Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2016 – 08:44 PM EDT

PDB ID	:	5AZ6
Title	:	Crystal structure of MBP-Tom20 fusion protein with a 2-residue spacer in the connector helix
Authors	:	Matsuoka, R.; Kohda, D.
Deposited on	:	2015-09-27
Resolution	:	2.56 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

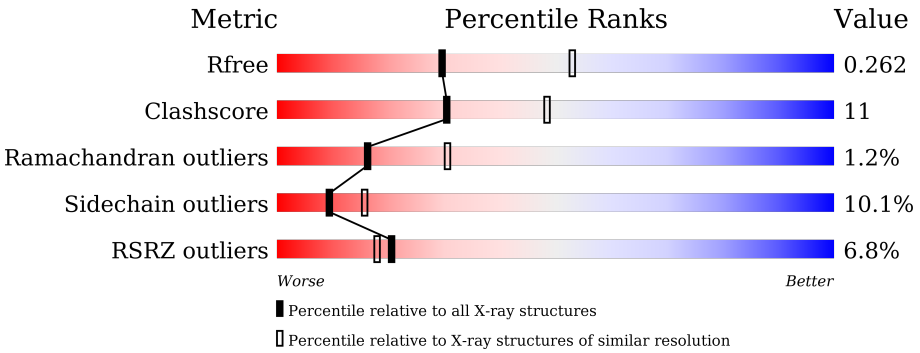
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.56 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}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	433	7% 78% 18%
1	B	433	6% 79% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6821 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.

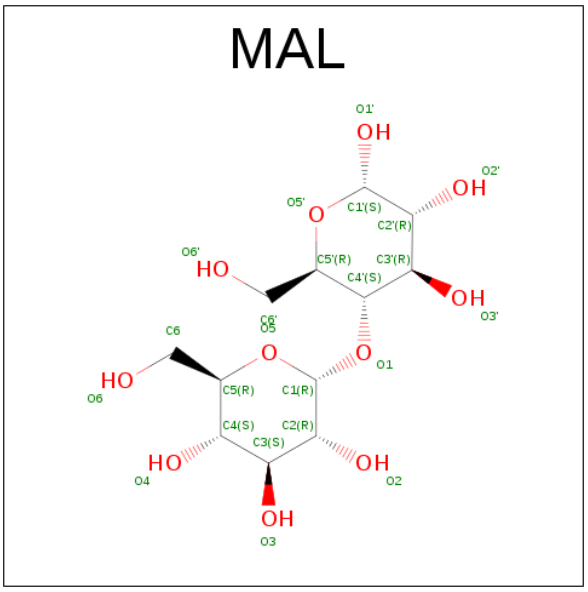
- Molecule 1 is a protein called Maltose-binding periplasmic protein,Mitochondrial import receptor subunit TOM20 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	433	Total	C	N	O	S	0	0	0
			3377	2177	548	643	9			
1	A	433	Total	C	N	O	S	0	0	0
			3377	2177	548	643	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0AEX9
B	313	VAL	ALA	engineered mutation	UNP P0AEX9
B	370	LYS	-	linker	UNP P0AEX9
B	371	GLU	-	linker	UNP P0AEX9
A	1	MET	-	initiating methionine	UNP P0AEX9
A	313	VAL	ALA	engineered mutation	UNP P0AEX9
A	370	LYS	-	linker	UNP P0AEX9
A	371	GLU	-	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	B	1	Total C O 23 12 11	0	0
2	A	1	Total C O 23 12 11	0	0

