



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2017 – 07:41 AM EDT

PDB ID : 5JST
Title : MBP fused MDV1 coiled coil
Authors : Kim, B.-W.; Song, H.K.
Deposited on : 2016-05-09
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

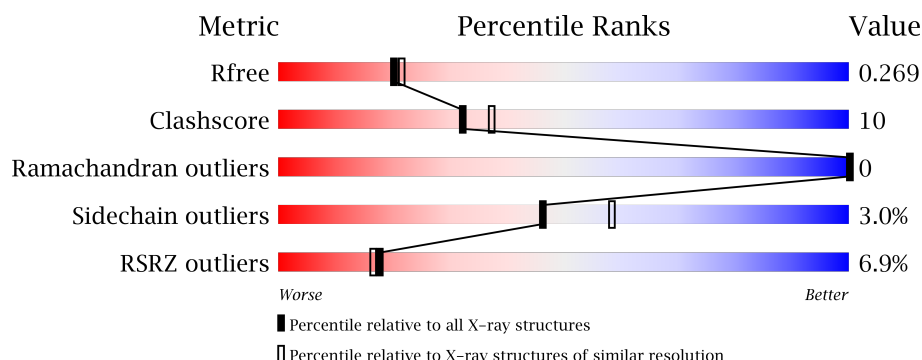
1 Overall quality at a glance

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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	443	<div> <div>3%</div> <div>82%</div> <div>14%</div> <div>••</div> </div>
1	B	443	<div> <div>10%</div> <div>74%</div> <div>23%</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	ACT	A	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6836 atoms, of which 14 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.

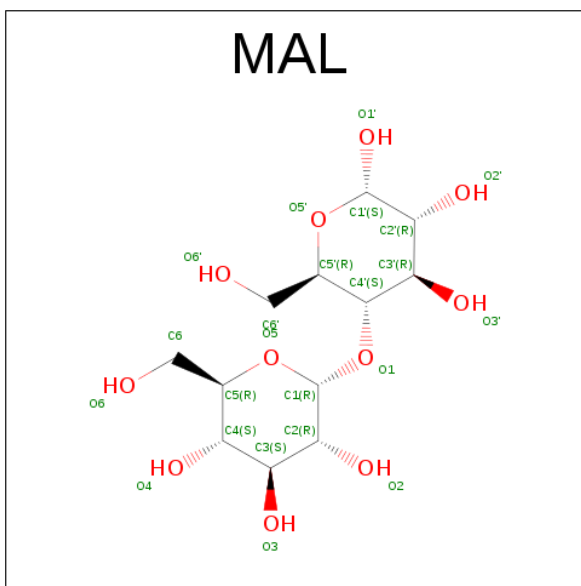
- Molecule 1 is a protein called Maltose-binding periplasmic protein, Mitochondrial division protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3250	2084	534	626	6			
1	B	432	Total	C	N	O	S	0	0	0
			3279	2100	540	633	6			

There are 24 discrepancies between the modelled and reference sequences:

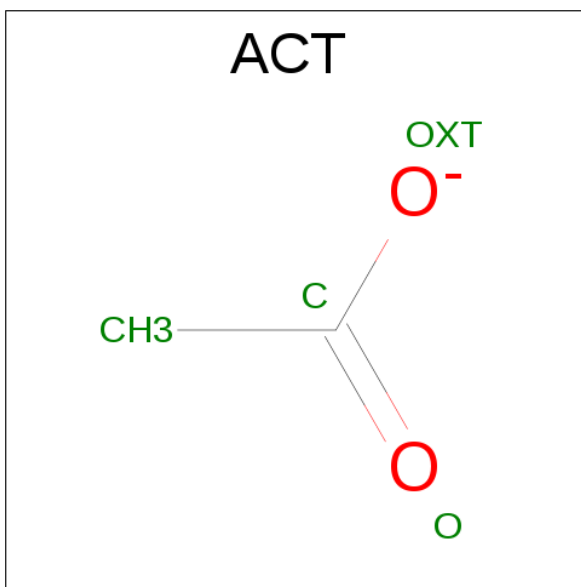
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0AEX9
A	82	ALA	ASP	engineered mutation	UNP P0AEX9
A	83	ALA	LYS	engineered mutation	UNP P0AEX9
A	239	ALA	LYS	engineered mutation	UNP P0AEX9
A	359	ALA	GLU	engineered mutation	UNP P0AEX9
A	362	ALA	LYS	engineered mutation	UNP P0AEX9
A	363	ALA	ASP	engineered mutation	UNP P0AEX9
A	367	ASN	-	linker	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	GLY	-	linker	UNP P0AEX9
B	0	MET	-	initiating methionine	UNP P0AEX9
B	82	ALA	ASP	engineered mutation	UNP P0AEX9
B	83	ALA	LYS	engineered mutation	UNP P0AEX9
B	239	ALA	LYS	engineered mutation	UNP P0AEX9
B	359	ALA	GLU	engineered mutation	UNP P0AEX9
B	362	ALA	LYS	engineered mutation	UNP P0AEX9
B	363	ALA	ASP	engineered mutation	UNP P0AEX9
B	367	ASN	-	linker	UNP P0AEX9
B	368	ALA	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	371	GLY	-	linker	UNP P0AEX9

