



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 01:07 AM EDT

PDB ID : 3L9I
Title : Myosin VI nucleotide-free (mdinsert2) L310G mutant crystal structure
Authors : Pylypenko, O.; Song, L.; Sweeney, L.H.; Houdusse, A.
Deposited on : 2010-01-05
Resolution : 2.20 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 : 2.23.2
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) : 2.23.2

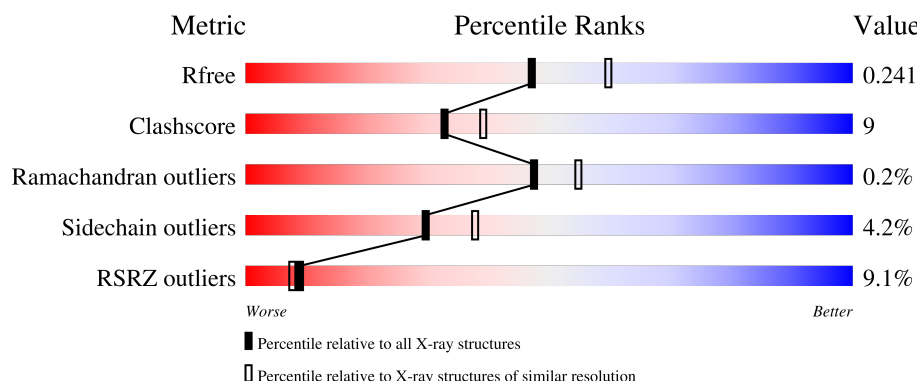
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


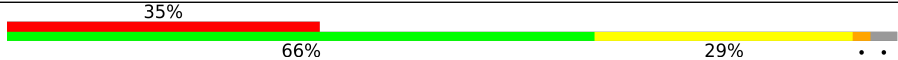
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	814	
2	C	149	

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	ACT	A	820	-	-	X	-
5	PO4	A	817	-	-	-	X
5	PO4	A	818	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8566 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-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	791	6546	4186	1127	1201	32	0	36	0

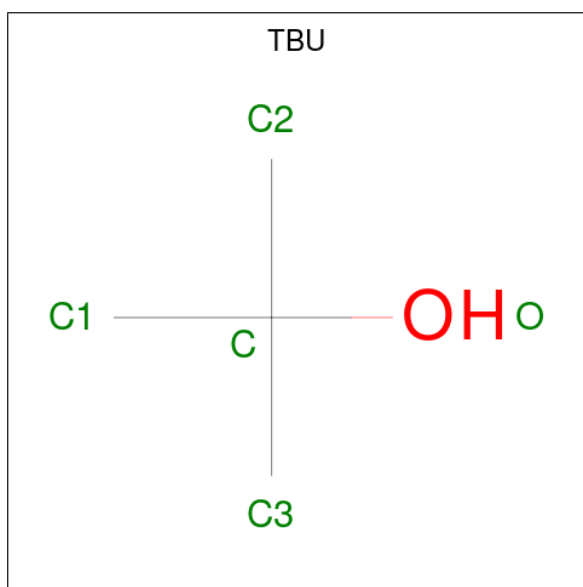
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	LEU	engineered mutation	UNP Q29122
A	?	-	LYS	SEE REMARK 999	UNP Q29122
A	547	VAL	GLY	SEE REMARK 999	UNP Q29122
A	572	ARG	ALA	SEE REMARK 999	UNP Q29122
A	573	ASP	TYR	SEE REMARK 999	UNP Q29122
A	714	LEU	VAL	SEE REMARK 999	UNP Q29122
A	721	TYR	SER	SEE REMARK 999	UNP Q29122
A	722	MET	LEU	SEE REMARK 999	UNP Q29122

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	145	1154	709	187	250	8	0	3	0

- Molecule 3 is TERTIARY-BUTYL ALCOHOL (three-letter code: TBU) (formula: C₄H₁₀O).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	Ca	0	0
			4	4		