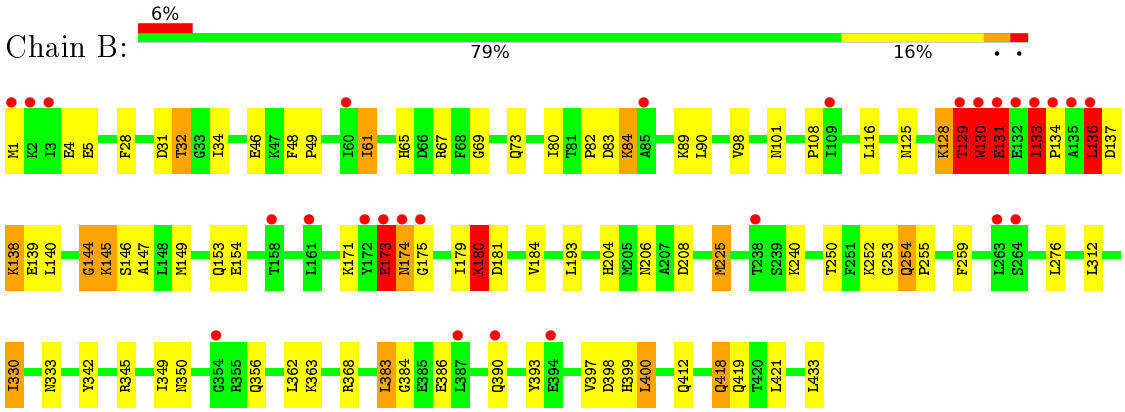
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	13	Total O 13 13	0	0
3	A	8	Total O 8 8	0	0

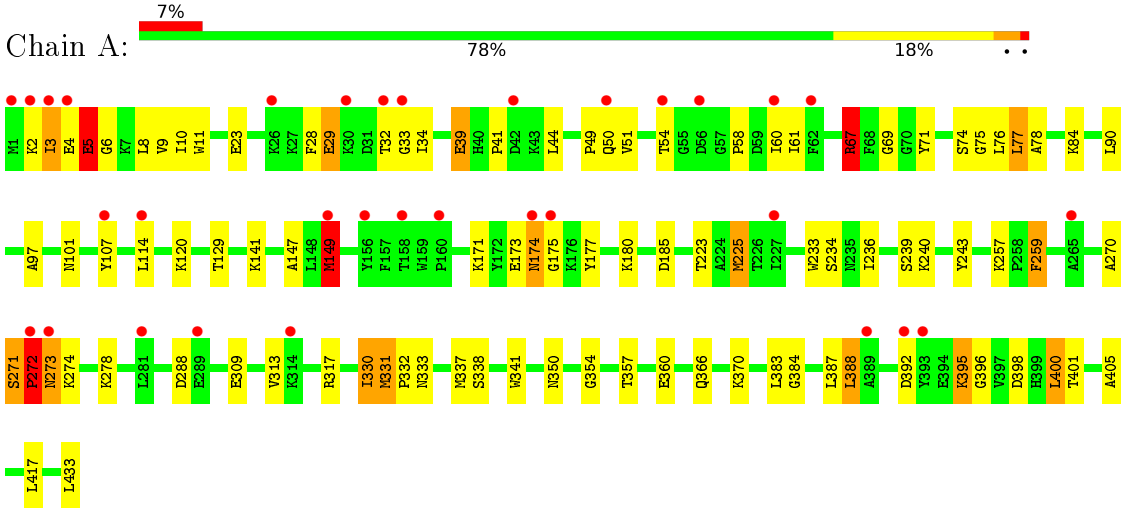
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 import receptor subunit TOM20 homolog



• Molecule 1: Maltose-binding periplasmic protein,Mitochondrial import receptor subunit TOM20 homolog



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.91Å 81.23Å 109.89Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	24.72 – 2.56 24.72 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.72-2.56) 99.4 (24.72-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.203 , 0.260 0.208 , 0.262	Depositor DCC
R_{free} test set	1784 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 35820 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6821	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 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MAL

