



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2026 – 04:09 am BST

PDB ID : 9H6S / pdb_00009h6s
Title : Structure of the V606M/W622L mutant of myosin UNC-54
Authors : Arnese, R.; Meinhart, A.; Deszcz, L.; Clausen, T.
Deposited on : 2024-10-25
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 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	:	1.8.4, CSD as541be (2020)
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

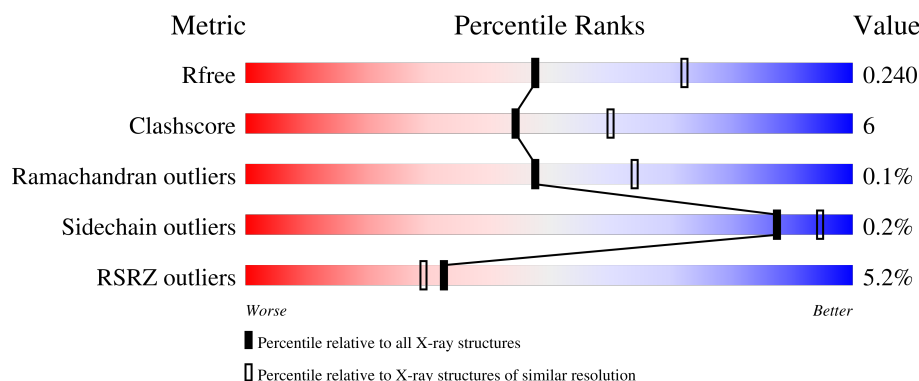
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	796	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div></div> </div> <div></div> </div>
1	B	796	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div></div> </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
3	GOL	A	802	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12395 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 Myosin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total	C	N	O	S	0	0	0
			6190	3929	1067	1151	43			
1	B	763	Total	C	N	O	S	0	0	0
			6152	3905	1057	1147	43			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	606	MET	VAL	engineered mutation	UNP P02566
A	622	LEU	TRP	engineered mutation	UNP P02566
A	791	HIS	-	expression tag	UNP P02566
A	792	HIS	-	expression tag	UNP P02566
A	793	HIS	-	expression tag	UNP P02566
A	794	HIS	-	expression tag	UNP P02566
A	795	HIS	-	expression tag	UNP P02566
A	796	HIS	-	expression tag	UNP P02566
B	606	MET	VAL	engineered mutation	UNP P02566
B	622	LEU	TRP	engineered mutation	UNP P02566
B	791	HIS	-	expression tag	UNP P02566
B	792	HIS	-	expression tag	UNP P02566
B	793	HIS	-	expression tag	UNP P02566
B	794	HIS	-	expression tag	UNP P02566
B	795	HIS	-	expression tag	UNP P02566
B	796	HIS	-	expression tag	UNP P02566

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

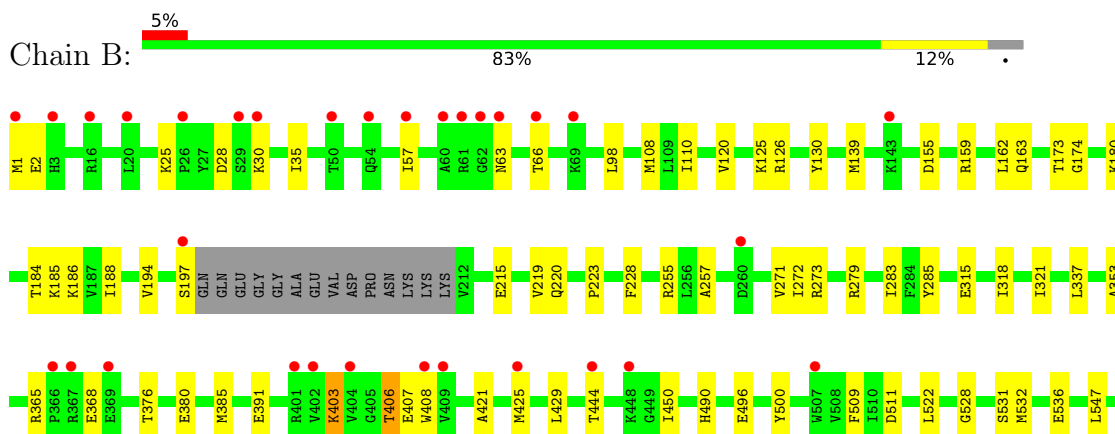
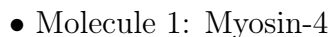