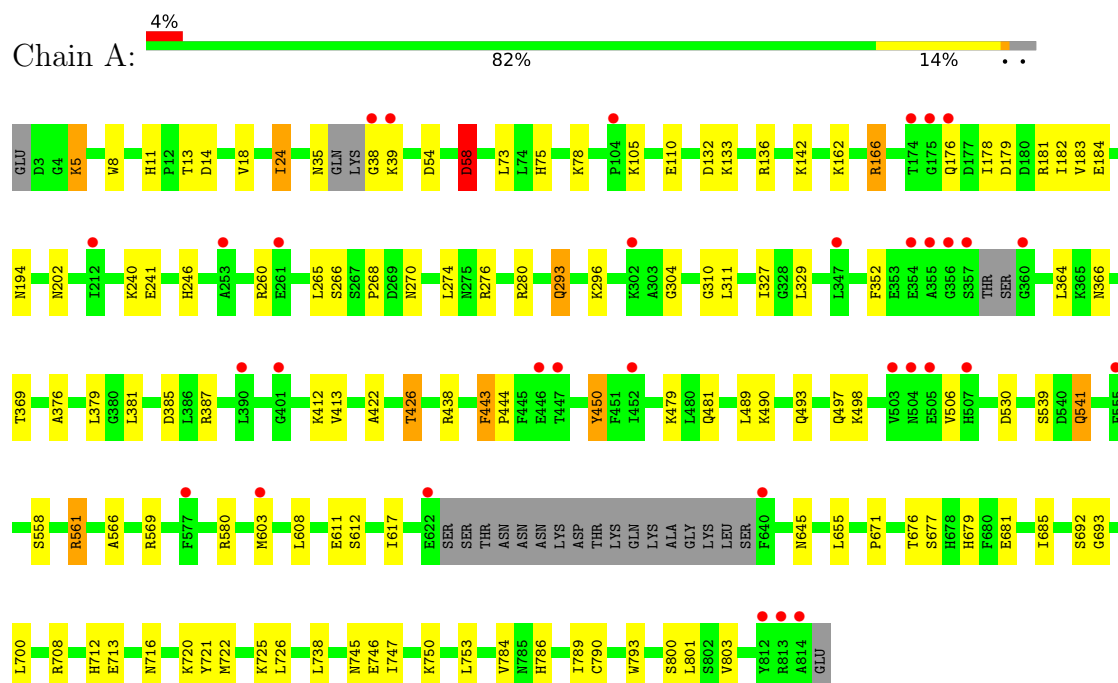
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	788	Total	O	0	0
			788	788		
7	C	41	Total	O	0	0
			41	41		

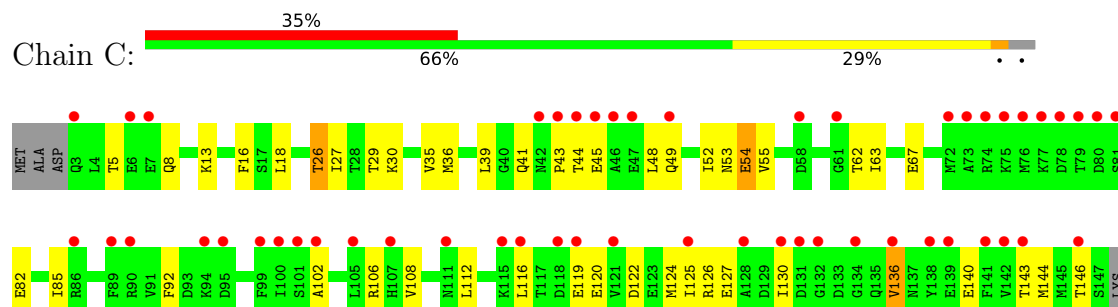
3 Residue-property plots [i](#)

