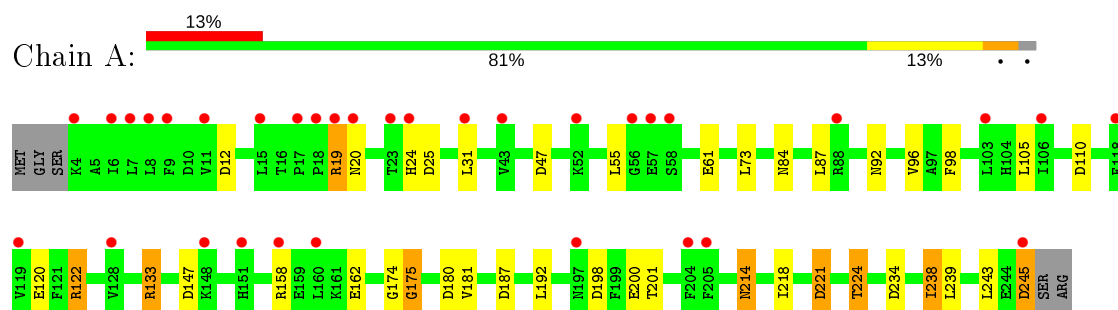
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total	O	0	0
			64	64		
5	B	134	Total	O	0	0
			134	134		
5	C	82	Total	O	0	0
			82	82		

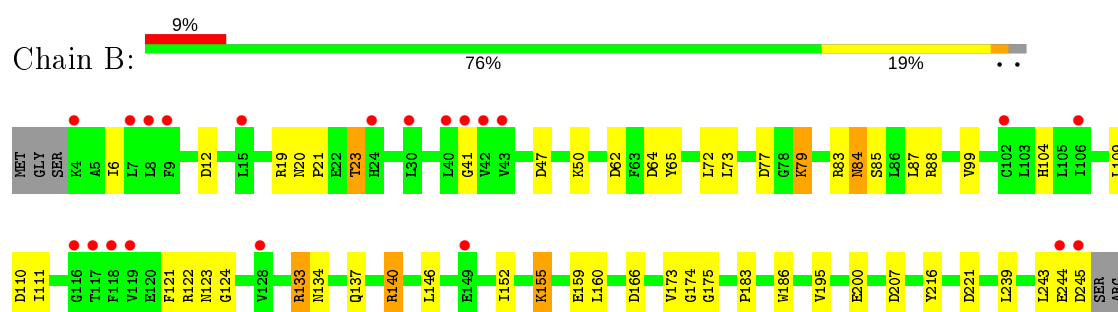
3 Residue-property plots [i](#)

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.

