WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:22 am GMT

PDB ID	:	5AZA
Title	:	Crystal structure of MBP-sAglB fusion protein with a 20-residue spacer in the connector helix
Authors	:	Matsuoka, R.; Kohda, D.
Deposited on	:	2015-09-27
Resolution	:	2.08 Å(reported)

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	:	trunk28620
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)	:	recalc28949
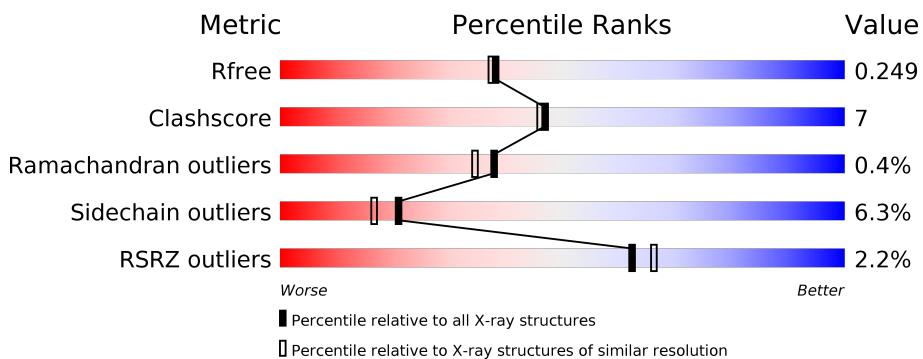
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
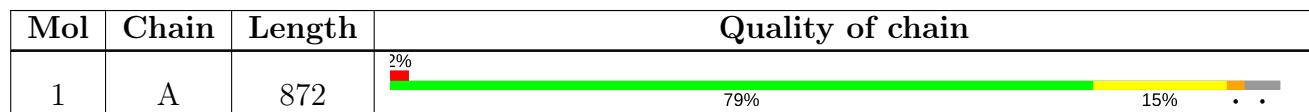
The reported resolution of this entry is 2.08 Å.

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	4955 (2.10-2.06)
Clashscore	112137	5537 (2.10-2.06)
Ramachandran outliers	110173	5483 (2.10-2.06)
Sidechain outliers	110143	5484 (2.10-2.06)
RSRZ outliers	101464	4991 (2.10-2.06)

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	872	

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	CA	A	902	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6733 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,Oligosaccharyl transferase stt3 subunit related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	836	6583	4239	1076	1256	12	0	4	0

There are 28 discrepancies between the modelled and reference sequences:
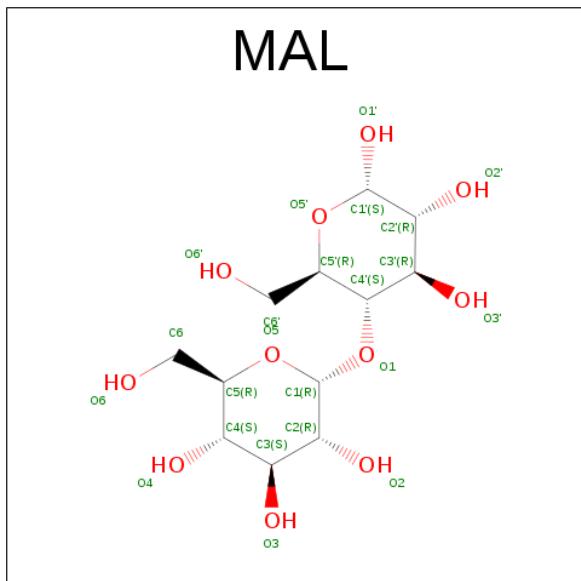
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0AEX9
A	312	VAL	ALA	engineered mutation	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ALA	-	linker	UNP P0AEX9
A	372	LYS	-	linker	UNP P0AEX9
A	373	ALA	-	linker	UNP P0AEX9
A	374	GLU	-	linker	UNP P0AEX9
A	375	ALA	-	linker	UNP P0AEX9
A	376	ALA	-	linker	UNP P0AEX9
A	377	ALA	-	linker	UNP P0AEX9
A	378	LYS	-	linker	UNP P0AEX9
A	379	ALA	-	linker	UNP P0AEX9
A	380	GLU	-	linker	UNP P0AEX9
A	381	ALA	-	linker	UNP P0AEX9
A	382	ALA	-	linker	UNP P0AEX9
A	383	ALA	-	linker	UNP P0AEX9
A	384	LYS	-	linker	UNP P0AEX9
A	385	ALA	-	linker	UNP P0AEX9
A	386	ALA	-	linker	UNP P0AEX9
A	387	ALA	-	linker	UNP P0AEX9
A	388	ALA	-	linker	UNP P0AEX9
A	866	HIS	-	expression tag	UNP I6V0B8
A	867	HIS	-	expression tag	UNP I6V0B8
A	868	HIS	-	expression tag	UNP I6V0B8
A	869	HIS	-	expression tag	UNP I6V0B8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	870	HIS	-	expression tag	UNP I6V0B8
A	871	HIS	-	expression tag	UNP I6V0B8