- Molecule 2 is MALTOSE (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



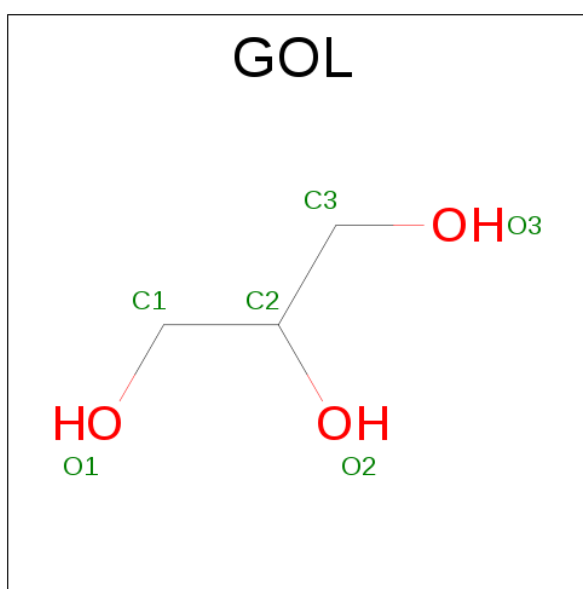
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C H O 7 2 3 2	0	0
3	A	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

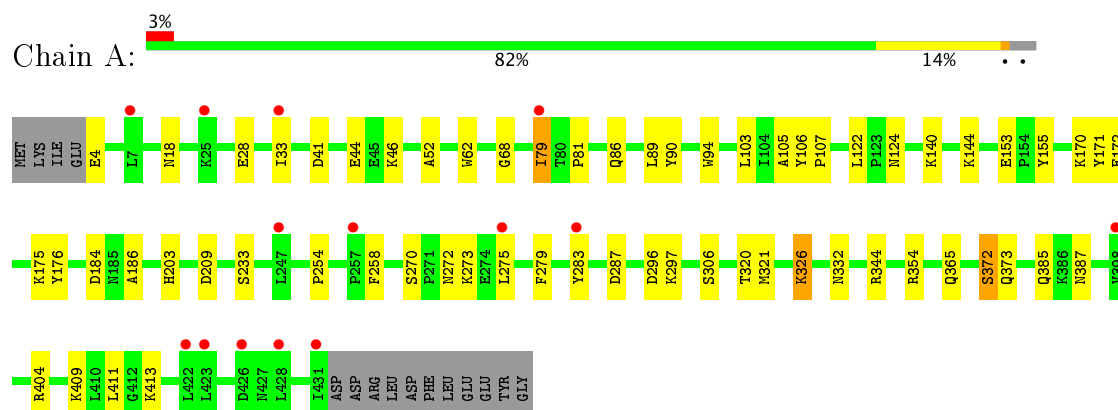
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	137	Total O 137 137	0	0
5	B	84	Total O 84 84	0	0

