Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 04:08 PM GMT

PDB ID	:	7B19
Title	:	Mutant Myosin-II-GGG motor domain
Authors	:	Ewert, W.; Preller, M.
Deposited on	:	2020-11-24
Resolution	:	2.55 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:

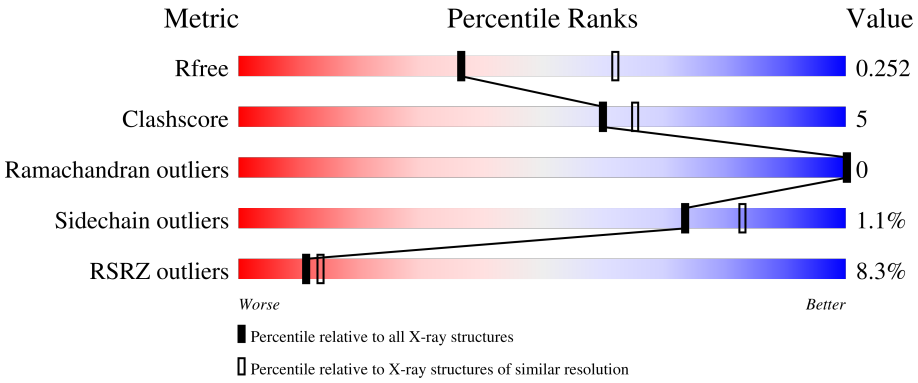
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	789	8% 85% 10% 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11930 atoms, of which 5801 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 Myosin-2 heavy chain,Myosin-2 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	750	11603	3750	5697	1016	1124	16	0	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP P08799
A	-9	HIS	-	expression tag	UNP P08799
A	-8	HIS	-	expression tag	UNP P08799
A	-7	HIS	-	expression tag	UNP P08799
A	-6	HIS	-	expression tag	UNP P08799
A	-5	HIS	-	expression tag	UNP P08799
A	-4	HIS	-	expression tag	UNP P08799
A	-3	HIS	-	expression tag	UNP P08799
A	-2	ASP	-	expression tag	UNP P08799
A	-1	GLY	-	expression tag	UNP P08799
A	0	THR	-	expression tag	UNP P08799
A	1	GLU	-	expression tag	UNP P08799
A	647	GLY	-	linker	UNP P08799
A	648	GLY	-	linker	UNP P08799
A	649	GLY	-	linker	UNP P08799
A	763	LEU	-	expression tag	UNP P08799
A	764	GLU	-	expression tag	UNP P08799
A	765	SER	-	expression tag	UNP P08799
A	766	ASN	-	expression tag	UNP P08799
A	767	GLU	-	expression tag	UNP P08799
A	768	PRO	-	expression tag	UNP P08799
A	769	PRO	-	expression tag	UNP P08799
A	770	MET	-	expression tag	UNP P08799
A	771	ASP	-	expression tag	UNP P08799
A	772	PHE	-	expression tag	UNP P08799
A	773	ASP	-	expression tag	UNP P08799
A	774	ASP	-	expression tag	UNP P08799

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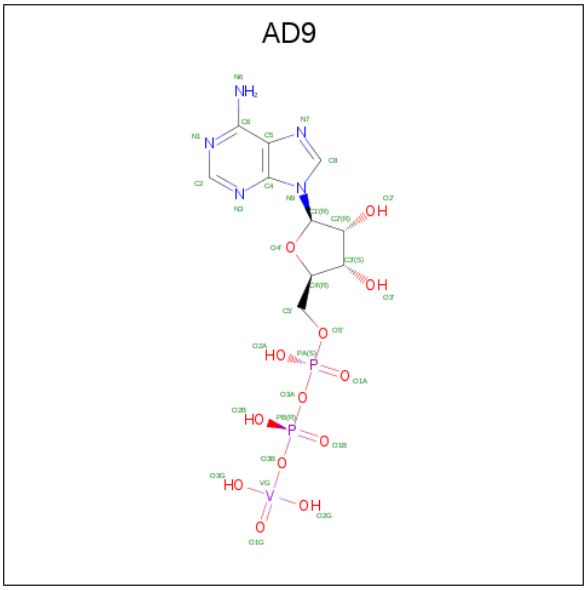
Chain	Residue	Modelled	Actual	Comment	Reference
A	775	ASP	-	expression tag	UNP P08799
A	776	ILE	-	expression tag	UNP P08799
A	777	PRO	-	expression tag	UNP P08799
A	778	PHE	-	expression tag	UNP P08799

- Molecule 2 is ADP METAVANADATE (three-letter code: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$).