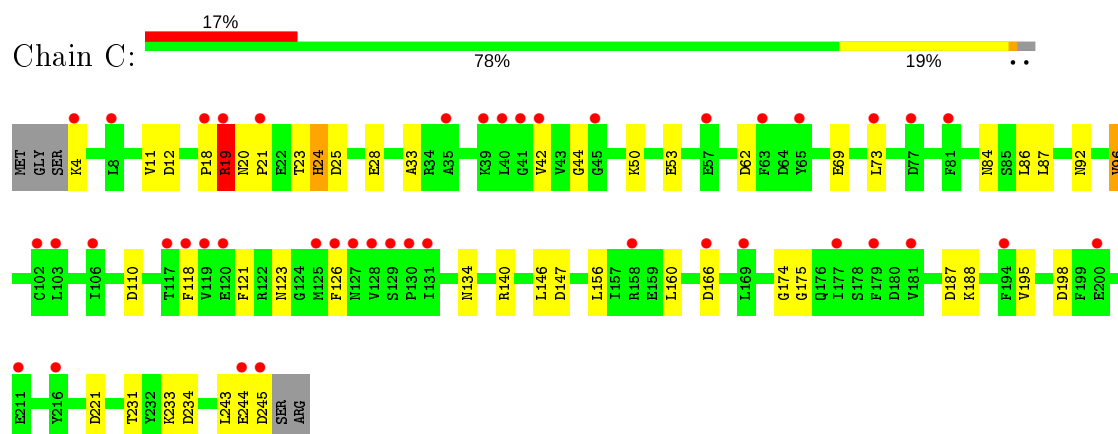
• Molecule 1: Phosphomannomutase



• Molecule 1: Phosphomannomutase



• Molecule 1: Phosphomannomutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.41Å 92.41Å 173.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.80 – 2.10 29.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.80-2.10) 99.8 (29.80-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.230 0.198 , 0.234	Depositor DCC
R_{free} test set	2572 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6201	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: MG, CL, CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/1995 (0.1%)	0.88	11/2684 (0.4%)
1	B	0.69	0/2006	0.90	12/2701 (0.4%)
1	C	0.63	2/1986 (0.1%)	0.88	9/2673 (0.3%)
All	All	0.64	3/5987 (0.1%)	0.88	32/8058 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	ASP	CG-OD2	6.35	1.40	1.25
1	A	61	GLU	CD-OE1	5.16	1.31	1.25
1	C	166	ASP	CG-OD1	5.12	1.37	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	180	ASP	CB-CG-OD2	8.20	125.68	118.30
1	A	122	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	245	ASP	CB-CG-OD2	8.08	125.58	118.30
1	C	19	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	12	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	221	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	122	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	110	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	147	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	147	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	133	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	207	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	187	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	198	ASP	CB-CG-OD2	5.49	123.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	62	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	62	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	234	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	64	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	133	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	187	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	25	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	140	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	47	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	140	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	198	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	245	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	110	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	221	ASP	CB-CG-OD2	5.02	122.81	118.30
1	B	122	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	12	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	1951	0	1907	14	0
1	B	1954	0	1909	32	0
1	C	1946	0	1898	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	13	0	5	2	0
4	B	26	0	10	8	0
4	C	26	0	10	9	0
5	A	64	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	134	0	0	4	0
5	C	82	0	0	4	0
All	All	6201	0	5739	74	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 6.

