



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:57 am BST

PDB ID : 2BKH
Title : Myosin VI nucleotide-free (MDInsert2) crystal structure
Authors : Menetrey, J.; Bahloul, A.; Yengo, C.; Wells, A.; Morris, C.; Sweeney, H.L.; Houdusse, A.
Deposited on : 2005-02-16
Resolution : 2.40 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

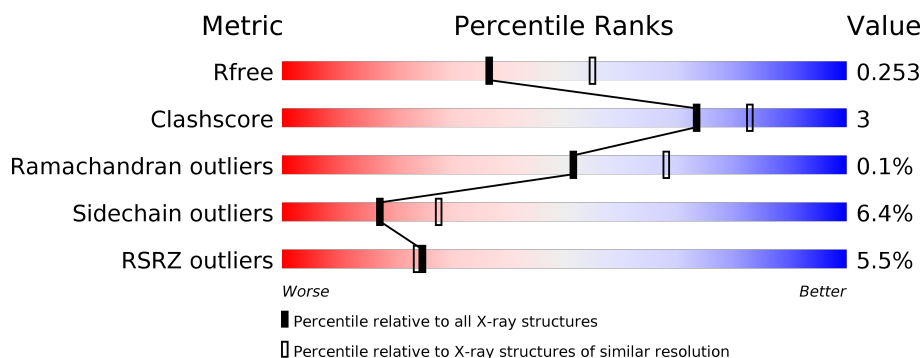
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	814	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div> <div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div> <div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div>
2	B	149	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div> <div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div> <div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></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
3	GOL	A	1818	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7728 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 UNCONVENTIONAL MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6340	4037	1099	1173	31			

- Molecule 2 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1063	656	169	230	8			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Ca	0	0
			4	4		

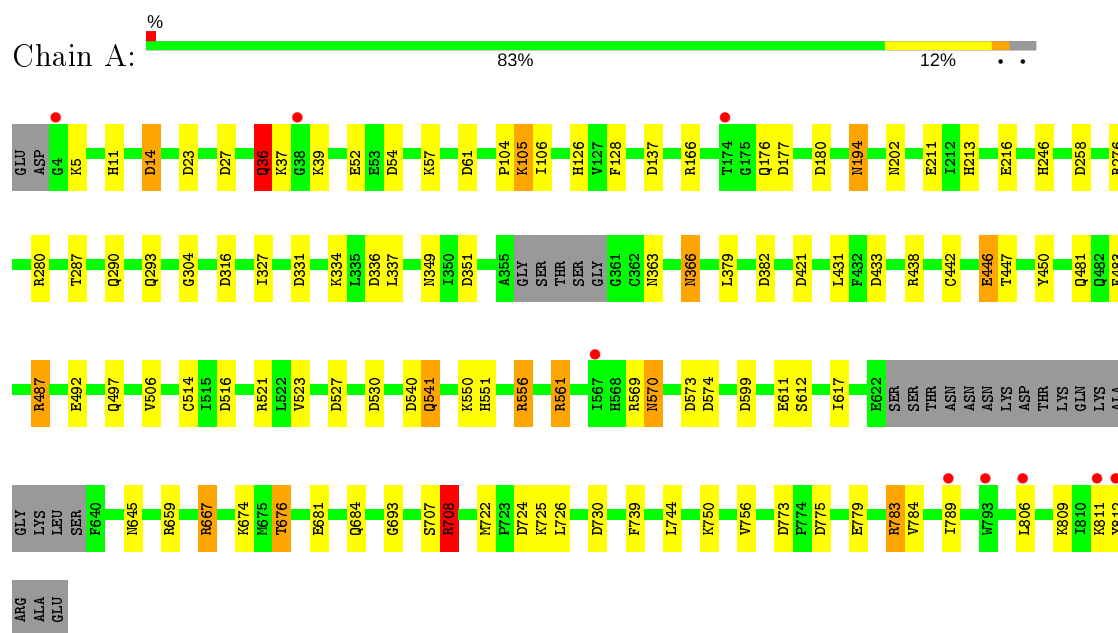
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	278	Total	O	0	0
			278	278		
5	B	7	Total	O	0	0
			7	7		