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	0.67	5/3455 (0.1%)	0.83	6/4688 (0.1%)
1	B	0.66	0/3455	0.79	4/4688 (0.1%)
All	All	0.67	5/6910 (0.1%)	0.81	10/9376 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	PRO	CA-C	6.16	1.65	1.52
1	A	273	ASN	CA-C	6.02	1.68	1.52
1	A	273	ASN	N-CA	5.96	1.58	1.46
1	A	272	PRO	N-CA	5.80	1.57	1.47
1	A	5	GLU	CA-C	5.08	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	173	GLU	N-CA-C	-6.14	94.43	111.00
1	A	272	PRO	N-CA-C	6.10	127.97	112.10
1	A	5	GLU	CA-C-N	6.07	128.33	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	LEU	CA-CB-CG	5.98	129.06	115.30
1	B	131	GLU	N-CA-C	5.94	127.03	111.00
1	A	5	GLU	N-CA-C	5.65	126.26	111.00
1	A	149	MET	CA-CB-CG	5.60	122.82	113.30
1	A	331	MET	CG-SD-CE	-5.09	92.05	100.20
1	B	67	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	SER	Peptide
1	B	130	TRP	Peptide
1	B	131	GLU	Peptide
1	B	144	GLY	Peptide
1	B	180	LYS	Peptide
1	B	31	ASP	Peptide

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	3377	0	3371	86	0
1	B	3377	0	3371	69	0
2	A	23	0	22	0	0
2	B	23	0	22	0	0
3	A	8	0	0	1	0
3	B	13	0	0	6	0
All	All	6821	0	6786	149	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 11.