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-VI



• 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	68.54Å 104.40Å 90.33Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	19.97 – 2.20 19.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-2.20) 99.6 (19.97-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.185 , 0.235 0.190 , 0.241	Depositor DCC
R_{free} test set	3209 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8566	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TBU, ACT, PO4, 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	0.70	0/6787	0.72	2/9134 (0.0%)
2	C	0.54	0/1175	0.64	0/1578
All	All	0.68	0/7962	0.71	2/10712 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	54	ASP	CB-CG-OD2	5.95	123.66	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6546	0	6627	101	0
2	C	1154	0	1086	43	0
3	A	5	0	10	0	0
4	A	8	0	6	3	0
5	A	20	0	0	0	0
6	C	4	0	0	0	0
7	A	788	0	0	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	41	0	0	1	0
All	All	8566	0	7729	134	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 9.

All (134) 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:493[B]:GLN:HE21	1:A:493[B]:GLN:HA	0.97	1.13
1:A:493[B]:GLN:HA	1:A:493[B]:GLN:NE2	1.81	0.95
1:A:493[B]:GLN:HE21	1:A:493[B]:GLN:CA	1.81	0.92
2:C:52:ILE:HG23	2:C:63:ILE:HD11	1.49	0.92
1:A:24:ILE:HD12	1:A:24:ILE:O	1.76	0.86
1:A:202:ASN:HD22	1:A:246:HIS:HE1	1.30	0.79
2:C:39:LEU:HD11	2:C:112:LEU:HD21	1.64	0.78
1:A:789:ILE:HD13	2:C:127:GLU:HG3	1.66	0.78
1:A:422:ALA:O	1:A:426[B]:THR:HG23	1.87	0.74
2:C:26:THR:HG23	2:C:62:THR:HB	1.69	0.74
1:A:329:LEU:HD11	1:A:438:ARG:HG2	1.71	0.73
1:A:801:LEU:HD12	1:A:801:LEU:O	1.90	0.71
1:A:692[B]:SER:OG	7:A:1121:HOH:O	2.09	0.71
1:A:789:ILE:HG21	2:C:127:GLU:HG3	1.74	0.69
1:A:24:ILE:HD12	1:A:24:ILE:C	2.12	0.69
2:C:5:THR:HG22	2:C:8:GLN:OE1	1.93	0.69
1:A:722:MET:HE3	1:A:726:LEU:HD22	1.75	0.67
1:A:202:ASN:ND2	1:A:246:HIS:HE1	1.92	0.67
1:A:5:LYS:HB3	1:A:5:LYS:NZ	2.10	0.67
1:A:722:MET:HE3	1:A:726:LEU:CD2	2.25	0.66
2:C:36:MET:HE3	2:C:43:PRO:HG3	1.78	0.66
1:A:376:ALA:HB1	1:A:381:LEU:O	1.97	0.65
2:C:36:MET:HE3	2:C:48:LEU:HD21	1.76	0.65
1:A:489:LEU:HD11	1:A:506:VAL:HG13	1.78	0.64
2:C:92:PHE:CD1	2:C:108:VAL:HG21	2.32	0.64
1:A:789:ILE:HD13	2:C:127:GLU:CG	2.31	0.61
1:A:176:GLN:HE21	1:A:181[A]:ARG:HH22	1.47	0.60