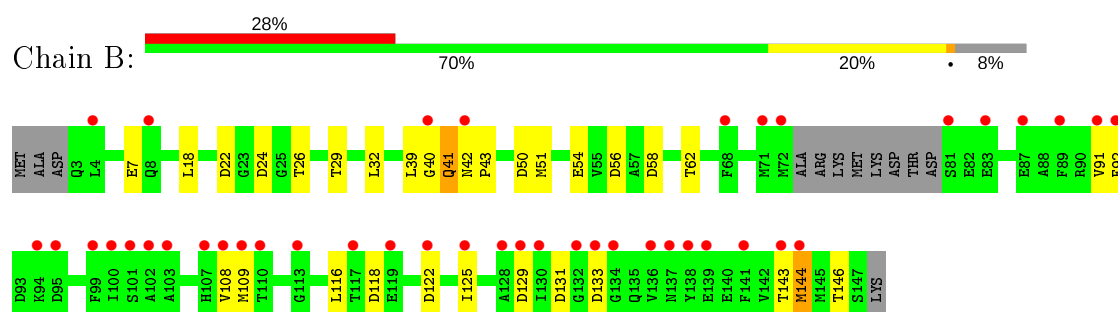
3 Residue-property plots [i](#)

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: UNCONVENTIONAL MYOSIN



• Molecule 2: CALMODULIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.57Å 104.44Å 90.28Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 55.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.40) 99.8 (55.18-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.206 , 0.254 0.207 , 0.253	Depositor DCC
R_{free} test set	2520 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7728	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: GOL, CA

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	0.51	0/6470	0.78	30/8715 (0.3%)
2	B	0.46	0/1074	0.86	10/1444 (0.7%)
All	All	0.50	0/7544	0.79	40/10159 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CB-CG-OD2	8.35	125.81	118.30
1	A	708	ARG	NE-CZ-NH2	-8.29	116.16	120.30
2	B	24	ASP	CB-CG-OD2	8.03	125.52	118.30
1	A	775	ASP	CB-CG-OD2	7.71	125.23	118.30
1	A	773	ASP	CB-CG-OD2	7.11	124.70	118.30
2	B	22	ASP	CB-CG-OD2	7.01	124.61	118.30
2	B	129	ASP	CB-CG-OD2	7.01	124.61	118.30
2	B	133	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	574	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	708	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	599	ASP	CB-CG-OD2	6.84	124.46	118.30
1	A	23	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	331	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	180	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	433	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	487	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	A	336	ASP	CB-CG-OD2	6.13	123.81	118.30
1	A	54	ASP	CB-CG-OD2	6.03	123.73	118.30
2	B	131	ASP	CB-CG-OD2	5.89	123.60	118.30
2	B	56	ASP	CB-CG-OD2	5.86	123.58	118.30
2	B	118	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	137	ASP	CB-CG-OD2	5.74	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	667	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	573	ASP	CB-CG-OD2	5.68	123.41	118.30
2	B	122	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	724	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	516	ASP	CB-CG-OD2	5.35	123.11	118.30
2	B	58	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	351	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	561	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	382	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	730	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	14	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	540	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	316	ASP	CB-CG-OD2	5.17	122.96	118.30
2	B	50	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	27	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	527	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	708	ARG	CG-CD-NE	-5.07	101.16	111.80

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	6340	0	6315	42	0
2	B	1063	0	984	7	0
3	A	36	0	48	1	0
4	B	4	0	0	0	0
5	A	278	0	0	2	0
5	B	7	0	0	0	0
All	All	7728	0	7347	48	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 3.