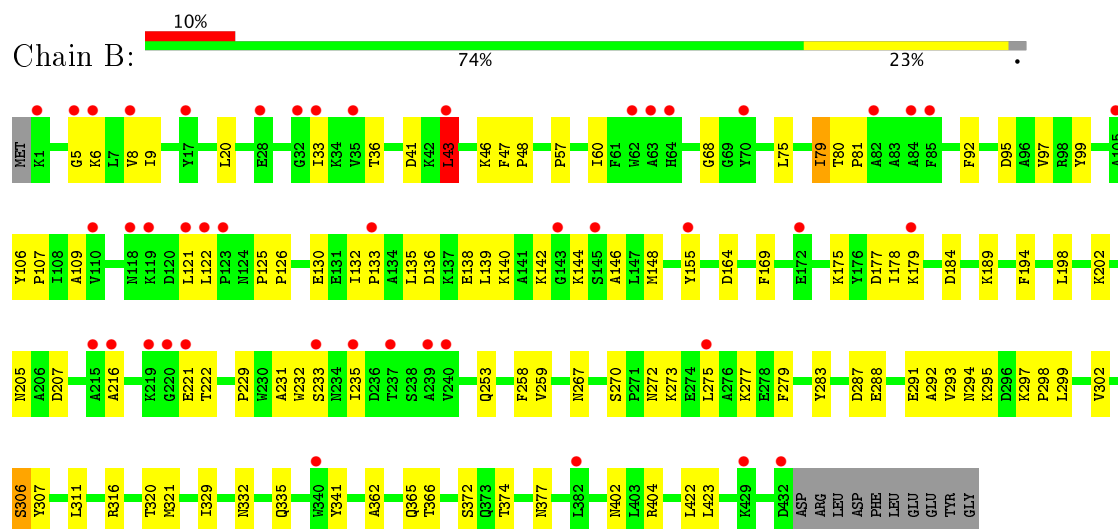
3 Residue-property plots

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: Maltose-binding periplasmic protein,Mitochondrial division protein 1



- Molecule 1: Maltose-binding periplasmic protein,Mitochondrial division protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.51Å 102.94Å 79.27Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	36.85 – 2.20 36.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.85-2.20) 93.2 (36.85-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.274 0.220 , 0.269	Depositor DCC
R_{free} test set	1886 reflections (3.95%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.014 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6836	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 4.40% 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: GOL, MAL, ACT

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	0.40	0/3320	0.53	0/4519
1	B	0.35	0/3349	0.51	1/4560 (0.0%)
All	All	0.38	0/6669	0.52	1/9079 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	LEU	CA-CB-CG	5.28	127.44	115.30

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	3250	0	3182	58	0
1	B	3279	0	3201	72	0
2	A	23	0	22	7	0
2	B	23	0	22	2	0
3	A	16	6	12	2	0
3	B	4	0	3	0	0
4	A	6	8	8	0	0
5	A	137	0	0	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	84	0	0	6	1
All	All	6822	14	6450	131	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 10.