2:C:29:THR:HG21	2:C:49[A]:GLN:HE21	1.66	0.60
1:A:352:PHE:HB2	1:A:413:VAL:HG13	1.83	0.59
1:A:132:ASP:OD1	1:A:136:ARG:NH1	2.34	0.59
1:A:558:SER:OG	1:A:580:ARG:NH1	2.36	0.59
1:A:75:HIS:ND1	7:A:1431:HOH:O	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HG22	1:A:182:ILE:HD12	1.84	0.57
1:A:790:CYS:HB3	2:C:144:MET:HE1	1.87	0.57
2:C:54:GLU:CD	2:C:55:VAL:HG13	2.26	0.56
2:C:52:ILE:HG23	2:C:63:ILE:CD1	2.31	0.56
1:A:270:ASN:ND2	7:A:1556:HOH:O	2.38	0.55
1:A:24:ILE:C	1:A:24:ILE:CD1	2.75	0.55
2:C:36:MET:CE	2:C:48:LEU:HD21	2.37	0.55
1:A:18[A]:VAL:HG22	7:A:970:HOH:O	2.07	0.55
1:A:364:LEU:HD22	1:A:387:ARG:HG3	1.89	0.54
1:A:366:ASN:O	1:A:369:THR:OG1	2.20	0.54
1:A:530:ASP:OD1	1:A:645:ASN:ND2	2.41	0.54
1:A:722:MET:HE1	1:A:738:LEU:HD13	1.89	0.54
1:A:541:GLN:HE21	1:A:541:GLN:H	1.55	0.53
1:A:310:GLY:O	1:A:311:LEU:HD23	2.09	0.53
1:A:479:LYS:HB3	1:A:655[B]:LEU:HD21	1.90	0.53
1:A:8:TRP:CZ3	1:A:18[A]:VAL:HG13	2.44	0.52
1:A:722:MET:CE	1:A:726:LEU:CD2	2.86	0.52
2:C:39:LEU:HD11	2:C:112:LEU:CD2	2.35	0.52
1:A:481:GLN:HE22	1:A:693:GLY:HA3	1.75	0.52
1:A:329:LEU:HD11	1:A:438:ARG:CG	2.40	0.52
1:A:11:HIS:HD2	1:A:13:THR:H	1.58	0.51
1:A:720:LYS:HE3	1:A:721:TYR:CZ	2.45	0.51
1:A:789:ILE:HG23	2:C:124:MET:HG2	1.93	0.51
1:A:385:ASP:HB3	1:A:608:LEU:HD11	1.93	0.50
1:A:561:ARG:NH2	7:A:1599:HOH:O	2.44	0.50
1:A:38:GLY:N	7:A:1586:HOH:O	2.44	0.50
1:A:240:LYS:NZ	1:A:241[B]:GLU:OE2	2.43	0.50
1:A:5:LYS:HB3	1:A:5:LYS:HZ2	1.76	0.49
1:A:379:LEU:O	1:A:612:SER:OG	2.24	0.49
1:A:364:LEU:HD13	1:A:387:ARG:CG	2.42	0.49
2:C:63:ILE:HA	2:C:67:GLU:OE1	2.12	0.49
1:A:260:ARG:HG2	1:A:265:LEU:HB2	1.95	0.49
1:A:671:PRO:HA	1:A:685:ILE:HD11	1.95	0.49
1:A:481:GLN:NE2	1:A:693:GLY:HA3	2.28	0.49
1:A:712:HIS:CE1	1:A:716:ASN:HD21	2.31	0.49
2:C:82:GLU:HG3	2:C:85:ILE:HD12	1.94	0.49
1:A:379:LEU:HA	1:A:617:ILE:CD1	2.43	0.48
1:A:498[A]:LYS:HE3	1:A:498[A]:LYS:HB2	1.48	0.48
2:C:144:MET:HA	2:C:144:MET:HE2	1.95	0.48
1:A:489:LEU:HD11	1:A:506:VAL:CG1	2.43	0.48
2:C:16:PHE:CD2	2:C:27:ILE:HD11	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASN:ND2	1:A:246:HIS:CE1	2.79	0.48
1:A:183:VAL:HG22	4:A:820:ACT:H2	1.95	0.47
1:A:443:PHE:N	1:A:444:PRO:CD	2.77	0.47
1:A:133[B]:LYS:NZ	7:A:1313:HOH:O	2.42	0.46
1:A:110:GLU:HB2	7:A:1270:HOH:O	2.14	0.46
1:A:700:LEU:C	1:A:700:LEU:HD23	2.36	0.46