All (74) 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)
4:C:3003[A]:CIT:O2	5:C:3084:HOH:O	1.61	1.16
1:C:231:THR:HG22	1:C:233:LYS:H	1.46	0.81
4:C:3003[B]:CIT:O1	5:C:3085:HOH:O	2.01	0.77
1:B:84:ASN:HD22	1:B:85:SER:H	1.38	0.70
1:B:19:ARG:HD2	5:B:3102:HOH:O	1.94	0.67
1:B:155:LYS:NZ	1:B:159:GLU:OE2	2.29	0.66
1:C:221:ASP:O	5:C:3050:HOH:O	2.14	0.65
1:A:221:ASP:O	5:A:3038:HOH:O	2.15	0.64
1:A:234:ASP:O	1:A:238:ILE:HD13	1.97	0.64
4:B:3002[A]:CIT:O2	5:B:3038:HOH:O	2.16	0.61
1:C:19:ARG:NH1	1:C:20:ASN:HD21	2.00	0.60
1:C:18:PRO:O	1:C:19:ARG:HG2	2.02	0.59
1:C:11:VAL:HG23	1:C:12:ASP:H	1.68	0.58
1:A:218:ILE:O	1:A:224:THR:HG21	2.04	0.57
1:B:50:LYS:HZ1	4:B:3002[B]:CIT:C6	2.18	0.57
1:A:19:ARG:O	1:A:20:ASN:ND2	2.39	0.56
1:B:83:ARG:HH11	1:B:123:ASN:HD21	1.54	0.56
1:B:175:GLY:HA3	4:B:3002[A]:CIT:C5	2.36	0.55
1:B:121:PHE:H	1:C:134:ASN:HD22	1.55	0.55
1:B:121:PHE:H	1:C:134:ASN:ND2	2.06	0.53
1:B:183:PRO:HD2	1:B:186:TRP:CE3	2.45	0.51
1:B:84:ASN:ND2	1:B:85:SER:H	2.06	0.51
1:C:50:LYS:HA	1:C:53:GLU:HG2	1.93	0.51
1:C:92:ASN:O	1:C:96:VAL:HG13	2.10	0.51
1:B:175:GLY:HA3	4:B:3002[A]:CIT:C4	2.41	0.51
1:A:214:ASN:C	1:A:214:ASN:HD22	2.15	0.49
1:B:134:ASN:HD22	1:C:121:PHE:H	1.60	0.49
1:B:216:TYR:OH	5:B:3119:HOH:O	2.20	0.49
1:B:23:THR:HG21	5:B:3103:HOH:O	2.13	0.49
1:A:120:GLU:OE1	1:A:122:ARG:HD3	2.14	0.48
1:B:50:LYS:NZ	4:B:3002[B]:CIT:O5	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLU:OE1	1:C:123:ASN:O	2.31	0.48
1:C:11:VAL:HG23	1:C:12:ASP:N	2.28	0.48
1:C:174:GLY:O	4:C:3003[A]:CIT:O3	2.32	0.47
1:A:98:PHE:CZ	1:A:181:VAL:HG11	2.49	0.47
1:C:86:LEU:HD21	1:C:126:PHE:CE2	2.49	0.47
1:B:84:ASN:HD22	1:B:85:SER:N	2.10	0.47
1:C:33:ALA:HA	1:C:243:LEU:HD21	1.95	0.47
1:A:174:GLY:O	1:A:175:GLY:O	2.32	0.47
1:B:83:ARG:HH11	1:B:123:ASN:ND2	2.11	0.47
1:C:50:LYS:NZ	4:C:3003[B]:CIT:O5	2.46	0.46
1:C:175:GLY:HA3	4:C:3003[A]:CIT:C4	2.46	0.46
1:B:50:LYS:NZ	4:B:3002[A]:CIT:O6	2.48	0.45
1:B:99[A]:VAL:HG11	1:C:118:PHE:CZ	2.50	0.45
1:C:19:ARG:HH11	1:C:19:ARG:CG	2.28	0.45
1:B:239:LEU:O	1:B:243:LEU:HG	2.15	0.45
1:B:133:ARG:HH12	4:B:3002[B]:CIT:H22	1.81	0.45
1:B:174:GLY:O	4:B:3002[A]:CIT:H42	2.17	0.45
1:A:174:GLY:HA3	5:A:3065:HOH:O	2.17	0.44
1:C:23:THR:HG22	1:C:24:HIS:N	2.33	0.44
1:A:175:GLY:H	4:A:3001:CIT:H42	1.82	0.44
1:A:239:LEU:O	1:A:243:LEU:HG	2.18	0.44
4:C:3003[A]:CIT:O4	4:C:3003[A]:CIT:O6	2.35	0.43
1:A:158:ARG:O	1:A:162:GLU:HG2	2.18	0.43
4:A:3001:CIT:H21	4:A:3001:CIT:O4	2.19	0.43
1:C:175:GLY:HA3	4:C:3003[A]:CIT:H41	2.00	0.43
1:B:111:ILE:HG21	1:B:152:ILE:HD13	2.01	0.43
1:B:72:LEU:HD13	1:B:124:GLY:HA3	2.01	0.42
1:C:174:GLY:O	4:C:3003[A]:CIT:H42	2.19	0.42
1:A:92:ASN:O	1:A:96:VAL:HG13	2.20	0.42
1:B:6:ILE:HD13	1:B:195[A]:VAL:HG21	2.02	0.41
1:A:133:ARG:HD2	5:A:3046:HOH:O	2.20	0.41
1:B:166:ASP:OD1	1:B:166:ASP:N	2.49	0.41
1:B:104:HIS:HE1	5:C:3006:HOH:O	2.03	0.41
1:B:20:ASN:HB3	1:B:21:PRO:HD2	2.03	0.41
1:C:18:PRO:O	1:C:20:ASN:ND2	2.53	0.41
1:B:137:GLN:OE1	1:B:140:ARG:HD3	2.20	0.41
1:B:77:ASP:O	1:B:79:LYS:HE2	2.20	0.41
1:B:134:ASN:ND2	1:C:121:PHE:H	2.18	0.41
1:C:44:GLY:HA2	1:C:188:LYS:HE3	2.02	0.41
1:C:19:ARG:HH11	1:C:19:ARG:HG2	1.86	0.41
1:C:20:ASN:HB3	1:C:21:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3003[A]:CIT:O6	4:C:3003[A]:CIT:C5	2.69	0.41
1:B:41:GLY:HA2	1:B:65:TYR:O	2.22	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	241/247 (98%)	230 (95%)	10 (4%)	1 (0%)	34	32
1	B	243/247 (98%)	239 (98%)	4 (2%)	0	100	100
1	C	240/247 (97%)	231 (96%)	9 (4%)	0	100	100
All	All	724/741 (98%)	700 (97%)	23 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLY

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	210/213 (99%)	193 (92%)	17 (8%)	11	8
1	B	212/213 (100%)	199 (94%)	13 (6%)	18	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	209/213 (98%)	194 (93%)	15 (7%)	14	11
All	All	631/639 (99%)	586 (93%)	45 (7%)	14	11