All (48) 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:202:ASN:HD22	1:A:246:HIS:HE1	1.30	0.78
1:A:202:ASN:ND2	1:A:246:HIS:HE1	1.86	0.73
1:A:541:GLN:HE21	1:A:541:GLN:H	1.40	0.69
1:A:659:ARG:NH2	5:A:2232:HOH:O	2.32	0.63
1:A:366:ASN:ND2	5:A:2129:HOH:O	2.31	0.62
1:A:287:THR:HA	1:A:290:GLN:HE21	1.67	0.60
1:A:523:VAL:O	1:A:551:HIS:HE1	1.84	0.60
2:B:39:LEU:HG	2:B:91:VAL:HG11	1.84	0.59
1:A:106:ILE:O	1:A:126:HIS:HE1	1.86	0.58
1:A:514:CYS:HB2	1:A:556:ARG:HD3	1.88	0.55
1:A:530:ASP:OD1	1:A:645:ASN:ND2	2.40	0.55
1:A:779:GLU:O	1:A:783:ARG:HG3	2.07	0.53
1:A:126:HIS:CD2	1:A:128:PHE:H	2.26	0.53
2:B:92:PHE:CE1	2:B:108:VAL:HG11	2.43	0.53
1:A:11:HIS:HD2	1:A:14:ASP:H	1.59	0.51
1:A:349:ASN:HD22	3:A:1818:GOL:C3	2.24	0.51
1:A:327:ILE:HB	1:A:442:CYS:SG	2.52	0.50
1:A:523:VAL:O	1:A:551:HIS:CE1	2.64	0.50
1:A:52:GLU:OE1	1:A:57:LYS:NZ	2.43	0.49
2:B:42:ASN:N	2:B:43:PRO:CD	2.76	0.49
1:A:211:GLU:OE1	1:A:213:HIS:HE1	1.96	0.48
2:B:42:ASN:N	2:B:43:PRO:HD3	2.28	0.48
1:A:104:PRO:O	1:A:105:LYS:HG3	2.13	0.48
1:A:722:MET:CE	1:A:726:LEU:HD22	2.43	0.48
1:A:337:LEU:HD23	1:A:431:LEU:HD11	1.96	0.48
1:A:674:LYS:HB2	1:A:676:THR:HG22	1.97	0.47
1:A:492:GLU:OE1	1:A:708:ARG:NH2	2.48	0.46
1:A:707:SER:C	1:A:708:ARG:HG3	2.34	0.46
2:B:40:GLY:O	2:B:41:GLN:NE2	2.49	0.46
1:A:806:LEU:HD13	2:B:32:LEU:HD11	1.99	0.45
1:A:523:VAL:HG12	1:A:550:LYS:HE2	1.99	0.44
1:A:211:GLU:OE1	1:A:213:HIS:CE1	2.71	0.44
2:B:144:MET:HE3	2:B:144:MET:HA	2.00	0.44
1:A:202:ASN:ND2	1:A:246:HIS:CE1	2.76	0.43
1:A:280:ARG:HD2	1:A:304:GLY:O	2.18	0.42
1:A:739:PHE:CE2	1:A:756:VAL:HG11	2.55	0.42
1:A:36:GLN:HB3	1:A:39:LYS:HG2	2.01	0.42
1:A:446:GLU:HG3	1:A:447:THR:N	2.34	0.42
1:A:681:GLU:HG2	1:A:684:GLN:NE2	2.35	0.41
1:A:379:LEU:O	1:A:612:SER:OG	2.31	0.41
1:A:722:MET:HE3	1:A:726:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:PHE:CD2	1:A:744:LEU:HD12	2.55	0.41
1:A:194:ASN:HD22	1:A:194:ASN:N	2.18	0.41
1:A:570:ASN:HD22	1:A:570:ASN:HA	1.65	0.41
1:A:483:PHE:O	1:A:487:ARG:HG2	2.21	0.40
1:A:481:GLN:NE2	1:A:693:GLY:HA3	2.35	0.40
1:A:739:PHE:CD2	1:A:744:LEU:CD1	3.03	0.40
1:A:379:LEU:HA	1:A:617:ILE:CD1	2.52	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	781/814 (96%)	754 (96%)	26 (3%)	1 (0%)	51	68
2	B	133/149 (89%)	129 (97%)	4 (3%)	0	100	100
All	All	914/963 (95%)	883 (97%)	30 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLN

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	698/721 (97%)	660 (95%)	38 (5%)	22	36
2	B	114/128 (89%)	100 (88%)	14 (12%)	4	6
All	All	812/849 (96%)	760 (94%)	52 (6%)	17	28

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	36	GLN
1	A	37	LYS
1	A	105	LYS
1	A	166	ARG
1	A	176	GLN
1	A	177	ASP
1	A	194	ASN
1	A	216	GLU
1	A	258	ASP
1	A	276	ARG
1	A	293	GLN
1	A	334	LYS
1	A	363	ASN
1	A	366	ASN
1	A	438	ARG
1	A	446	GLU
1	A	450	TYR
1	A	497	GLN
1	A	506	VAL
1	A	521	ARG
1	A	541	GLN
1	A	556	ARG
1	A	561	ARG
1	A	569	ARG
1	A	570	ASN
1	A	611	GLU
1	A	667	ARG
1	A	676	THR
1	A	708	ARG
1	A	725	LYS
1	A	750	LYS
1	A	783	ARG
1	A	784	VAL
1	A	789	ILE

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Mol	Chain	Res	Type
1	A	809	LYS
1	A	811	LYS
1	A	812	TYR
2	B	7	GLU
2	B	18	LEU
2	B	26	THR
2	B	29	THR
2	B	41	GLN
2	B	51	MET
2	B	54	GLU
2	B	62	THR
2	B	109	MET
2	B	116	LEU
2	B	125	ILE
2	B	143	THR
2	B	144	MET
2	B	146	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	36	GLN
1	A	47	GLN
1	A	126	HIS
1	A	194	ASN
1	A	202	ASN
1	A	213	HIS
1	A	246	HIS
1	A	290	GLN
1	A	293	GLN
1	A	383	GLN
1	A	417	ASN
1	A	418	ASN
1	A	481	GLN
1	A	485	ASN
1	A	493	GLN
1	A	533	ASN
1	A	541	GLN
1	A	551	HIS
1	A	568	HIS
1	A	570	ASN