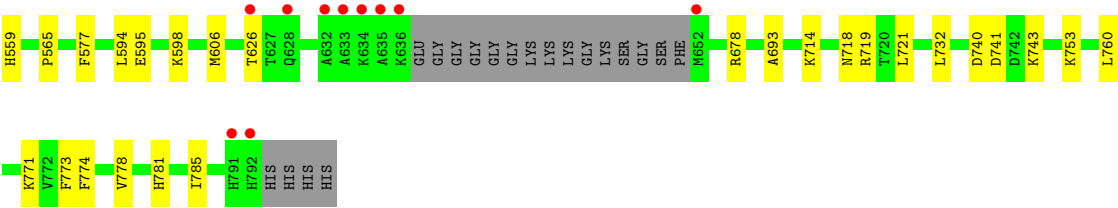
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	B	21	Total 21	O 21	0	0

- Molecule 1: Myosin-4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.03Å 124.27Å 96.96Å 90.00° 109.88° 90.00°	Depositor
Resolution (Å)	76.78 – 2.40 76.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (76.78-2.40) 88.0 (76.78-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.17 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.212 , 0.240 0.212 , 0.240	Depositor DCC
R_{free} test set	6134 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12395	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: FMT, GOL

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	0.14	0/6320	0.37	0/8514
1	B	0.15	0/6280	0.37	0/8462
All	All	0.14	0/12600	0.37	0/16976

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	6190	0	6133	88	1
1	B	6152	0	6093	63	1
2	A	3	0	1	0	0
2	B	3	0	1	0	0
3	A	6	0	8	5	0
4	A	20	0	0	0	0
4	B	21	0	0	0	0
All	All	12395	0	12236	147	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 6.