All (131) 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:79:ILE:HG23	1:A:81:PRO:HD3	1.35	1.03
1:A:175:LYS:HD2	1:A:176:TYR:H	1.25	1.01
1:B:404:ARG:NH1	5:B:602:HOH:O	2.07	0.86
1:A:79:ILE:HD11	1:A:106:TYR:CD1	2.11	0.85
1:B:79:ILE:HG23	1:B:81:PRO:HD3	1.60	0.83
1:B:140:LYS:NZ	1:B:202:LYS:O	2.13	0.81
1:B:402:ASN:OD1	5:B:601:HOH:O	1.99	0.81
1:A:33:ILE:HD13	1:A:275:LEU:HD13	1.63	0.80
1:A:79:ILE:HG22	1:A:103:LEU:HB2	1.63	0.80
1:A:86:GLN:NE2	5:A:605:HOH:O	2.14	0.80
1:B:92:PHE:HA	1:B:95:ASP:OD2	1.84	0.78
1:B:164:ASP:OD1	1:B:253:GLN:NE2	2.16	0.78
1:A:413:LYS:NZ	5:A:607:HOH:O	2.19	0.75
1:A:411:LEU:O	5:A:601:HOH:O	2.03	0.74
1:A:79:ILE:HD11	1:A:106:TYR:CG	2.22	0.74
1:A:155:TYR:HB2	2:A:501:MAL:C6'	2.19	0.73
1:A:175:LYS:HD2	1:A:176:TYR:N	2.02	0.69
1:A:270:SER:O	1:A:273:LYS:NZ	2.26	0.69
1:A:203:HIS:NE2	5:A:609:HOH:O	2.26	0.68
1:A:155:TYR:HB2	2:A:501:MAL:H6'2	1.75	0.67
2:A:501:MAL:O3	5:A:603:HOH:O	2.12	0.66
1:A:287:ASP:OD1	1:A:306:SER:OG	2.14	0.65
1:A:79:ILE:HD11	1:A:106:TYR:CE1	2.31	0.65
1:A:44:GLU:OE2	5:A:604:HOH:O	2.13	0.64
1:A:372:SER:N	5:A:612:HOH:O	2.30	0.64
1:B:79:ILE:HG13	1:B:106:TYR:CE1	2.34	0.63
1:A:153:GLU:OE1	1:A:344:ARG:NH1	2.32	0.61
1:B:335:GLN:HA	1:B:374:THR:HG21	1.82	0.60
1:B:292:ALA:HA	1:B:295:LYS:NZ	2.16	0.60
1:A:175:LYS:CD	1:A:176:TYR:H	2.07	0.60
1:B:287:ASP:OD1	1:B:306:SER:OG	2.19	0.59
1:A:41:ASP:O	1:A:46:LYS:HE2	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TYR:HB2	2:A:501:MAL:H5'	1.85	0.58
1:A:89:LEU:HD22	1:A:94:TRP:CZ2	2.37	0.58
1:B:99:TYR:OH	5:B:603:HOH:O	2.15	0.58
1:B:5:GLY:O	1:B:33:ILE:HG23	2.02	0.58
1:B:307:TYR:CE2	1:B:311:LEU:HD11	2.39	0.57
1:B:140:LYS:HA	1:B:144:LYS:O	2.04	0.57
1:B:148:MET:SD	1:B:222:THR:HG21	2.44	0.57
1:B:80:THR:O	1:B:277:LYS:NZ	2.30	0.57
1:B:341:TYR:OH	5:B:604:HOH:O	2.17	0.57
1:B:8:VAL:HG12	1:B:36:THR:HB	1.86	0.56
1:A:186:ALA:H	3:A:503:ACT:H2	1.69	0.56
1:A:89:LEU:HD23	1:A:107:PRO:HG2	1.88	0.56
1:B:6:LYS:O	1:B:272:ASN:ND2	2.39	0.56
1:A:4:GLU:N	1:A:272:ASN:HD21	2.04	0.55
1:B:109:ALA:HA	1:B:302:VAL:HA	1.88	0.55
1:B:47:PHE:HB2	1:B:60:ILE:HD12	1.88	0.55
1:B:177:ASP:OD1	1:B:179:LYS:HG2	2.06	0.55
1:A:68:GLY:HA3	1:A:332:ASN:O	2.06	0.55
1:A:155:TYR:HB2	2:A:501:MAL:C5'	2.37	0.54
1:B:33:ILE:HD13	1:B:275:LEU:HD13	1.90	0.54
1:B:122:LEU:HD21	1:B:126:PRO:HD3	1.91	0.53
1:B:92:PHE:HB2	5:B:657:HOH:O	2.09	0.53
1:A:254:PRO:HB3	1:A:326:LYS:HD3	1.90	0.52
1:A:86:GLN:CD	5:A:605:HOH:O	2.42	0.52
1:A:4:GLU:N	1:A:4:GLU:OE1	2.42	0.52
1:A:33:ILE:HD13	1:A:275:LEU:CD1	2.37	0.52
1:B:279:PHE:O	1:B:283:TYR:HB2	2.10	0.52
1:A:18:ASN:HB2	1:A:296:ASP:OD2	2.10	0.52
1:B:270:SER:O	1:B:273:LYS:NZ	2.44	0.51
1:B:205:ASN:OD1	1:B:207:ASP:HB2	2.10	0.51
1:B:216:ALA:HB1	1:B:222:THR:HG23	1.93	0.51
1:B:68:GLY:HA3	1:B:332:ASN:O	2.10	0.51
1:A:387:ASN:ND2	5:A:606:HOH:O	2.18	0.51
2:B:501:MAL:O2'	5:B:605:HOH:O	2.18	0.50
1:A:33:ILE:CD1	1:A:275:LEU:HD22	2.42	0.49