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Mol	Chain	Res	Type
1	A	581	HIS
1	A	678	HIS
1	A	745	ASN
2	B	49	GLN
2	B	53	ASN
2	B	111	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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
3	GOL	A	1813	-	5,5,5	0.55	0	5,5,5	0.61	0
3	GOL	A	1817	-	5,5,5	0.38	0	5,5,5	0.23	0
3	GOL	A	1814	-	5,5,5	0.38	0	5,5,5	0.39	0
3	GOL	A	1815	-	5,5,5	0.45	0	5,5,5	0.23	0
3	GOL	A	1816	-	5,5,5	0.28	0	5,5,5	0.46	0
3	GOL	A	1818	-	5,5,5	0.36	0	5,5,5	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1813	-	-	2/4/4/4	-
3	GOL	A	1817	-	-	2/4/4/4	-
3	GOL	A	1814	-	-	2/4/4/4	-
3	GOL	A	1815	-	-	1/4/4/4	-
3	GOL	A	1816	-	-	2/4/4/4	-
3	GOL	A	1818	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1818	GOL	O1-C1-C2-O2
3	A	1813	GOL	O1-C1-C2-C3
3	A	1814	GOL	O1-C1-C2-C3
3	A	1818	GOL	O1-C1-C2-C3
3	A	1816	GOL	O2-C2-C3-O3
3	A	1817	GOL	O1-C1-C2-C3
3	A	1816	GOL	C1-C2-C3-O3
3	A	1818	GOL	C1-C2-C3-O3
3	A	1813	GOL	O1-C1-C2-O2
3	A	1817	GOL	O1-C1-C2-O2
3	A	1814	GOL	O1-C1-C2-O2
3	A	1815	GOL	O2-C2-C3-O3
3	A	1818	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1818	GOL	1	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	787/814 (96%)	-0.07	9 (1%) 80 79	25, 43, 66, 76	0
2	B	137/149 (91%)	1.48	42 (30%) 0 0	53, 77, 85, 86	0
All	All	924/963 (95%)	0.16	51 (5%) 25 24	25, 45, 80, 86	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	134	GLY	5.7
2	B	94	LYS	5.5
2	B	128	ALA	5.1
2	B	92	PHE	5.0
2	B	102	ALA	4.7
2	B	141	PHE	4.6
2	B	137	ASN	4.1
2	B	136	VAL	3.8
2	B	129	ASP	3.8
2	B	81	SER	3.7
1	A	789	ILE	3.4
1	A	793	TRP	3.4
2	B	138	TYR	3.3
2	B	107	HIS	3.2
1	A	567	ILE	3.2
2	B	119	GLU	3.1
2	B	101	SER	3.0
2	B	42	ASN	3.0
2	B	99	PHE	3.0
1	A	812	TYR	3.0
2	B	133	ASP	2.9
2	B	72	MET	2.9
2	B	130	ILE	2.8
2	B	91	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	95	ASP	2.8
2	B	8	GLN	2.8
1	A	4	GLY	2.7
2	B	103	ALA	2.7
1	A	174	THR	2.6
2	B	40	GLY	2.6
2	B	68	PHE	2.5
2	B	132	GLY	2.5
2	B	122	ASP	2.4
2	B	89	PHE	2.4
2	B	71	MET	2.4
2	B	113	GLY	2.3
1	A	806	LEU	2.3
2	B	109	MET	2.2
2	B	100	ILE	2.2
2	B	87	GLU	2.2
2	B	4	LEU	2.2
1	A	38	GLY	2.2
2	B	83	GLU	2.2
2	B	110	THR	2.1
2	B	139	GLU	2.1
2	B	108	VAL	2.1
2	B	143	THR	2.1
1	A	811	LYS	2.1
2	B	144	MET	2.1
2	B	125	ILE	2.0
2	B	117	THR	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(Å ²)	Q<0.9
3	GOL	A	1818	6/6	0.66	0.41	77,78,79,79	0
3	GOL	A	1814	6/6	0.87	0.23	63,66,67,68	0
3	GOL	A	1817	6/6	0.87	0.14	65,67,68,68	0
3	GOL	A	1816	6/6	0.89	0.24	55,55,56,57	0
4	CA	B	1150	1/1	0.90	0.09	91,91,91,91	0
3	GOL	A	1815	6/6	0.92	0.20	45,47,48,51	0
4	CA	B	1151	1/1	0.93	0.09	90,90,90,90	0
3	GOL	A	1813	6/6	0.96	0.17	46,48,50,50	0
4	CA	B	1149	1/1	0.97	0.04	71,71,71,71	0
4	CA	B	1148	1/1	0.98	0.05	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.