All (147) 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:1:MET:HE3	1:B:63:ASN:HA	1.61	0.82
1:A:761:SER:H	1:A:764:MET:HE2	1.47	0.78
1:B:391:GLU:H	1:B:391:GLU:CD	1.92	0.75
1:A:177:GLY:H	3:A:802:GOL:H11	1.50	0.75
1:A:39:GLU:OE1	1:A:39:GLU:N	2.21	0.71
1:A:142:ARG:NE	1:A:145:GLU:OE2	2.25	0.68
1:A:613:LYS:HA	1:A:613:LYS:HE2	1.75	0.67
1:B:271:VAL:HG23	1:B:272:ILE:HG23	1.77	0.66
1:A:235:ARG:NH1	1:A:467:PHE:HA	2.12	0.65
1:B:159:ARG:O	1:B:163:GLN:HG3	1.96	0.65
1:B:718:ASN:HB2	1:B:774:PHE:HB2	1.77	0.65
1:A:159:ARG:O	1:A:163:GLN:HG3	1.98	0.64
1:A:496:GLU:OE2	1:A:719:ARG:NH2	2.33	0.61
1:A:235:ARG:HH12	1:A:467:PHE:HA	1.64	0.61
1:A:45:GLY:HA3	1:A:57:ILE:HD13	1.82	0.60
1:A:627:THR:HG22	1:A:630:GLU:HG3	1.82	0.60
1:A:43:LEU:HD12	1:A:59:THR:HB	1.86	0.58
1:A:173:THR:OG1	1:A:678:ARG:HD2	2.04	0.58
1:A:425:MET:HE1	1:A:606:MET:SD	2.44	0.57
1:B:28:ASP:OD1	1:B:30:LYS:HG2	2.05	0.57
1:A:1:MET:CE	1:B:63:ASN:HA	2.35	0.56
1:A:491:HIS:CE1	1:A:674:PRO:HD2	2.42	0.55
1:B:279:ARG:HG2	1:B:285:TYR:CZ	2.42	0.54
1:A:503:GLU:HG2	1:A:773:PHE:CE1	2.42	0.54
1:B:257:ALA:HA	1:B:450:ILE:HB	1.88	0.54
1:A:80:PHE:O	1:A:83:THR:OG1	2.25	0.54
1:A:108:MET:HA	1:A:108:MET:HE2	1.90	0.54
1:A:28:ASP:OD1	1:A:30:LYS:HG2	2.07	0.53
1:A:376:THR:O	1:A:380:GLU:HG3	2.07	0.53
1:B:173:THR:OG1	1:B:678:ARG:HD2	2.08	0.53
1:B:496:GLU:CD	1:B:719:ARG:HH22	2.17	0.53
1:A:446:ASP:OD1	1:A:452:ARG:NH2	2.41	0.53
1:A:185:LYS:HE3	1:A:219:VAL:HG21	1.90	0.53
1:B:522:LEU:HB2	1:B:559:HIS:CE1	2.43	0.53
1:B:139:MET:HE2	1:B:194:VAL:HG12	1.89	0.53
1:A:155:ASP:O	1:A:159:ARG:HG2	2.09	0.53
1:A:185:LYS:HE2	1:A:215:GLU:OE2	2.09	0.53
1:B:528:GLY:O	1:B:532:MET:HG3	2.09	0.52
1:A:279:ARG:HG2	1:A:285:TYR:CZ	2.44	0.52
1:B:130:TYR:HB3	1:B:186:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:CYS:O	1:A:598:LYS:NZ	2.39	0.52
1:A:718:ASN:HB2	1:A:774:PHE:HB2	1.92	0.52
1:A:172:ILE:HD12	1:A:677:ILE:HB	1.92	0.52
1:B:185:LYS:HE2	1:B:215:GLU:OE1	2.09	0.52
1:B:365:ARG:HB3	1:B:368:GLU:HB2	1.92	0.52
1:B:490:HIS:ND1	1:B:511:ASP:OD2	2.40	0.52
1:A:337:LEU:HD22	1:A:444:THR:HG21	1.91	0.51
1:A:744:LYS:NZ	1:A:748:GLU:OE2	2.43	0.51
1:A:755:VAL:HG21	1:A:762:GLU:HG3	1.92	0.51