1:A:52:ALA:O	1:A:385:GLN:HG3	2.11	0.49
1:B:320:THR:HG22	1:B:321:MET:CE	2.43	0.49
1:B:155:TYR:HB2	2:B:501:MAL:H62	1.95	0.49
1:B:216:ALA:HB1	1:B:222:THR:CG2	2.43	0.48
1:A:140:LYS:HD3	1:A:144:LYS:O	2.13	0.48
1:A:79:ILE:HD11	1:A:106:TYR:CD2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLU:OE1	1:B:288:GLU:N	2.30	0.47
1:A:90:TYR:CE1	5:A:608:HOH:O	2.56	0.47
1:B:142:LYS:HG2	1:B:142:LYS:O	2.14	0.47
1:A:90:TYR:OH	5:A:608:HOH:O	2.21	0.46
1:B:41:ASP:O	1:B:46:LYS:HE2	2.16	0.46
1:B:320:THR:HG22	1:B:321:MET:HE2	1.97	0.46
1:B:292:ALA:HA	1:B:295:LYS:HZ3	1.81	0.46
1:B:292:ALA:HA	1:B:295:LYS:HZ2	1.81	0.46
1:A:155:TYR:CB	2:A:501:MAL:H6'2	2.43	0.45
1:B:135:LEU:O	1:B:139:LEU:HG	2.15	0.45
1:A:90:TYR:HE1	5:A:608:HOH:O	1.98	0.45
1:B:122:LEU:HD13	1:B:135:LEU:HD11	1.98	0.45
1:B:291:GLU:O	1:B:295:LYS:HG2	2.16	0.45
1:A:184:ASP:HB2	1:A:365:GLN:OE1	2.17	0.45
1:B:135:LEU:HG	1:B:139:LEU:CD1	2.47	0.45
1:B:130:GLU:N	1:B:130:GLU:OE1	2.44	0.45
1:A:79:ILE:HG22	1:A:103:LEU:CB	2.42	0.45
1:A:171:TYR:O	1:A:172:GLU:HG3	2.18	0.44
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.53	0.44
1:A:62:TRP:HE1	2:A:501:MAL:H2'	1.83	0.44
1:B:8:VAL:HG23	1:B:57:PRO:HA	1.99	0.44
1:A:79:ILE:HD12	1:A:105:ALA:C	2.37	0.44
1:A:413:LYS:HB3	1:A:413:LYS:HE2	1.71	0.44
1:A:186:ALA:N	3:A:503:ACT:H2	2.32	0.43
1:B:43:LEU:HD23	1:B:43:LEU:C	2.38	0.43
1:B:144:LYS:HD2	1:B:221:GLU:HA	2.00	0.43
1:B:169:PHE:CD1	1:B:178:ILE:HA	2.53	0.43
1:A:320:THR:HG22	1:A:321:MET:HE2	2.00	0.43
1:A:321:MET:CE	1:A:321:MET:HA	2.49	0.43
1:B:132:ILE:N	1:B:133:PRO:CD	2.81	0.43
1:A:209:ASP:HB2	5:A:693:HOH:O	2.18	0.43
1:B:121:LEU:CD2	1:B:142:LYS:HE3	2.48	0.43
1:B:184:ASP:HB2	1:B:365:GLN:OE1	2.19	0.43
1:B:231:ALA:O	1:B:235:ILE:HG13	2.19	0.43
1:B:177:ASP:OD1	1:B:179:LYS:CG	2.67	0.43
1:B:362:ALA:O	1:B:366:THR:HG23	2.19	0.42
1:B:233:SER:OG	1:B:298:PRO:HD3	2.19	0.42
1:B:259:VAL:HB	1:B:329:ILE:HA	2.02	0.42
1:B:9:ILE:HG21	1:B:20:LEU:HD21	2.01	0.42
1:B:233:SER:OG	1:B:297:LYS:HA	2.19	0.42
1:A:79:ILE:HD12	1:A:105:ALA:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:VAL:HG11	1:B:299:LEU:HD21	2.02	0.42
1:B:48:PRO:HA	1:B:75:LEU:HD13	2.01	0.41
1:B:232:TRP:CH2	1:B:316:ARG:HB3	2.55	0.41
1:B:122:LEU:HD21	1:B:125:PRO:HA	2.02	0.41
1:A:354:ARG:NH2	1:B:46:LYS:HD3	2.35	0.41
1:B:97:VAL:HG21	1:B:107:PRO:HD3	2.02	0.41
1:B:294:ASN:OD1	1:B:298:PRO:HA	2.19	0.41
1:A:233:SER:HB3	1:A:297:LYS:HD3	2.01	0.41
1:B:288:GLU:H	1:B:288:GLU:CD	2.17	0.41
1:A:279:PHE:O	1:A:283:TYR:HB2	2.20	0.41
1:A:28:GLU:HG3	1:A:33:ILE:O	2.21	0.41
1:B:184:ASP:HB2	1:B:365:GLN:CD	2.41	0.41
1:B:194:PHE:CE2	1:B:198:LEU:HD11	2.56	0.41
1:A:33:ILE:HD12	1:A:275:LEU:HD22	2.03	0.41
1:B:57:PRO:O	1:B:267:ASN:HB2	2.21	0.41
1:B:184:ASP:O	1:B:189:LYS:HE3	2.21	0.40
1:B:136:ASP:HA	1:B:146:ALA:HB2	2.03	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)
5:A:688:HOH:O	5:B:634:HOH:O[3_455]	2.05	0.15