All (149) 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:B:130:TRP:HA	3:B:610:HOH:O	1.49	1.12
1:A:6:GLY:H	1:A:273:ASN:C	1.62	1.03
1:A:5:GLU:O	1:A:271:SER:CB	2.08	1.02
1:B:133:ILE:O	1:B:137:ASP:N	1.92	1.02
1:A:5:GLU:CD	1:A:274:LYS:HG3	1.80	1.01
1:B:128:LYS:O	1:B:130:TRP:N	1.99	0.95
1:A:5:GLU:HA	1:A:272:PRO:C	1.87	0.94
1:B:131:GLU:OE2	1:B:134:PRO:HG3	1.65	0.94
1:A:270:ALA:O	1:A:271:SER:HB2	1.65	0.93
1:B:129:THR:O	1:B:250:THR:OG1	1.92	0.86
1:B:145:LYS:HG3	1:B:145:LYS:O	1.78	0.83
1:A:5:GLU:O	1:A:271:SER:OG	1.97	0.82
1:A:5:GLU:O	1:A:271:SER:C	2.17	0.82
1:B:130:TRP:HB2	1:B:250:THR:O	1.80	0.81
1:A:5:GLU:CD	1:A:274:LYS:CG	2.49	0.81
1:A:173:GLU:O	1:A:175:GLY:N	2.14	0.81
1:A:5:GLU:OE2	1:A:274:LYS:HG3	1.82	0.80
1:A:5:GLU:O	1:A:272:PRO:N	2.15	0.79
1:B:175:GLY:CA	1:A:174:ASN:O	2.30	0.78
1:B:175:GLY:N	1:A:174:ASN:O	2.17	0.77
1:A:5:GLU:H	1:A:274:LYS:H	1.36	0.74
1:B:130:TRP:CD1	1:B:134:PRO:HB3	2.23	0.73
1:A:5:GLU:O	1:A:271:SER:CA	2.36	0.73
1:A:5:GLU:OE2	1:A:274:LYS:HE3	1.89	0.73
1:A:5:GLU:N	1:A:273:ASN:HA	2.03	0.73
1:B:32:THR:HG22	1:B:34:ILE:H	1.52	0.73
1:A:5:GLU:HA	1:A:272:PRO:CA	2.19	0.72
1:B:175:GLY:HA2	1:A:174:ASN:O	1.89	0.72
1:A:392:ASP:HB3	1:A:395:LYS:HE3	1.72	0.71
1:A:270:ALA:O	1:A:271:SER:CB	2.40	0.70
1:A:6:GLY:N	1:A:273:ASN:C	2.44	0.67
1:A:5:GLU:H	1:A:274:LYS:N	1.92	0.67
1:A:6:GLY:N	1:A:273:ASN:N	2.44	0.65
1:A:5:GLU:OE1	1:A:274:LYS:CA	2.44	0.65
1:A:350:ASN:O	1:A:354:GLY:O	2.14	0.65
1:B:134:PRO:O	1:B:138:LYS:HB2	2.00	0.62
1:B:174:ASN:HB3	1:A:175:GLY:O	1.99	0.62
1:B:144:GLY:HA3	3:B:609:HOH:O	2.00	0.61
1:B:69:GLY:HA3	1:B:333:ASN:O	1.99	0.61
1:B:129:THR:HG22	1:B:250:THR:OG1	1.99	0.61
1:B:145:LYS:HB2	3:B:612:HOH:O	2.00	0.61
1:B:131:GLU:HA	1:B:134:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLU:OE1	1:A:274:LYS:HG3	2.02	0.60
1:B:136:LEU:O	1:B:140:LEU:HB2	2.02	0.60
1:A:5:GLU:CA	1:A:272:PRO:C	2.68	0.59
1:B:384:GLY:HA3	1:B:400:LEU:HD13	1.84	0.59
1:B:144:GLY:CA	3:B:609:HOH:O	2.51	0.59
1:B:138:LYS:HG2	1:B:204:HIS:NE2	2.18	0.58
1:A:5:GLU:C	1:A:273:ASN:N	2.58	0.57
1:A:107:TYR:OH	1:A:278:LYS:HD3	2.05	0.57
1:B:34:ILE:HD13	1:B:276:LEU:HD13	1.86	0.57
1:B:133:ILE:HA	1:B:136:LEU:HB2	1.86	0.57
1:B:130:TRP:O	1:B:133:ILE:N	2.39	0.56
1:A:5:GLU:HG2	1:A:274:LYS:NZ	2.21	0.56
1:A:392:ASP:CB	1:A:395:LYS:HE3	2.35	0.56
1:B:418:GLN:NE2	1:B:419:GLN:OE1	2.39	0.55
1:A:3:ILE:HG22	1:A:4:GLU:C	2.27	0.54
1:B:145:LYS:CG	1:B:145:LYS:O	2.55	0.53
1:B:136:LEU:O	1:B:140:LEU:N	2.40	0.53
1:A:177:TYR:CE2	1:A:332:PRO:HB3	2.44	0.53
1:B:174:ASN:C	1:A:175:GLY:HA3	2.28	0.53
1:B:393:TYR:O	1:B:397:VAL:HG22	2.09	0.52
1:B:154:GLU:OE1	1:B:345:ARG:NH1	2.43	0.52
1:A:69:GLY:HA3	1:A:333:ASN:O	2.09	0.52
1:B:83:ASP:O	1:B:84:LYS:CB	2.58	0.52
1:A:5:GLU:O	1:A:271:SER:HB3	2.03	0.52
1:A:28:PHE:CE1	1:A:32:THR:HG21	2.46	0.51
1:A:387:LEU:HD23	1:A:395:LYS:HB2	1.93	0.51
1:A:5:GLU:HG2	1:A:274:LYS:CE	2.41	0.51
1:B:179:ILE:O	1:B:180:LYS:CG	2.58	0.51
1:B:145:LYS:HA	3:B:612:HOH:O	2.10	0.51
1:B:179:ILE:O	1:B:180:LYS:HG2	2.10	0.51
1:B:179:ILE:O	1:B:180:LYS:CB	2.57	0.51
1:B:130:TRP:CB	1:B:250:THR:O	2.53	0.50
1:A:6:GLY:N	1:A:273:ASN:CA	2.74	0.50
1:A:173:GLU:O	1:A:174:ASN:C	2.50	0.50
1:B:171:LYS:HD3	1:B:181:ASP:OD2	2.12	0.50
1:A:331:MET:HE3	1:A:341:TRP:HZ2	1.78	0.49
1:B:250:THR:HG22	1:B:255:PRO:HA	1.94	0.49
1:B:28:PHE:O	1:B:32:THR:HB	2.13	0.49