1:B:273:ARG:HH21	1:B:595:GLU:CD	2.18	0.50
1:B:337:LEU:HD22	1:B:444:THR:HG21	1.92	0.50
1:A:286:GLN:HB3	1:A:327:PHE:HB2	1.94	0.50
1:B:429:LEU:HD21	1:B:606:MET:HE1	1.94	0.50
1:A:142:ARG:NH2	1:B:66:THR:O	2.45	0.50
1:A:142:ARG:HH21	1:B:66:THR:HG1	1.55	0.50
1:A:188:ILE:HD13	1:A:218:ILE:HD13	1.93	0.49
1:A:740:ASP:OD1	1:A:741:ASP:N	2.45	0.49
1:B:565:PRO:HD3	1:B:577:PHE:HA	1.94	0.49
1:A:421:ALA:O	1:A:425:MET:HB2	2.11	0.49
1:A:496:GLU:HG3	1:A:500:TYR:CE2	2.47	0.49
1:B:185:LYS:HE3	1:B:219:VAL:HG21	1.94	0.49
1:A:279:ARG:HG2	1:A:285:TYR:CE2	2.48	0.49
1:B:721:LEU:HD13	1:B:771:LYS:HG2	1.95	0.48
1:A:294:GLU:H	1:A:294:GLU:CD	2.21	0.48
1:A:196:ALA:C	1:A:255:ARG:HH12	2.22	0.48
1:B:318:ILE:HB	1:B:321:ILE:HB	1.95	0.48
1:B:108:MET:HE3	1:B:125:LYS:HE2	1.96	0.48
1:B:403:LYS:HG3	1:B:407:GLU:C	2.38	0.48
1:A:569:LYS:HE3	1:A:569:LYS:HB2	1.58	0.47
1:B:376:THR:O	1:B:380:GLU:HG3	2.14	0.47
1:A:761:SER:N	1:A:764:MET:HE2	2.22	0.47
1:A:150:LEU:HD12	1:A:677:ILE:HD13	1.95	0.47
1:B:740:ASP:OD1	1:B:741:ASP:N	2.47	0.47
1:B:35:ILE:HD13	1:B:57:ILE:HD11	1.96	0.47
1:A:318:ILE:HB	1:A:321:ILE:HB	1.96	0.47
1:B:184:THR:O	1:B:188:ILE:HG12	2.14	0.47
1:A:220:GLN:O	1:A:223:PRO:HD2	2.15	0.46
1:A:565:PRO:HD3	1:A:577:PHE:HA	1.96	0.46
1:B:403:LYS:HD2	1:B:406:THR:O	2.15	0.46
1:B:25:LYS:HA	1:B:25:LYS:HD2	1.77	0.46
1:A:176:SER:HA	3:A:802:GOL:H11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:SER:HB3	1:B:255:ARG:NH1	2.31	0.46
1:B:279:ARG:HG2	1:B:285:TYR:CE2	2.51	0.46
1:A:743:LYS:HA	1:A:743:LYS:HD3	1.75	0.46
1:A:742:ASP:HB3	1:A:745:LYS:HD2	1.97	0.46
1:B:760:LEU:HD21	1:B:778:VAL:HG13	1.98	0.45
1:B:403:LYS:HB2	1:B:408:TRP:HA	1.99	0.45
1:A:735:LYS:HD2	1:A:735:LYS:N	2.29	0.45
1:A:142:ARG:HB2	1:A:145:GLU:OE2	2.17	0.45
1:A:68:LYS:HG3	1:A:71:LEU:HD13	1.99	0.45
1:B:155:ASP:O	1:B:159:ARG:HG2	2.17	0.45
1:B:353:ALA:HB2	1:B:385:MET:HB2	1.99	0.45
1:A:27:TYR:HE1	1:A:75:MET:HG2	1.82	0.45
1:B:98:LEU:HD21	1:B:693:ALA:HB1	1.99	0.45
1:B:279:ARG:HG3	1:B:315:GLU:O	2.17	0.45
1:A:279:ARG:HG3	1:A:315:GLU:O	2.17	0.45
1:A:268:LYS:HE3	1:A:427:LYS:HB3	1.98	0.44
1:B:421:ALA:O	1:B:425:MET:HE2	2.17	0.44
1:B:718:ASN:C	1:B:719:ARG:HG3	2.42	0.44