• 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 23	C 12	O 11	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
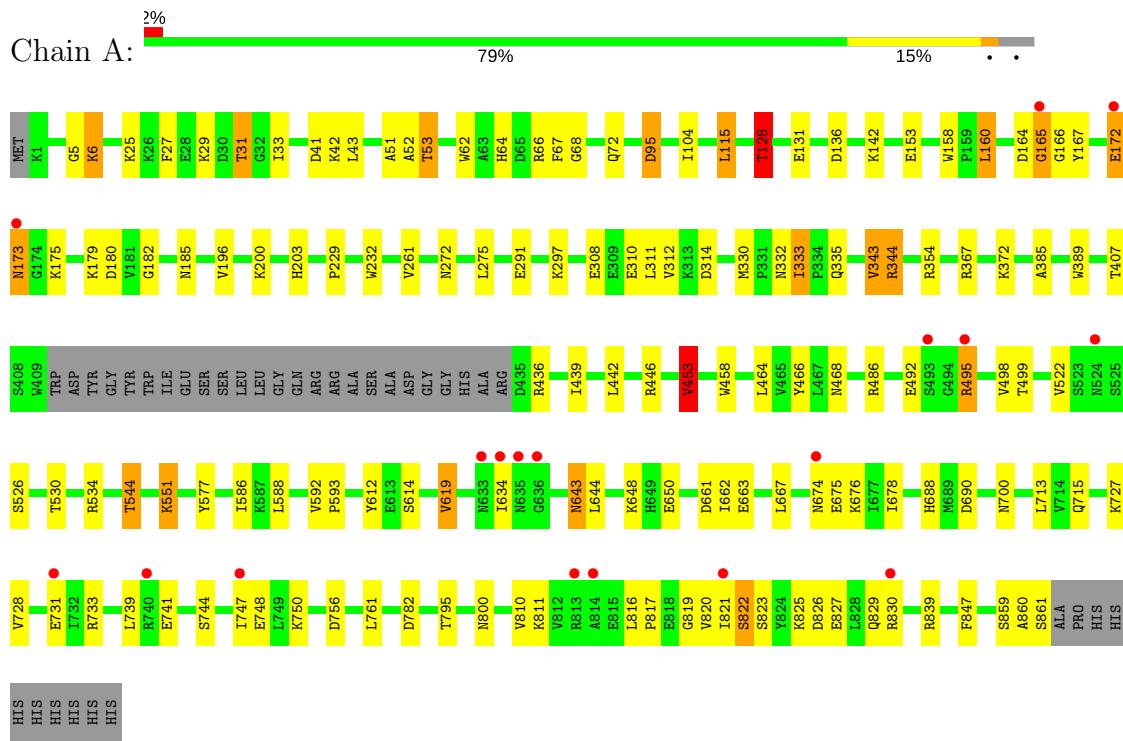
• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total 126	O 126	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,Oligosaccharyl transferase stt3 subunit related protein