1:A:392:ASP:C	1:A:395:LYS:HE3	2.33	0.48
1:A:259:PHE:O	3:A:601:HOH:O	2.20	0.48
1:A:388:LEU:HD13	1:A:396:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:TRP:CD1	3:B:610:HOH:O	2.56	0.47
1:A:97:ALA:HB2	1:A:330:ILE:HD11	1.97	0.47
1:B:116:LEU:HD21	1:B:225:MET:HE1	1.97	0.47
1:B:129:THR:O	1:B:131:GLU:N	2.48	0.47
1:A:180:LYS:HE2	1:A:405:ALA:O	2.14	0.47
1:A:3:ILE:HG22	1:A:4:GLU:O	2.15	0.47
1:A:5:GLU:H	1:A:273:ASN:HA	1.79	0.47
1:A:5:GLU:OE1	1:A:274:LYS:N	2.47	0.47
1:B:48:PHE:CG	1:B:61:ILE:HD12	2.50	0.47
1:B:250:THR:HB	1:B:254:GLN:O	2.16	0.46
1:B:383:LEU:HB3	1:B:399:HIS:ND1	2.30	0.46
1:B:174:ASN:CA	1:A:175:GLY:HA3	2.46	0.46
1:A:78:ALA:CB	1:A:274:LYS:HE2	2.46	0.46
1:A:3:ILE:HB	1:A:274:LYS:HD2	1.97	0.45
1:A:236:ILE:HG22	1:A:243:TYR:CD1	2.52	0.45
1:A:5:GLU:OE1	1:A:274:LYS:HA	2.14	0.45
1:B:153:GLN:HA	1:B:349:ILE:HD11	1.98	0.45
1:A:332:PRO:HG2	1:A:337:MET:SD	2.56	0.45
1:B:136:LEU:O	1:B:140:LEU:CB	2.65	0.45
1:A:331:MET:CE	1:A:341:TRP:HZ2	2.30	0.45
1:A:39:GLU:C	1:A:41:PRO:HD3	2.38	0.45
1:B:342:TYR:CD2	1:B:368:ARG:NH2	2.85	0.45
1:A:5:GLU:C	1:A:272:PRO:N	2.69	0.44
1:A:5:GLU:OE1	1:A:274:LYS:CB	2.66	0.44
1:A:398:ASP:O	1:A:401:THR:HB	2.17	0.44
1:A:147:ALA:O	1:A:225:MET:HG2	2.18	0.44
1:A:6:GLY:HA2	1:A:271:SER:OG	2.17	0.44
1:B:173:GLU:O	1:B:174:ASN:C	2.55	0.44
1:B:46:GLU:O	1:B:49:PRO:HD2	2.17	0.44
1:A:236:ILE:CG2	1:A:243:TYR:CD1	3.01	0.44
1:A:5:GLU:N	1:A:273:ASN:CA	2.77	0.44
1:A:357:THR:HG23	1:A:360:GLU:H	1.83	0.43
1:A:67:ARG:HH11	1:A:67:ARG:CG	2.31	0.43
1:A:149:MET:HB2	1:A:223:THR:HG21	2.01	0.43
1:B:131:GLU:HG3	1:B:252:LYS:N	2.33	0.43
1:B:131:GLU:HG3	1:B:253:GLY:H	1.82	0.43
1:A:29:GLU:O	1:A:33:GLY:N	2.47	0.43
1:A:5:GLU:HG2	1:A:274:LYS:HZ2	1.81	0.43
1:B:206:ASN:HB3	1:B:208:ASP:OD1	2.19	0.43
1:B:147:ALA:O	1:B:225:MET:HG3	2.19	0.42
1:B:350:ASN:ND2	1:B:356:GLN:OE1	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TRP:CH2	1:A:317:ARG:HB3	2.53	0.42
1:B:133:ILE:CG2	1:B:136:LEU:HB3	2.49	0.42
1:A:10:ILE:HG12	1:A:60:ILE:HB	2.00	0.42
1:B:89:LYS:C	1:B:90:LEU:HD23	2.40	0.42
1:B:65:HIS:CE1	1:B:330:ILE:HD13	2.55	0.42
1:B:129:THR:C	1:B:250:THR:H	2.23	0.42
1:B:32:THR:HG23	1:B:34:ILE:HD12	2.01	0.42
1:A:49:PRO:HG3	1:A:71:TYR:CE1	2.55	0.41
1:A:6:GLY:N	1:A:273:ASN:H	2.16	0.41
1:B:133:ILE:HG23	1:B:136:LEU:HB3	2.01	0.41
1:B:134:PRO:HA	1:B:137:ASP:CB	2.50	0.41
1:B:80:ILE:HD12	1:B:82:PRO:HD3	2.02	0.41
1:A:309:GLU:O	1:A:313:VAL:HG13	2.20	0.41
1:A:384:GLY:HA3	1:A:400:LEU:HD13	2.02	0.41
1:A:185:ASP:HB2	1:A:366:GLN:HB2	2.03	0.41
1:A:5:GLU:CA	1:A:273:ASN:N	2.83	0.41
1:B:146:SER:OG	1:B:149:MET:CE	2.69	0.41
1:B:193:LEU:HD22	1:B:362:LEU:HD21	2.02	0.41
1:A:29:GLU:HG3	1:A:34:ILE:O	2.21	0.41
1:A:75:GLY:O	1:A:77:LEU:N	2.51	0.41
1:A:11:TRP:CD1	1:A:58:PRO:HB3	2.57	0.40
1:A:5:GLU:CD	1:A:274:LYS:CD	2.90	0.40
1:A:90:LEU:HD12	1:A:90:LEU:N	2.36	0.40
1:A:74:SER:HB2	1:A:76:LEU:HD22	2.02	0.40
1:B:98:VAL:HG21	1:B:108:PRO:HD3	2.03	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	431/433 (100%)	405 (94%)	22 (5%)	4 (1%)	21 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	431/433 (100%)	401 (93%)	24 (6%)	6 (1%)	14 25
All	All	862/866 (100%)	806 (94%)	46 (5%)	10 (1%)	16 30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	LYS
1	B	129	THR
1	A	8	LEU
1	A	174	ASN
1	A	271	SER
1	B	130	TRP
1	B	5	GLU
1	A	272	PRO
1	B	125	ASN
1	B	133	ILE