1:A:268:PRO:HB3	1:A:274:LEU:HD13	1.98	0.46
1:A:490:LYS:NZ	7:A:1323:HOH:O	2.45	0.46
2:C:49[B]:GLN:HE21	2:C:53:ASN:HD21	1.63	0.45
2:C:63:ILE:HD13	2:C:63:ILE:N	2.32	0.45
2:C:26:THR:HG22	7:C:620:HOH:O	2.15	0.45
1:A:179:ASP:O	1:A:183:VAL:HG23	2.16	0.45
1:A:676:THR:HG22	1:A:677:SER:O	2.17	0.45
1:A:162[B]:LYS:CG	4:A:820:ACT:H1	2.47	0.44
1:A:280:ARG:HD2	1:A:304:GLY:O	2.17	0.44
1:A:364:LEU:HD13	1:A:387:ARG:HG3	1.99	0.44
1:A:790:CYS:O	1:A:793:TRP:HB2	2.18	0.44
1:A:800:SER:HA	2:C:39:LEU:HD23	2.00	0.44
1:A:746:GLU:O	1:A:750:LYS:NZ	2.41	0.44
1:A:142[A]:LYS:HD2	1:A:450:TYR:OH	2.18	0.44
2:C:35:VAL:O	2:C:39:LEU:HD13	2.18	0.43
1:A:162[B]:LYS:HG3	4:A:820:ACT:H1	1.99	0.43
1:A:293[B]:GLN:HE21	1:A:293[B]:GLN:HB3	1.55	0.43
1:A:11:HIS:CD2	1:A:14:ASP:H	2.35	0.43
2:C:130:ILE:HD12	2:C:140:GLU:HG2	2.00	0.43
1:A:202:ASN:HB2	1:A:311:LEU:HD11	1.99	0.43
1:A:479:LYS:HE2	1:A:655[B]:LEU:CD2	2.48	0.43
1:A:58:ASP:OD1	1:A:58:ASP:C	2.57	0.42
1:A:184:GLU:HG3	7:A:883:HOH:O	2.19	0.42
2:C:144:MET:HE2	2:C:144:MET:CA	2.48	0.42
1:A:78:LYS:NZ	7:A:1561:HOH:O	2.49	0.42
1:A:493[B]:GLN:OE1	1:A:506:VAL:HG12	2.20	0.42
2:C:102:ALA:O	2:C:106:ARG:CB	2.67	0.42
1:A:5:LYS:HB3	1:A:5:LYS:HZ3	1.85	0.42
1:A:293[A]:GLN:HE22	1:A:296:LYS:NZ	2.18	0.42
2:C:36:MET:HB2	2:C:36:MET:HE2	1.91	0.42
1:A:11:HIS:CD2	1:A:13:THR:H	2.36	0.42
1:A:789:ILE:HG21	2:C:127:GLU:CG	2.47	0.42
1:A:803:VAL:HG21	2:C:39:LEU:HD22	2.01	0.41
2:C:122:ASP:HA	2:C:125:ILE:HD12	2.02	0.41
2:C:122:ASP:O	2:C:126[A]:ARG:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:HIS:NE2	1:A:681:GLU:OE2	2.51	0.41
1:A:412:LYS:NZ	7:A:1593:HOH:O	2.51	0.41
2:C:63:ILE:HG23	2:C:67:GLU:HB2	2.02	0.41
1:A:364:LEU:HD13	1:A:387:ARG:HG2	2.03	0.41
1:A:566:ALA:HB1	1:A:569[A]:ARG:HH12	1.85	0.41
1:A:722:MET:HE2	1:A:726:LEU:HD23	2.01	0.41
1:A:786:HIS:ND1	2:C:127:GLU:OE1	2.53	0.41
1:A:11:HIS:HD2	1:A:14:ASP:H	1.67	0.41
1:A:713[B]:GLU:CD	7:A:1137:HOH:O	2.58	0.41
1:A:166:ARG:HD3	1:A:179:ASP:OD2	2.21	0.41
1:A:566:ALA:O	1:A:569[A]:ARG:NH1	2.54	0.41
2:C:112:LEU:HA	2:C:112:LEU:HD23	1.84	0.41
1:A:745:ASN:HD21	1:A:747:ILE:HB	1.85	0.41
2:C:13:LYS:O	2:C:16:PHE:HB3	2.21	0.41
2:C:30[B]:LYS:HA	2:C:30[B]:LYS:HD2	1.89	0.41
2:C:18:LEU:HD12	2:C:18:LEU:HA	1.93	0.40
2:C:62:THR:C	2:C:63:ILE:HD13	2.42	0.40
1:A:793:TRP:HH2	2:C:136:VAL:HG21	1.87	0.40
2:C:16:PHE:CE2	2:C:27:ILE:CD1	3.05	0.40