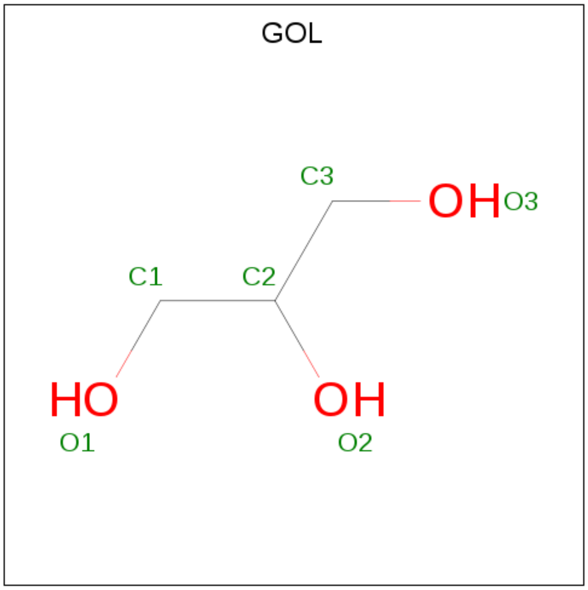


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	V	0	0
			45	10	14	5	13	2	1		

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

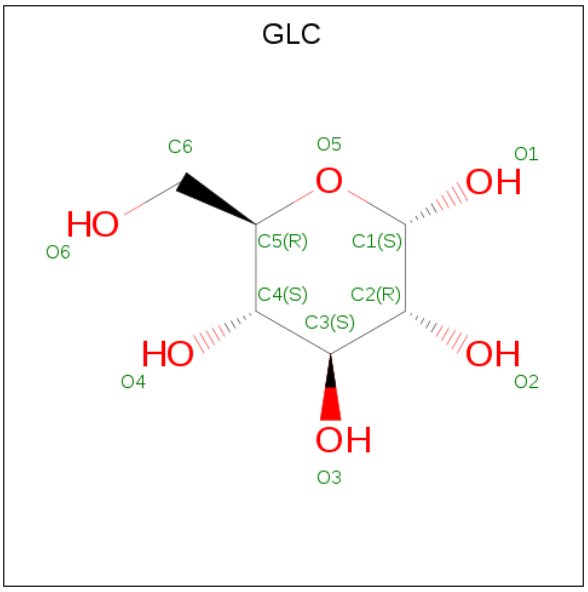
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



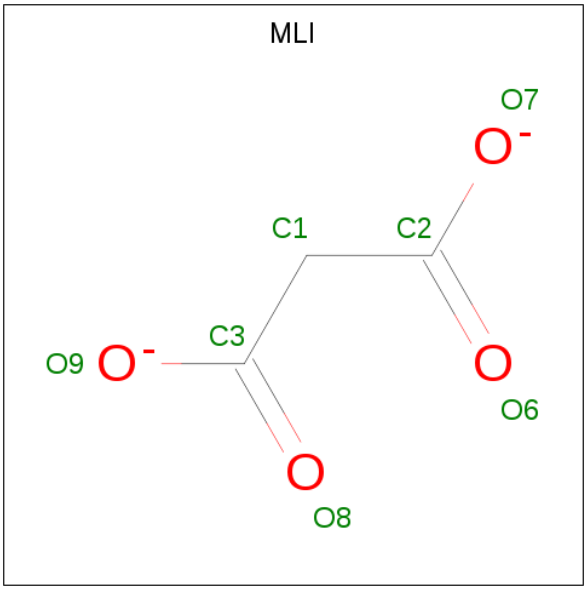
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			24	6	12	6		

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			9	3	2	4		
6	A	1	Total	C	H	O	0	0
			9	3	2	4		
6	A	1	Total	C	H	O	0	0
			9	3	2	4		