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	353/353 (100%)	316 (90%)	37 (10%)	8 14
1	B	353/353 (100%)	319 (90%)	34 (10%)	10 18
All	All	706/706 (100%)	635 (90%)	71 (10%)	9 16

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	4	GLU
1	B	32	THR
1	B	61	ILE
1	B	73	GLN
1	B	101	ASN

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Mol	Chain	Res	Type
1	B	128	LYS
1	B	129	THR
1	B	130	TRP
1	B	133	ILE
1	B	136	LEU
1	B	138	LYS
1	B	139	GLU
1	B	145	LYS
1	B	173	GLU
1	B	174	ASN
1	B	180	LYS
1	B	184	VAL
1	B	225	MET
1	B	240	LYS
1	B	254	GLN
1	B	259	PHE
1	B	312	LEU
1	B	330	ILE
1	B	363	LYS
1	B	383	LEU
1	B	386	GLU
1	B	390	GLN
1	B	398	ASP
1	B	400	LEU
1	B	412	GLN
1	B	418	GLN
1	B	421	LEU
1	B	433	LEU
1	A	2	LYS
1	A	3	ILE
1	A	5	GLU
1	A	9	VAL
1	A	23	GLU
1	A	29	GLU
1	A	39	GLU
1	A	44	LEU
1	A	50	GLN
1	A	51	VAL
1	A	54	THR
1	A	61	ILE
1	A	67	ARG
1	A	77	LEU