1:A:721:LEU:HD23	1:A:771:LYS:HG2	1.99	0.44
1:A:245:PHE:CZ	1:A:457:GLY:HA3	2.51	0.44
1:B:403:LYS:HD2	1:B:406:THR:C	2.43	0.44
1:B:536:GLU:HG2	1:B:547:LEU:HB2	1.98	0.44
1:B:1:MET:HB3	1:B:2:GLU:H	1.56	0.44
1:A:181:THR:H	3:A:802:GOL:C3	2.30	0.44
1:A:217:GLN:O	1:A:221:THR:HG23	2.18	0.44
1:A:605:VAL:O	1:A:609:MET:HG3	2.18	0.44
1:B:391:GLU:CD	1:B:391:GLU:N	2.70	0.44
1:A:354:HIS:ND1	1:A:426:ALA:HB1	2.33	0.43
1:B:421:ALA:O	1:B:425:MET:HB2	2.18	0.43
1:A:308:TYR:HA	1:A:359:ASN:OD1	2.19	0.43
1:A:603:ASP:OD2	1:A:628:GLN:NE2	2.50	0.43
1:B:110:ILE:O	1:B:120:VAL:HA	2.19	0.43
1:A:172:ILE:CD1	1:A:677:ILE:HB	2.49	0.43
1:A:609:MET:HB3	1:A:618:LEU:HD21	2.00	0.43
1:A:532:MET:HE2	1:A:532:MET:HB3	1.87	0.43
1:A:161:MET:HB3	1:A:161:MET:HE2	1.72	0.42
1:A:736:GLU:OE1	1:A:736:GLU:N	2.46	0.42
1:B:228:PHE:CZ	1:B:283:ILE:HG12	2.54	0.42
1:A:39:GLU:HG2	1:A:40:GLU:HG2	2.01	0.42
1:B:220:GLN:O	1:B:223:PRO:HD2	2.19	0.42
1:A:92:LEU:HB3	1:A:709:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:GLY:O	1:A:532:MET:HG3	2.19	0.42
1:B:594:LEU:O	1:B:598:LYS:HG3	2.19	0.42
1:A:291:PHE:CD2	1:A:292:ARG:HG3	2.54	0.42
1:A:395:LYS:HB2	1:A:395:LYS:HE3	1.75	0.42
1:A:487:PHE:CZ	1:A:674:PRO:HG3	2.55	0.42
1:B:743:LYS:HD3	1:B:743:LYS:HA	1.77	0.41
1:A:181:THR:OG1	3:A:802:GOL:H31	2.19	0.41
1:A:353:ALA:HB2	1:A:385:MET:CB	2.50	0.41
1:B:174:GLY:O	1:B:180:LYS:HE3	2.20	0.41
1:A:34:TRP:CZ2	1:A:75:MET:HE2	2.56	0.41
1:A:180:LYS:N	3:A:802:GOL:H32	2.36	0.41
1:A:255:ARG:HG2	1:A:450:ILE:HD13	2.02	0.41
1:A:610:LYS:NZ	1:A:623:GLN:HA	2.35	0.41
1:B:130:TYR:CD1	1:B:186:LYS:HG3	2.56	0.41
1:B:321:ILE:HD13	1:B:321:ILE:HA	1.92	0.41
1:A:579:MET:HE2	1:A:588:TYR:CE2	2.56	0.41
1:B:781:HIS:NE2	1:B:785:ILE:HD11	2.35	0.41
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.92	0.41
1:A:4:GLU:HG3	1:A:9:TRP:NE1	2.36	0.40
1:A:173:THR:HG23	1:A:678:ARG:NH1	2.37	0.40
1:B:500:TYR:HE2	1:B:773:PHE:CD2	2.39	0.40
1:B:509:PHE:CZ	1:B:714:LYS:HE2	2.56	0.40
1:A:722:HIS:HB2	1:A:723:PRO:HD3	2.03	0.40
1:A:490:HIS:ND1	1:A:511:ASP:OD2	2.50	0.40
1:B:732:LEU:O	1:B:753:LYS:HE2	2.22	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:325:GLU:OE2	1:B:126:ARG:NE[2_655]	2.16	0.04