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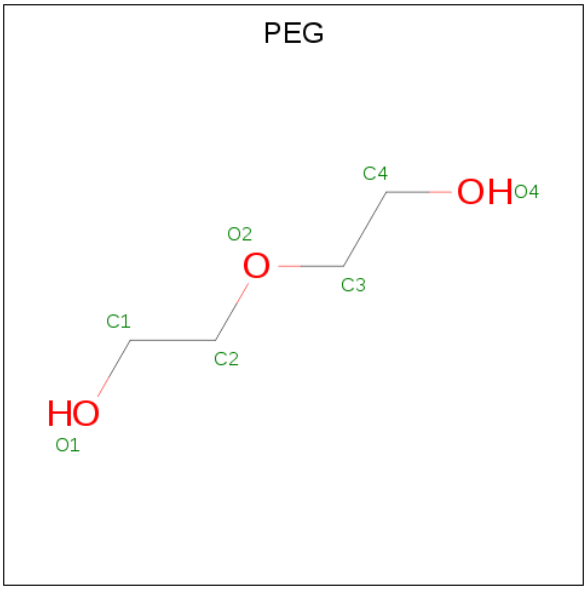
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			9	3	2	4		
6	A	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			17	4	10	3		
7	A	1	Total	C	H	O	0	0
			17	4	10	3		

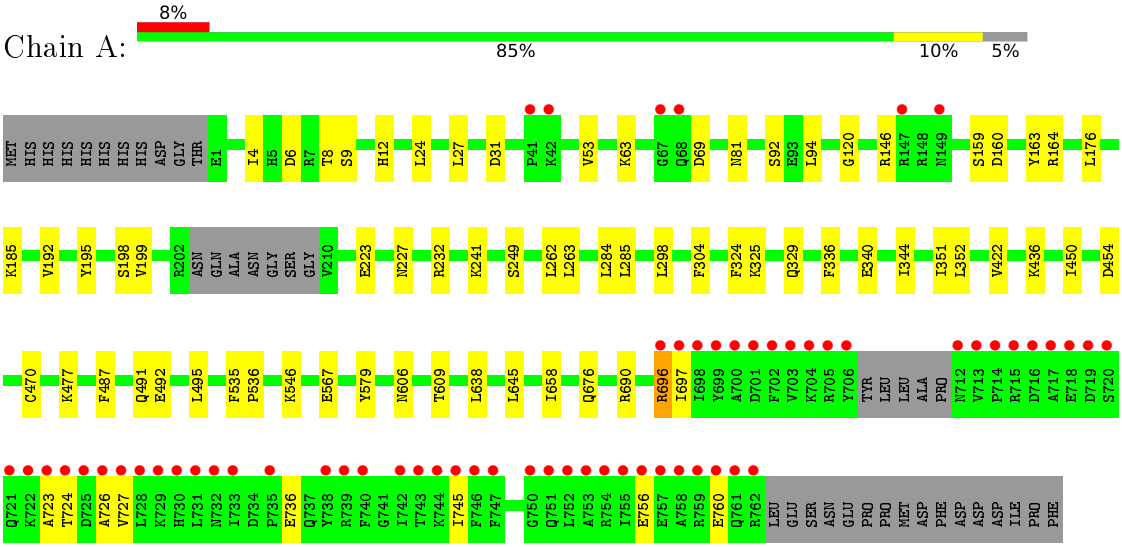
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	94	Total	O	0	0
			94	94		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Myosin-2 heavy chain,Myosin-2 heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	89.19Å 149.03Å 153.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.59 – 2.55 44.59 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.59-2.55) 99.6 (44.59-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.206 , 0.252 0.206 , 0.252	Depositor DCC
R_{free} test set	1675 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11930	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MG, MLI, GLC, AD9, PEG

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	0.35	0/6020	0.54	0/8137

There are no bond length outliers.

There are no bond angle outliers.

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	5906	5697	5740	50	0
2	A	31	14	12	1	0
3	A	1	0	0	0	0
4	A	36	48	48	0	0
5	A	12	12	12	4	0
6	A	35	10	10	0	0
7	A	14	20	20	3	0
8	A	94	0	0	0	0
All	All	6129	5801	5842	55	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 5.