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Mol	Chain	Res	Type
1	A	84	LYS
1	A	101	ASN
1	A	114	LEU
1	A	120	LYS
1	A	129	THR
1	A	141	LYS
1	A	149	MET
1	A	171	LYS
1	A	225	MET
1	A	234	SER
1	A	240	LYS
1	A	257	LYS
1	A	259	PHE
1	A	288	ASP
1	A	330	ILE
1	A	338	SER
1	A	370	LYS
1	A	383	LEU
1	A	388	LEU
1	A	395	LYS
1	A	400	LEU
1	A	417	LEU
1	A	433	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	GLN
1	B	174	ASN
1	B	254	GLN
1	B	390	GLN
1	A	283	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)

2 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	0.75	0	35,35,35	1.21	6 (17%)
2	MAL	B	501	-	24,24,24	0.54	0	35,35,35	0.87	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
2	MAL	A	501	-	-	0/8/48/48	0/2/2/2
2	MAL	B	501	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	MAL	O2-C2-C3	-2.68	104.31	110.36
2	A	501	MAL	O4-C4-C3	-2.62	104.46	110.36
2	A	501	MAL	O2'-C2'-C3'	-2.42	104.91	110.36
2	A	501	MAL	O1-C1-C2	-2.33	102.35	108.12
2	A	501	MAL	O4-C4-C5	2.23	115.09	109.23
2	A	501	MAL	O2'-C2'-C1'	2.35	114.88	109.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	433/433 (100%)	0.28	32 (7%)	17	15	37, 61, 90, 154	0
1	B	433/433 (100%)	0.20	27 (6%)	24	21	35, 53, 84, 119	0
All	All	866/866 (100%)	0.24	59 (6%)	20	18	35, 56, 89, 154	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	LEU	11.8
1	B	135	ALA	9.8
1	A	1	MET	9.2
1	B	129	THR	7.4
1	A	272	PRO	7.2
1	A	3	ILE	6.3
1	A	2	LYS	6.3
1	B	132	GLU	5.6
1	B	1	MET	4.6
1	B	387	LEU	4.2
1	B	2	LYS	3.9
1	A	392	ASP	3.8
1	A	30	LYS	3.8
1	A	174	ASN	3.7
1	B	354	GLY	3.6
1	B	172	TYR	3.5
1	A	60	ILE	3.3
1	B	174	ASN	3.3
1	A	227	ILE	3.2
1	A	149	MET	3.0
1	B	133	ILE	3.0
1	A	175	GLY	3.0
1	B	134	PRO	3.0
1	A	265	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	161	LEU	2.8
1	A	107	TYR	2.8
1	B	175	GLY	2.7
1	B	263	LEU	2.7
1	B	390	GLN	2.7
1	B	85	ALA	2.6
1	A	393	TYR	2.6
1	B	238	THR	2.6
1	B	3	ILE	2.5
1	A	389	ALA	2.5
1	A	50	GLN	2.5
1	B	131	GLU	2.5
1	A	26	LYS	2.5
1	B	130	TRP	2.5
1	B	109	ILE	2.5
1	A	42	ASP	2.5
1	A	33	GLY	2.4
1	A	273	ASN	2.4
1	B	264	SER	2.3
1	B	173	GLU	2.3
1	A	281	LEU	2.2
1	A	56	ASP	2.2
1	B	394	GLU	2.2
1	B	158	THR	2.2
1	A	54	THR	2.2
1	B	60	ILE	2.1
1	A	4	GLU	2.1
1	A	289	GLU	2.1
1	A	32	THR	2.1
1	A	160	PRO	2.1
1	A	314	LYS	2.1
1	A	156	TYR	2.1
1	A	114	LEU	2.1
1	A	62	PHE	2.0
1	A	158	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. 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MAL	A	501	23/23	0.96	0.13	-0.85	37,44,51,55	0
2	MAL	B	501	23/23	0.97	0.11	-1.19	33,36,42,45	0

6.5 Other polymers (i)

There are no such residues in this entry.