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.47Å 100.47Å 140.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.08 43.57 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.08) 99.8 (43.57-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.196 , 0.248 0.204 , 0.249	Depositor DCC
R_{free} test set	2902 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6733	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, 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	0.85	1/6733 (0.0%)	0.93	18/9140 (0.2%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	ASP	CB-CG	5.29	1.62	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ASP	CB-CG-OD1	9.54	126.88	118.30
1	A	53	THR	N-CA-C	-7.45	90.90	111.00
1	A	551	LYS	CD-CE-NZ	6.69	127.08	111.70
1	A	344	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	53	THR	C-N-CA	-6.38	108.89	122.30
1	A	160	LEU	CB-CG-CD2	6.29	121.70	111.00
1	A	367	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	839	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	661	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	128	THR	N-CA-CB	-5.66	99.55	110.30
1	A	53	THR	CA-C-N	5.35	126.91	116.20
1	A	756	ASP	CB-CG-OD1	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	LEU	CB-CG-CD2	5.21	119.86	111.00
1	A	95	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	453	VAL	N-CA-CB	-5.15	100.16	111.50
1	A	344	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	53	THR	O-C-N	-5.03	114.66	123.20
1	A	314	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	GLY	Peptide
1	A	172	GLU	Peptide

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	6583	0	6540	94	0
2	A	23	0	22	0	0
3	A	1	0	0	0	0
4	A	126	0	0	13	0
All	All	6733	0	6562	94	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 7.