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	24	HIS
1	A	25	ASP
1	A	31	LEU
1	A	55	LEU
1	A	73	LEU
1	A	84	ASN
1	A	87	LEU
1	A	105	LEU
1	A	133	ARG
1	A	192	LEU
1	A	200	GLU
1	A	201	THR
1	A	214	ASN
1	A	224	THR
1	A	238	ILE
1	A	245	ASP
1	B	23	THR
1	B	73	LEU
1	B	79	LYS
1	B	84	ASN
1	B	87	LEU
1	B	88	ARG
1	B	109	LEU
1	B	146	LEU
1	B	155	LYS
1	B	160	LEU
1	B	173	VAL
1	B	200	GLU
1	B	244	GLU
1	C	4	LYS
1	C	19	ARG
1	C	24	HIS
1	C	28	GLU
1	C	42	VAL
1	C	73	LEU

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Mol	Chain	Res	Type
1	C	84	ASN
1	C	87	LEU
1	C	96	VAL
1	C	146	LEU
1	C	156	LEU
1	C	160	LEU
1	C	195	VAL
1	C	244	GLU
1	C	245	ASP

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	20	ASN
1	A	84	ASN
1	A	123	ASN
1	A	134	ASN
1	A	214	ASN
1	B	51	GLN
1	B	84	ASN
1	B	123	ASN
1	B	134	ASN
1	B	193	GLN
1	C	20	ASN
1	C	84	ASN
1	C	134	ASN
1	C	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	CIT	B	3002[A]	-	3,12,12	1.83	1 (33%)	3,17,17	3.67	1 (33%)
4	CIT	B	3002[B]	-	3,12,12	1.08	0	3,17,17	3.69	2 (66%)
4	CIT	C	3003[A]	-	3,12,12	1.59	1 (33%)	3,17,17	4.98	1 (33%)
4	CIT	C	3003[B]	-	3,12,12	1.15	0	3,17,17	1.66	1 (33%)
4	CIT	A	3001	-	3,12,12	1.62	1 (33%)	3,17,17	0.86	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
4	CIT	B	3002[A]	-	-	5/6/16/16	-
4	CIT	B	3002[B]	-	-	6/6/16/16	-
4	CIT	C	3003[A]	-	-	3/6/16/16	-
4	CIT	C	3003[B]	-	-	6/6/16/16	-
4	CIT	A	3001	-	-	1/6/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3002[A]	CIT	C4-C3	-2.65	1.51	1.54
4	C	3003[A]	CIT	O7-C3	2.25	1.46	1.43
4	A	3001	CIT	O7-C3	2.20	1.46	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3003[A]	CIT	C3-C2-C1	-8.33	101.64	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3002[A]	CIT	C3-C4-C5	-6.10	105.22	114.98
4	B	3002[B]	CIT	C3-C4-C5	4.68	122.48	114.98
4	B	3002[B]	CIT	C3-C2-C1	4.35	121.95	114.98
4	C	3003[B]	CIT	C3-C4-C5	2.79	119.45	114.98

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3002[A]	CIT	C1-C2-C3-C6
4	C	3003[A]	CIT	C1-C2-C3-C6
4	B	3002[B]	CIT	C1-C2-C3-O7
4	B	3002[B]	CIT	C1-C2-C3-C4
4	B	3002[B]	CIT	C1-C2-C3-C6
4	B	3002[B]	CIT	C6-C3-C4-C5
4	C	3003[B]	CIT	C2-C3-C4-C5
4	C	3003[B]	CIT	O7-C3-C4-C5
4	C	3003[B]	CIT	C6-C3-C4-C5
4	B	3002[B]	CIT	O7-C3-C4-C5
4	C	3003[A]	CIT	C1-C2-C3-O7
4	C	3003[A]	CIT	C1-C2-C3-C4
4	B	3002[A]	CIT	C1-C2-C3-O7
4	B	3002[A]	CIT	C1-C2-C3-C4
4	A	3001	CIT	O7-C3-C4-C5
4	B	3002[B]	CIT	C2-C3-C4-C5
4	C	3003[B]	CIT	C1-C2-C3-C4
4	B	3002[A]	CIT	C6-C3-C4-C5
4	C	3003[B]	CIT	C1-C2-C3-C6
4	B	3002[A]	CIT	O7-C3-C4-C5
4	C	3003[B]	CIT	C1-C2-C3-O7

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3002[A]	CIT	5	0
4	B	3002[B]	CIT	3	0
4	C	3003[A]	CIT	7	0
4	C	3003[B]	CIT	2	0
4	A	3001	CIT	2	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 ⓘ