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	426/443 (96%)	415 (97%)	11 (3%)	0	100	100
1	B	430/443 (97%)	418 (97%)	12 (3%)	0	100	100
All	All	856/886 (97%)	833 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	328/357 (92%)	318 (97%)	10 (3%)	46	58
1	B	330/357 (92%)	320 (97%)	10 (3%)	46	58
All	All	658/714 (92%)	638 (97%)	20 (3%)	46	58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	122	LEU
1	A	124	ASN
1	A	170	LYS
1	A	258	PHE
1	A	326	LYS
1	A	372	SER
1	A	373	GLN
1	A	404	ARG
1	A	409	LYS
1	B	43	LEU
1	B	79	ILE
1	B	138	GLU
1	B	175	LYS
1	B	258	PHE
1	B	306	SER
1	B	372	SER
1	B	377	ASN
1	B	422	LEU
1	B	423	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

8 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	MAL	A	501	-	24,24,24	0.79	0	35,35,35	2.15	13 (37%)
3	ACT	A	502	-	1,3,3	1.51	0	0,3,3	0.00	-
3	ACT	A	503	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
3	ACT	A	504	-	1,3,3	1.88	0	0,3,3	0.00	-
3	ACT	A	505	-	1,3,3	1.38	0	0,3,3	0.00	-
4	GOL	A	506	-	5,5,5	0.35	0	5,5,5	0.11	0
2	MAL	B	501	-	24,24,24	0.56	0	35,35,35	1.01	1 (2%)
3	ACT	B	502	-	1,3,3	1.81	0	0,3,3	0.00	-