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	761/796 (96%)	751 (99%)	10 (1%)	0	100	100
1	B	757/796 (95%)	742 (98%)	14 (2%)	1 (0%)	48	64
All	All	1518/1592 (95%)	1493 (98%)	24 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	403	LYS

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	673/692 (97%)	673 (100%)	0	100	100
1	B	669/692 (97%)	666 (100%)	3 (0%)	84	92
All	All	1342/1384 (97%)	1339 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	406	THR
1	B	531	SER
1	B	626	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	220	GLN
1	A	491	HIS
1	A	561	ASN

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Mol	Chain	Res	Type
1	A	611	GLN
1	A	793	HIS
1	B	3	HIS
1	B	486	GLN
1	B	491	HIS
1	B	561	ASN
1	B	623	GLN
1	B	673	HIS
1	B	727	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	FMT	A	801	-	2,2,2	0.62	0	1,1,1	0.20	0
3	GOL	A	802	-	5,5,5	0.32	0	5,5,5	0.47	0
2	FMT	B	801	-	2,2,2	0.62	0	1,1,1	0.20	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	802	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	GOL	O1-C1-C2-C3
3	A	802	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	GOL	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	767/796 (96%)	0.41	39 (5%)	33 30	37, 56, 87, 142	0
1	B	763/796 (95%)	0.38	41 (5%)	31 28	38, 53, 97, 145	0
All	All	1530/1592 (96%)	0.39	80 (5%)	33 29	37, 54, 92, 145	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	SER	4.9
1	B	29	SER	4.4
1	B	402	VAL	4.0
1	B	408	TRP	3.7
1	B	1	MET	3.6
1	B	63	ASN	3.6
1	A	652	MET	3.5
1	A	635	ALA	3.5
1	B	632	ALA	3.5
1	B	791	HIS	3.5
1	B	366	PRO	3.4
1	A	196	ALA	3.3
1	B	367	ARG	3.2
1	B	260	ASP	3.2
1	B	652	MET	3.2
1	B	404	VAL	3.2
1	A	29	SER	3.2
1	A	636	LYS	3.1
1	A	1	MET	3.1
1	A	211	LYS	3.0
1	A	632	ALA	3.0
1	A	508	VAL	3.0
1	A	444	THR	3.0
1	A	54	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	631	ALA	2.9
1	A	369	GLU	2.9
1	B	57	ILE	2.8
1	B	792	HIS	2.8
1	B	20	LEU	2.8
1	B	636	LYS	2.8
1	A	3	HIS	2.8
1	B	409	VAL	2.7
1	B	50	THR	2.7
1	A	51	LYS	2.7
1	B	197	SER	2.7
1	A	403	LYS	2.6
1	A	447	GLN	2.6
1	A	24	SER	2.5
1	B	66	THR	2.5
1	A	366	PRO	2.5
1	B	633	ALA	2.5
1	A	210	LYS	2.5
1	A	506	GLN	2.5
1	B	3	HIS	2.4
1	B	26	PRO	2.4
1	B	628	GLN	2.4
1	B	635	ALA	2.4
1	B	62	GLY	2.4
1	A	235	ARG	2.4
1	A	601	LEU	2.4
1	B	30	LYS	2.4
1	B	507	TRP	2.4
1	A	39	GLU	2.3
1	A	212	VAL	2.3
1	B	626	THR	2.3
1	B	60	ALA	2.2
1	A	690	MET	2.2
1	B	69	LYS	2.2
1	A	367	ARG	2.2
1	B	16	ARG	2.2
1	B	425	MET	2.2
1	A	425	MET	2.2
1	B	54	GLN	2.2
1	B	444	THR	2.1
1	A	67	LEU	2.1
1	A	405	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	401	ARG	2.1
1	A	634	LYS	2.1
1	B	634	LYS	2.1
1	A	537	CYS	2.1
1	A	365	ARG	2.1
1	A	580	ARG	2.1
1	A	391	GLU	2.1
1	A	762	GLU	2.1
1	A	260	ASP	2.1
1	A	319	ASP	2.1
1	B	143	LYS	2.0
1	B	61	ARG	2.0
1	B	369	GLU	2.0
1	B	448	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 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(\AA^2)	Q<0.9
3	GOL	A	802	6/6	0.71	0.17	59,60,66,70	0
2	FMT	B	801	3/3	0.73	0.23	50,50,51,52	0
2	FMT	A	801	3/3	0.75	0.23	48,48,50,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.