All (55) 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)
2:A:801:AD9:O4'	2:A:801:AD9:C1'	1.64	1.23
1:A:4:ILE:CD1	1:A:146:ARG:NH1	2.04	1.19
1:A:4:ILE:CD1	1:A:146:ARG:HH12	1.53	1.19
1:A:4:ILE:HD12	1:A:146:ARG:HH12	1.10	1.12
1:A:4:ILE:HD11	1:A:146:ARG:NH1	1.71	1.01
1:A:4:ILE:HD12	1:A:146:ARG:NH1	1.77	0.87
1:A:6:ASP:O	1:A:9:SER:OG	2.06	0.72
1:A:745:ILE:HG23	1:A:745:ILE:O	1.89	0.71
1:A:6:ASP:OD1	1:A:8:THR:OG1	2.08	0.69
5:A:805:GLC:H62	5:A:805:GLC:H2	1.75	0.68
1:A:4:ILE:CD1	1:A:146:ARG:HH11	2.03	0.66
1:A:325:LYS:O	1:A:329:GLN:HG3	1.98	0.64
1:A:81:ASN:ND2	1:A:94:LEU:HD22	2.15	0.60
1:A:195:TYR:CZ	1:A:199:VAL:HG21	2.40	0.57
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.88	0.56
1:A:696:ARG:O	1:A:697:ILE:HD13	2.06	0.55
1:A:477:LYS:HD3	1:A:638:LEU:HD21	1.88	0.55
1:A:53:VAL:HG11	1:A:63:LYS:HG3	1.88	0.55
1:A:24:LEU:HA	1:A:27:LEU:HD12	1.89	0.55
1:A:606:ASN:HA	1:A:609:THR:HG22	1.89	0.55
1:A:262:LEU:HD11	1:A:470:CYS:HB3	1.92	0.52
1:A:723:ALA:O	1:A:726:ALA:HB3	2.11	0.51
1:A:284:LEU:HD12	1:A:324:PHE:CZ	2.46	0.51
1:A:285:LEU:HD23	1:A:298:LEU:HD13	1.94	0.50
1:A:94:LEU:O	1:A:690:ARG:NH2	2.44	0.50
1:A:176:LEU:HD21	1:A:645:LEU:HD22	1.94	0.49
1:A:492:GLU:HA	1:A:495:LEU:HD12	1.95	0.48
1:A:736:GLU:OE1	1:A:736:GLU:O	2.31	0.48
1:A:263:LEU:H	7:A:809:PEG:H11	1.78	0.48
1:A:262:LEU:CD2	7:A:816:PEG:C4	2.91	0.48
1:A:745:ILE:CG2	1:A:745:ILE:O	2.59	0.48
1:A:223:GLU:O	1:A:227:ASN:HB2	2.13	0.48
1:A:340:GLU:O	1:A:344:ILE:HG13	2.14	0.47
1:A:159:SER:OG	1:A:192:VAL:HG22	2.14	0.47
1:A:535:PHE:CD2	1:A:536:PRO:HD2	2.49	0.47
1:A:336:PHE:CE1	1:A:436:LYS:HG2	2.49	0.47
5:A:805:GLC:H2	5:A:805:GLC:C6	2.43	0.47
1:A:696:ARG:HD2	1:A:696:ARG:H	1.80	0.46
1:A:567:GLU:HA	1:A:579:TYR:O	2.15	0.46
1:A:160:ASP:O	1:A:164:ARG:HG2	2.16	0.46
1:A:756:GLU:O	1:A:760:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD21	1:A:298:LEU:HD22	1.98	0.45
1:A:724:THR:HA	1:A:727:VAL:HB	1.98	0.44
1:A:63:LYS:CE	1:A:69:ASP:OD1	2.66	0.44
5:A:805:GLC:C2	5:A:805:GLC:C6	2.96	0.43
5:A:805:GLC:H62	5:A:805:GLC:C2	2.47	0.43
1:A:487:PHE:O	1:A:491:GLN:HG3	2.18	0.43
1:A:658:ILE:HG22	1:A:676:GLN:NE2	2.33	0.43
1:A:241:LYS:HE3	1:A:454:ASP:OD2	2.19	0.42
1:A:185:LYS:HE2	1:A:185:LYS:HB2	1.83	0.42
1:A:262:LEU:CD2	7:A:816:PEG:H42	2.50	0.41
1:A:63:LYS:HE2	1:A:69:ASP:OD1	2.21	0.41
1:A:92:SER:OG	1:A:120:GLY:HA2	2.21	0.40
1:A:304:PHE:CD2	1:A:352:LEU:HB3	2.57	0.40