All (94) 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:95:ASP:HB3	4:A:1115:HOH:O	1.26	1.26
1:A:522:VAL:HB	4:A:1091:HOH:O	1.52	1.08
1:A:167:TYR:O	1:A:179:LYS:HE3	1.73	0.89
1:A:530:THR:HG22	4:A:1046:HOH:O	1.74	0.88
1:A:72:GLN:HG3	4:A:1005:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:HIS:HE1	4:A:1118:HOH:O	1.64	0.79
1:A:64:HIS:HD2	1:A:261:VAL:H	1.31	0.75
1:A:688:HIS:HE1	1:A:690:ASP:OD1	1.72	0.71
1:A:522:VAL:HG12	1:A:522:VAL:O	1.91	0.70
1:A:128:THR:HB	1:A:131:GLU:OE1	1.92	0.68
1:A:663:GLU:OE2	1:A:688:HIS:HD2	1.76	0.67
1:A:64:HIS:CD2	1:A:261:VAL:H	2.12	0.67
1:A:827:GLU:HA	1:A:830:ARG:HG3	1.79	0.65
1:A:819:GLY:O	1:A:823:SER:CB	2.45	0.64
1:A:486:ARG:NH1	1:A:782:ASP:OD1	2.27	0.64
1:A:27:PHE:O	1:A:31:THR:HB	1.98	0.63
1:A:196:VAL:CG1	1:A:200:LYS:HD2	2.29	0.63
1:A:95:ASP:CB	4:A:1115:HOH:O	2.07	0.62
1:A:308:GLU:O	1:A:312:VAL:HG23	2.00	0.62
1:A:182:GLY:O	1:A:185:ASN:ND2	2.31	0.62
1:A:544:THR:CG2	4:A:1077:HOH:O	2.45	0.62
1:A:643:ASN:HD22	1:A:643:ASN:C	2.03	0.62
1:A:196:VAL:HG12	1:A:200:LYS:HD2	1.80	0.61
1:A:644:LEU:O	1:A:860:ALA:HA	2.01	0.60
1:A:31:THR:HG22	1:A:33:ILE:H	1.67	0.59
1:A:747:ILE:O	1:A:811:LYS:HA	2.01	0.59
1:A:819:GLY:O	1:A:823:SER:HB3	2.02	0.59
1:A:164:ASP:O	1:A:165:GLY:O	2.21	0.58
1:A:820:VAL:HG23	1:A:821:ILE:H	1.70	0.57
1:A:544:THR:HG23	4:A:1077:HOH:O	2.06	0.56
1:A:196:VAL:HG12	1:A:200:LYS:CD	2.35	0.56
1:A:739:LEU:HD11	1:A:747:ILE:HD11	1.86	0.56
1:A:68:GLY:HA3	1:A:332:ASN:O	2.06	0.56
1:A:297[A]:LYS:HD3	4:A:1052:HOH:O	2.05	0.56
1:A:128:THR:HG22	1:A:131:GLU:H	1.71	0.55
1:A:5:GLY:H	1:A:272:ASN:HD21	1.54	0.55
1:A:741:GLU:HA	1:A:816:LEU:HD23	1.88	0.54
1:A:650:GLU:HA	1:A:700:ASN:HD22	1.71	0.54
1:A:136:ASP:OD2	1:A:203:HIS:HD2	1.90	0.54
1:A:51:ALA:O	1:A:53:THR:O	2.26	0.54
1:A:663:GLU:H	1:A:715:GLN:HE22	1.54	0.53
1:A:312:VAL:HG12	1:A:312:VAL:O	2.08	0.53
1:A:663:GLU:H	1:A:715:GLN:NE2	2.07	0.53
1:A:727:LYS:HA	1:A:731:GLU:O	2.08	0.53
1:A:822:SER:HA	1:A:825:LYS:HB3	1.91	0.52
1:A:498:VAL:HG11	1:A:577:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ILE:HA	1:A:715:GLN:HE22	1.76	0.51
1:A:464:LEU:N	1:A:464:LEU:HD12	2.25	0.51
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.46	0.51
1:A:663:GLU:CD	1:A:688:HIS:HD2	2.14	0.51
1:A:498:VAL:HG11	1:A:577:TYR:CG	2.47	0.50
1:A:64:HIS:HE1	1:A:330:MET:O	1.94	0.49
1:A:164:ASP:C	1:A:165:GLY:O	2.51	0.48
1:A:33:ILE:HD13	1:A:275:LEU:HD22	1.95	0.48
1:A:31:THR:CG2	1:A:33:ILE:H	2.27	0.48
1:A:643:ASN:HB2	1:A:859:SER:O	2.13	0.48
1:A:67:PHE:HB3	1:A:104:ILE:HD12	1.96	0.47
1:A:544:THR:HG21	1:A:593:PRO:HD2	1.97	0.47
1:A:741:GLU:OE1	1:A:821:ILE:O	2.33	0.47
1:A:52:ALA:C	1:A:53:THR:O	2.49	0.47
1:A:690:ASP:HB3	4:A:1088:HOH:O	2.14	0.47
1:A:819:GLY:O	1:A:823:SER:HB2	2.14	0.47
1:A:172:GLU:O	1:A:173:ASN:HB2	2.14	0.47
1:A:62:TRP:CD1	1:A:66:ARG:HG3	2.50	0.47
1:A:612:TYR:HB3	1:A:619:VAL:HG13	1.96	0.47
1:A:62:TRP:HB3	1:A:67:PHE:HE1	1.80	0.46
1:A:820:VAL:HG23	1:A:821:ILE:N	2.29	0.46
1:A:728:VAL:HG23	1:A:733:ARG:HG3	1.98	0.46
1:A:495:ARG:HG3	1:A:495:ARG:HH11	1.81	0.45
1:A:551:LYS:CE	4:A:1016:HOH:O	2.64	0.45
1:A:153:GLU:OE1	1:A:344:ARG:NH1	2.50	0.45
1:A:522:VAL:CG1	1:A:522:VAL:O	2.63	0.45
1:A:31:THR:HG23	1:A:33:ILE:HD12	1.98	0.44
1:A:643:ASN:OD1	1:A:861:SER:C	2.56	0.44
1:A:522:VAL:HA	1:A:526:SER:O	2.17	0.44
1:A:544:THR:HG22	4:A:1077:HOH:O	2.14	0.44
1:A:442:LEU:HD12	1:A:446:ARG:HG3	2.00	0.44
1:A:466:TYR:CE2	1:A:468:ASN:HB2	2.53	0.43
1:A:385:ALA:O	1:A:389:TRP:HD1	2.01	0.43
1:A:6:LYS:HA	1:A:33:ILE:HG23	2.00	0.43
1:A:498:VAL:CG1	1:A:499:THR:N	2.82	0.42
1:A:436:ARG:HG2	1:A:458:TRP:CZ2	2.55	0.42
1:A:439:ILE:HG23	1:A:453:VAL:HG22	2.01	0.42
1:A:748:GLU:HA	1:A:810:VAL:O	2.20	0.42
1:A:158:TRP:CH2	1:A:343:VAL:HG22	2.54	0.42
1:A:817:PRO:O	1:A:820:VAL:HG22	2.20	0.41
1:A:586:ILE:HG22	1:A:592:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:HD12	1:A:335:GLN:HB2	2.03	0.41
1:A:495:ARG:HB3	1:A:495:ARG:CZ	2.49	0.41
1:A:172:GLU:OE2	1:A:372:LYS:NZ	2.51	0.41
1:A:498:VAL:HG12	1:A:499:THR:N	2.35	0.41
1:A:203:HIS:CE1	4:A:1118:HOH:O	2.52	0.40
1:A:33:ILE:CD1	1:A:275:LEU:HD22	2.51	0.40
1:A:761:LEU:HD13	1:A:847:PHE:CZ	2.57	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	836/872 (96%)	809 (97%)	24 (3%)	3 (0%)	38	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	GLY
1	A	800	ASN
1	A	674	ASN