There are no symmetry-related clashes.

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	820/814 (101%)	797 (97%)	22 (3%)	1 (0%)	51	60
2	C	146/149 (98%)	136 (93%)	9 (6%)	1 (1%)	22	22
All	All	966/963 (100%)	933 (97%)	31 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
2	C	45	GLU

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	732/720 (102%)	705 (96%)	27 (4%)	34	43
2	C	126/128 (98%)	116 (92%)	10 (8%)	12	12
All	All	858/848 (101%)	821 (96%)	37 (4%)	30	36

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	24	ILE
1	A	35	ASN
1	A	39	LYS
1	A	58	ASP
1	A	166	ARG
1	A	194	ASN
1	A	266	SER
1	A	276	ARG
1	A	293[A]	GLN
1	A	293[B]	GLN
1	A	327	ILE
1	A	426[A]	THR
1	A	426[B]	THR
1	A	443	PHE
1	A	450	TYR
1	A	497	GLN
1	A	539	SER
1	A	541	GLN
1	A	561	ARG
1	A	603[A]	MET
1	A	603[B]	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	611	GLU
1	A	708	ARG
1	A	725	LYS
1	A	753	LEU
1	A	784	VAL
2	C	26	THR
2	C	41	GLN
2	C	44	THR
2	C	54	GLU
2	C	116	LEU
2	C	119	GLU
2	C	120	GLU
2	C	136	VAL
2	C	143	THR
2	C	146	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	47	GLN
1	A	176	GLN
1	A	194	ASN
1	A	202	ASN
1	A	246	HIS
1	A	290	GLN
1	A	383	GLN
1	A	417	ASN
1	A	418	ASN
1	A	465	HIS
1	A	481	GLN
1	A	485	ASN
1	A	533	ASN
1	A	541	GLN
1	A	678	HIS
1	A	716	ASN
1	A	745	ASN
2	C	53	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
5	PO4	A	818	-	4,4,4	0.94	0	6,6,6	0.46	0
5	PO4	A	819	-	4,4,4	0.75	0	6,6,6	0.51	0
5	PO4	A	816	-	4,4,4	0.83	0	6,6,6	0.53	0
4	ACT	A	1	-	1,3,3	0.32	0	0,3,3	-	-
3	TBU	A	7134	-	4,4,4	0.42	0	6,6,6	1.10	1 (16%)
4	ACT	A	820	-	1,3,3	0.88	0	0,3,3	-	-
5	PO4	A	817	-	4,4,4	0.85	0	6,6,6	0.72	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7134	TBU	O-C-C3	2.05	113.36	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	820	ACT	3	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	791/814 (97%)	-0.02	33 (4%) 36 34	30, 45, 67, 98	0
2	C	145/149 (97%)	1.57	52 (35%) 0 0	46, 80, 95, 102	0
All	All	936/963 (97%)	0.23	85 (9%) 9 8	30, 47, 86, 102	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	812	TYR	7.7