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	242/247 (97%)	0.67	33 (13%) 3 4	45, 49, 53, 63	0
1	B	242/247 (97%)	0.56	21 (8%) 10 13	43, 49, 57, 71	0
1	C	242/247 (97%)	0.82	43 (17%) 1 1	43, 49, 54, 62	0
All	All	726/741 (97%)	0.68	97 (13%) 3 4	43, 49, 54, 71	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ARG	5.5
1	A	245	ASP	5.5
1	C	128	VAL	5.2
1	C	119	VAL	5.0
1	C	126	PHE	4.9
1	C	19	ARG	4.8
1	C	200	GLU	4.2
1	C	245	ASP	4.2
1	A	9	PHE	4.2
1	B	40	LEU	4.2
1	A	24	HIS	4.1
1	A	18	PRO	4.1
1	A	20	ASN	4.0
1	B	9	PHE	3.8
1	C	211	GLU	3.7
1	B	42	VAL	3.7
1	A	15	LEU	3.6
1	A	56	GLY	3.6
1	A	4	LYS	3.6
1	C	129	SER	3.6
1	B	41	GLY	3.5
1	A	205	PHE	3.5
1	A	8	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	3.4
1	C	181	VAL	3.4
1	C	40	LEU	3.4
1	C	244	GLU	3.3
1	A	43	VAL	3.3
1	B	128	VAL	3.3
1	B	245	ASP	3.2
1	A	128	VAL	3.2
1	C	169	LEU	3.2
1	B	15	LEU	3.1
1	B	4	LYS	3.1
1	C	81	PHE	3.1
1	A	119	VAL	3.1
1	C	166	ASP	3.1
1	C	216	TYR	3.0
1	C	118	PHE	3.0
1	B	43	VAL	2.9
1	A	158	ARG	2.9
1	B	149	GLU	2.9
1	C	73	LEU	2.9
1	C	57	GLU	2.9
1	A	103	LEU	2.8
1	C	194	PHE	2.8
1	A	11	VAL	2.8
1	C	127	ASN	2.8
1	C	158	ARG	2.7
1	A	23	THR	2.7
1	A	17	PRO	2.7
1	C	130	PRO	2.7
1	C	4	LYS	2.7
1	B	7	LEU	2.7
1	C	102	CYS	2.6
1	A	204	PHE	2.6
1	C	42	VAL	2.6
1	C	21	PRO	2.6
1	C	117	THR	2.5
1	A	106	ILE	2.5
1	C	103	LEU	2.5
1	C	45	GLY	2.5
1	A	118	PHE	2.5
1	C	35	ALA	2.5
1	B	106	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	8	LEU	2.5
1	C	106	ILE	2.5
1	B	117	THR	2.4
1	A	197	ASN	2.4
1	A	57	GLU	2.4
1	B	244	GLU	2.4
1	B	116	GLY	2.4
1	A	58	SER	2.4
1	B	8	LEU	2.4
1	C	41	GLY	2.4
1	B	102	CYS	2.4
1	B	24	HIS	2.4
1	A	148	LYS	2.3
1	C	63	PHE	2.3
1	C	65	TYR	2.3
1	B	30	LEU	2.3
1	C	39	LYS	2.3
1	C	125	MET	2.3
1	C	131	ILE	2.3
1	B	119	VAL	2.3
1	C	179	PHE	2.2
1	C	77	ASP	2.2
1	C	177	ILE	2.2
1	B	118	PHE	2.2
1	A	160	LEU	2.2
1	A	6	ILE	2.1
1	C	18	PRO	2.1
1	A	88	ARG	2.1
1	A	151	HIS	2.1
1	A	52	LYS	2.1
1	C	120	GLU	2.0
1	A	31	LEU	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

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(Å ²)	Q<0.9
3	MG	A	2002	1/1	0.50	0.25	70,70,70,70	0
3	MG	B	2001	1/1	0.63	0.39	63,63,63,63	0
4	CIT	C	3003[A]	13/13	0.70	0.31	42,48,49,52	13
4	CIT	C	3003[B]	13/13	0.70	0.31	40,51,54,54	13
3	MG	C	2003	1/1	0.74	0.23	74,74,74,74	0
4	CIT	B	3002[A]	13/13	0.81	0.25	41,44,48,48	13
4	CIT	B	3002[B]	13/13	0.81	0.25	32,41,42,45	13
4	CIT	A	3001	13/13	0.85	0.28	73,81,86,87	0
2	CL	A	1001	1/1	0.96	0.05	37,37,37,37	1
2	CL	B	1002	1/1	0.99	0.04	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.