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
2	MAL	A	501	-	-	0/8/48/48	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	A	502	-	-	0/0/0/0	0/0/0/0
3	ACT	A	503	-	-	0/0/0/0	0/0/0/0
3	ACT	A	504	-	-	0/0/0/0	0/0/0/0
3	ACT	A	505	-	-	0/0/0/0	0/0/0/0
4	GOL	A	506	-	-	0/4/4/4	0/0/0/0
2	MAL	B	501	-	-	0/8/48/48	0/2/2/2
3	ACT	B	502	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	ACT	CH3-C	2.26	1.51	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MAL	C2'-C3'-C4'	-4.78	99.70	109.61
2	A	501	MAL	C1-O1-C4'	-4.45	107.16	118.00
2	A	501	MAL	C3-C4-C5	-3.79	103.55	110.22
2	A	501	MAL	O5'-C5'-C4'	-3.61	102.36	109.75
2	A	501	MAL	C1'-C2'-C3'	-3.01	105.22	110.65
2	B	501	MAL	O6-C6-C5	-2.17	104.04	111.34
2	A	501	MAL	C1-O5-C5	2.03	117.55	113.72
2	A	501	MAL	C1-C2-C3	2.24	114.13	109.98
2	A	501	MAL	O1'-C1'-C2'	2.26	115.81	109.42
2	A	501	MAL	O1-C1-C2	2.81	114.45	108.11
2	A	501	MAL	O1-C4'-C3'	2.93	114.25	107.19
2	A	501	MAL	O1-C4'-C5'	2.95	116.59	109.34
2	A	501	MAL	O2'-C2'-C1'	3.06	116.11	109.75
2	A	501	MAL	O5-C1-C2	3.80	117.62	110.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MAL	7	0
3	A	503	ACT	2	0
2	B	501	MAL	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	428/443 (96%)	0.40	14 (3%) 47 44	35, 54, 84, 101	0
1	B	432/443 (97%)	0.75	45 (10%) 7 6	37, 63, 95, 117	0
All	All	860/886 (97%)	0.57	59 (6%) 18 16	35, 58, 92, 117	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	VAL	6.0
1	B	35	VAL	5.1
1	B	32	GLY	4.4
1	A	426	ASP	4.2
1	B	121	LEU	4.1
1	A	428	LEU	4.1
1	B	216	ALA	4.1
1	A	423	LEU	3.7
1	B	239	ALA	3.4
1	B	33	ILE	3.4
1	B	145	SER	3.4
1	B	235	ILE	3.4
1	A	283	TYR	3.3
1	B	5	GLY	3.2
1	B	123	PRO	3.2
1	B	6	LYS	3.2
1	B	17	TYR	3.2
1	A	33	ILE	3.2
1	B	275	LEU	3.0
1	B	432	ASP	3.0
1	B	122	LEU	3.0
1	B	429	LYS	2.9
1	B	143	GLY	2.9
1	B	179	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	219	LYS	2.8
1	B	220	GLY	2.7
1	B	63	ALA	2.7
1	A	247	LEU	2.7
1	B	340	TRP	2.7
1	A	422	LEU	2.6
1	B	70	TYR	2.5
1	B	62	TRP	2.5
1	B	172	GLU	2.5
1	B	84	ALA	2.3
1	B	215	ALA	2.3
1	A	25	LYS	2.2
1	B	8	VAL	2.2
1	B	43	LEU	2.2
1	B	237	THR	2.2
1	B	119	LYS	2.2
1	B	155	TYR	2.2
1	B	64	HIS	2.2
1	B	105	ALA	2.2
1	B	1	LYS	2.2
1	A	7	LEU	2.1
1	A	275	LEU	2.1
1	B	382	LEU	2.1
1	B	85	PHE	2.1
1	B	28	GLU	2.1
1	A	431	ILE	2.1
1	A	398	VAL	2.1
1	B	118	ASN	2.1
1	B	82	ALA	2.1
1	B	233	SER	2.0
1	A	257	PRO	2.0
1	B	133	PRO	2.0
1	B	110	VAL	2.0
1	B	221	GLU	2.0
1	A	79	ILE	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MAL	B	501	23/23	0.92	0.24	1.10	44,50,56,59	0
3	ACT	A	504	4/4	0.84	0.18	1.01	62,67,75,75	0
2	MAL	A	501	23/23	0.93	0.17	0.86	42,49,56,61	0
3	ACT	A	503	4/4	0.73	0.26	-	53,61,62,66	0
4	GOL	A	506	6/6	0.75	0.21	-	68,82,98,99	0
3	ACT	A	505	4/4	0.73	0.29	-	105,113,126,126	0
3	ACT	B	502	4/4	0.84	0.45	-	74,75,77,79	0
3	ACT	A	502	4/4	0.88	0.21	-	73,81,84,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.