1:A:163:TYR:HA	1:A:450:ILE:HD11	2.02	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	744/789 (94%)	733 (98%)	11 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	625/689 (91%)	618 (99%)	7 (1%)	73 83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	31	ASP
1	A	198	SER
1	A	232	ARG
1	A	249	SER
1	A	546	LYS
1	A	696	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	GLN
1	A	500	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	750/789 (95%)	0.61	62 (8%)	11	13	32, 50, 117, 282	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	730	HIS	9.1
1	A	753	ALA	9.0
1	A	758	ALA	8.9
1	A	702	PHE	7.6
1	A	726	ALA	7.5
1	A	728	LEU	7.0
1	A	699	TYR	6.6
1	A	752	LEU	6.6
1	A	756	GLU	6.2
1	A	703	VAL	6.0
1	A	713	VAL	6.0
1	A	745	ILE	5.9
1	A	714	PRO	5.8
1	A	733	ILE	5.8
1	A	697	ILE	5.7
1	A	729	LYS	5.6
1	A	761	GLN	5.6
1	A	732	ASN	5.3
1	A	720	SER	5.1
1	A	742	ILE	5.0
1	A	724	THR	5.0
1	A	760	GLU	5.0
1	A	712	ASN	4.8
1	A	757	GLU	4.7
1	A	747	PHE	4.7
1	A	719	ASP	4.7
1	A	759	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	701	ASP	4.6
1	A	715	ARG	4.4
1	A	755	ILE	4.2
1	A	735	PRO	4.2
1	A	706	TYR	3.9
1	A	727	VAL	3.9
1	A	754	ARG	3.7
1	A	723	ALA	3.7
1	A	696	ARG	3.7
1	A	717	ALA	3.6
1	A	750	GLY	3.5
1	A	722	LYS	3.5
1	A	738	TYR	3.4
1	A	721	GLN	3.2
1	A	725	ASP	3.2
1	A	740	PHE	3.2
1	A	704	LYS	3.2
1	A	762	ARG	3.1
1	A	731	LEU	3.0
1	A	718	GLU	2.9
1	A	700	ALA	2.9
1	A	746	PHE	2.9
1	A	716	ASP	2.9
1	A	41	PRO	2.7
1	A	67	GLY	2.7
1	A	744	LYS	2.5
1	A	698	ILE	2.5
1	A	751	GLN	2.5
1	A	149	ASN	2.5
1	A	705	ARG	2.3
1	A	743	THR	2.3
1	A	147	ARG	2.2
1	A	42	LYS	2.0
1	A	739	ARG	2.0
1	A	68	GLN	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 monosaccharides 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, 95^{th} 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
4	GOL	A	807	6/6	0.69	0.16	67,92,110,111	0
7	PEG	A	816	7/7	0.74	0.31	63,116,150,150	0
5	GLC	A	805	12/12	0.76	0.24	90,103,121,123	0
6	MLI	A	810	7/7	0.77	0.32	69,74,97,97	0
6	MLI	A	808	7/7	0.78	0.26	51,60,70,70	0
4	GOL	A	803	6/6	0.78	0.15	55,72,81,87	0
4	GOL	A	815	6/6	0.78	0.22	66,83,96,102	0
4	GOL	A	804	6/6	0.81	0.37	48,62,80,80	0
6	MLI	A	814	7/7	0.81	0.19	58,70,79,80	0
6	MLI	A	806	7/7	0.83	0.42	59,80,83,86	0
7	PEG	A	809	7/7	0.85	0.23	51,63,77,78	0
6	MLI	A	813	7/7	0.86	0.29	71,81,97,99	0
4	GOL	A	811	6/6	0.89	0.21	52,70,76,87	0
4	GOL	A	812	6/6	0.91	0.26	50,61,80,80	0
2	AD9	A	801	31/31	0.97	0.18	25,44,56,63	0
3	MG	A	802	1/1	0.99	0.29	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.