2	C	130	ILE	5.9
2	C	78	ASP	5.8
1	A	357	SER	5.8
1	A	814	ALA	5.3
1	A	360	GLY	5.2
2	C	139	GLU	5.1
2	C	76	MET	5.1
2	C	75	LYS	5.1
2	C	79	THR	5.0
2	C	94	LYS	4.9
1	A	503	VAL	4.9
2	C	73	ALA	4.7
1	A	175	GLY	4.5
2	C	105	LEU	4.5
1	A	38	GLY	4.3
1	A	356	GLY	4.3
2	C	134	GLY	4.3
2	C	131	ASP	4.2
2	C	138	TYR	4.2
1	A	813	ARG	4.2
2	C	99	PHE	4.1
2	C	100	ILE	3.9
2	C	3	GLN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	81	SER	3.8
2	C	58	ASP	3.7
2	C	80	ASP	3.7
2	C	146	THR	3.7
2	C	95	ASP	3.6
2	C	77	LYS	3.5
1	A	104	PRO	3.4
1	A	640	PHE	3.3
1	A	505	GLU	3.3
2	C	143	THR	3.3
1	A	446[A]	GLU	3.3
1	A	174	THR	3.2
2	C	45	GLU	3.2
2	C	101	SER	3.2
1	A	39	LYS	3.2
2	C	74	ARG	3.1
2	C	141	PHE	3.1
2	C	132	GLY	3.1
2	C	6	GLU	3.0
2	C	116	LEU	2.8
2	C	118	ASP	2.8
2	C	136	VAL	2.8
1	A	447	THR	2.8
2	C	128	ALA	2.6
1	A	354	GLU	2.6
2	C	107	HIS	2.6
1	A	555	PHE	2.6
2	C	142	VAL	2.5
1	A	507[A]	HIS	2.5
2	C	7	GLU	2.5
2	C	46	ALA	2.5
1	A	253	ALA	2.5
1	A	176	GLN	2.5
1	A	390	LEU	2.5
2	C	49[A]	GLN	2.4
2	C	121	VAL	2.4
1	A	452	ILE	2.4
2	C	102	ALA	2.4
2	C	125	ILE	2.3
1	A	401	GLY	2.3
2	C	89	PHE	2.3
1	A	504	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	2.3
2	C	111	ASN	2.3
2	C	72	MET	2.2
1	A	302	LYS	2.2
2	C	47	GLU	2.2
2	C	90	ARG	2.2
1	A	622	GLU	2.2
2	C	115	LYS	2.2
2	C	43	PRO	2.2
2	C	44	THR	2.2
1	A	577	PHE	2.1
1	A	261	GLU	2.1
1	A	212	ILE	2.1
2	C	119	GLU	2.1
2	C	61	GLY	2.1
1	A	347	LEU	2.1
1	A	603[A]	MET	2.1
2	C	42	ASN	2.0
2	C	86	ARG	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, 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
6	CA	C	1150	1/1	0.60	0.19	86,86,86,86	0
5	PO4	A	817	5/5	0.79	0.58	91,92,93,93	0
5	PO4	A	818	5/5	0.80	0.56	94,95,95,96	0
5	PO4	A	819	5/5	0.87	0.76	88,89,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ACT	A	1	4/4	0.89	0.24	51,52,53,53	0
4	ACT	A	820	4/4	0.92	0.30	67,67,67,67	0
5	PO4	A	816	5/5	0.92	0.43	82,82,83,84	0
6	CA	C	1151	1/1	0.93	0.15	88,88,88,88	0
6	CA	C	1149	1/1	0.94	0.05	70,70,70,70	0
3	TBU	A	7134	5/5	0.95	0.15	48,48,49,49	0
6	CA	C	1148	1/1	0.96	0.03	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.