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	690/716 (96%)	647 (94%)	43 (6%)	21	17

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	25	LYS
1	A	29	LYS
1	A	31	THR
1	A	41	ASP
1	A	42	LYS
1	A	43	LEU
1	A	115	LEU
1	A	128	THR
1	A	142	LYS
1	A	160	LEU
1	A	173	ASN
1	A	175	LYS
1	A	180	ASP
1	A	291	GLU
1	A	310	GLU
1	A	311	LEU
1	A	333	ILE
1	A	343	VAL
1	A	354	ARG
1	A	407	THR
1	A	453	VAL
1	A	492	GLU
1	A	495	ARG
1	A	534	ARG
1	A	544	THR
1	A	588	LEU
1	A	614	SER
1	A	619	VAL
1	A	634	ILE
1	A	643	ASN
1	A	648	LYS
1	A	667	LEU
1	A	675	GLU
1	A	676	LYS
1	A	678	ILE
1	A	713	LEU
1	A	744	SER

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Mol	Chain	Res	Type
1	A	750	LYS
1	A	795	THR
1	A	822	SER
1	A	826	ASP
1	A	829	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	64	HIS
1	A	100	ASN
1	A	173	ASN
1	A	201	ASN
1	A	203	HIS
1	A	218	ASN
1	A	253	GLN
1	A	272	ASN
1	A	282	ASN
1	A	325	GLN
1	A	335	GLN
1	A	399	ASN
1	A	474	ASN
1	A	524	ASN
1	A	607	ASN
1	A	616	ASN
1	A	643	ASN
1	A	688	HIS
1	A	700	ASN
1	A	715	GLN
1	A	737	ASN
1	A	829	GLN

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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#|Z| > 2$
2	MAL	A	901	-	24,24,24	0.66	0	35,35,35	1.37	3 (8%)

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	901	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	MAL	C4-C3-C2	-2.60	106.24	110.84
2	A	901	MAL	O2'-C2'-C3'	-2.30	105.35	110.36
2	A	901	MAL	O5'-C1'-C2'	4.21	117.02	110.04

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, 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(Å²)	Q<0.9
1	A	836/872 (95%)	-0.12	18 (2%)	62	66	23, 35, 67, 91	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	813	ARG	4.0
1	A	633	ASN	3.1
1	A	635	ASN	2.9
1	A	634	ILE	2.8
1	A	731	GLU	2.8
1	A	814	ALA	2.8
1	A	165	GLY	2.8
1	A	495	ARG	2.6
1	A	493	SER	2.5
1	A	636	GLY	2.5
1	A	674	ASN	2.5
1	A	747	ILE	2.5
1	A	740	ARG	2.4
1	A	172	GLU	2.4
1	A	173	ASN	2.3
1	A	821	ILE	2.2
1	A	830	ARG	2.1
1	A	524	ASN	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	CA	A	902	1/1	0.97	0.13	2.29	25,25,25,25	0
2	MAL	A	901	23/23	0.97	0.12	0.11	22,26,30,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.