Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:15 AM GMT

PDB ID	:	3OAI
Title	:	Crystal structure of the extra-cellular domain of human myelin protein zero
Authors	:	Liu, Z.; Wang, Y.; Brunzelle, J.; Kovari, I.A.; Sohi, J.; Kamholz, J.; Kovari, L.C.
Deposited on	:	2010-08-05
Resolution	:	2.10 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:

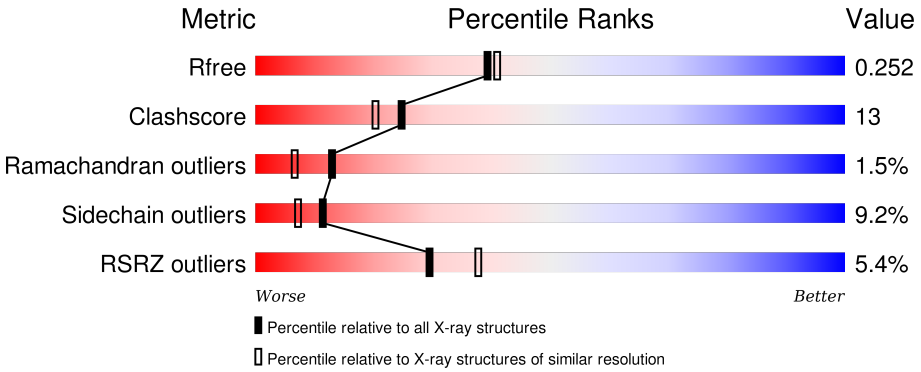
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	507	5% 75% 17%
1	B	507	6% 72% 19% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8212 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, Myelin protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3831	2463	626	734	8			
1	B	488	Total	C	N	O	S	0	0	0
			3831	2463	626	734	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	ASN	-	LINKER	UNP D3QK41
A	368	ASN	-	LINKER	UNP D3QK41
A	369	ASN	-	LINKER	UNP D3QK41
A	370	ASN	-	LINKER	UNP D3QK41
A	371	ASN	-	LINKER	UNP D3QK41
A	372	ASN	-	LINKER	UNP D3QK41
A	373	ASN	-	LINKER	UNP D3QK41
A	374	ASN	-	LINKER	UNP D3QK41
A	375	ASN	-	LINKER	UNP D3QK41
A	376	ASN	-	LINKER	UNP D3QK41
A	377	ASN	-	LINKER	UNP D3QK41
A	378	ASN	-	LINKER	UNP D3QK41
A	379	ASN	-	LINKER	UNP D3QK41
A	380	ASN	-	LINKER	UNP D3QK41
A	381	ASN	-	LINKER	UNP D3QK41
A	382	ASN	-	LINKER	UNP D3QK41
A	383	ASN	-	LINKER	UNP D3QK41
A	384	ASN	-	LINKER	UNP D3QK41
A	385	ASN	-	LINKER	UNP D3QK41
A	386	ASN	-	LINKER	UNP D3QK41
A	1016	GLN	ARG	CONFLICT	UNP P25189
B	367	ASN	-	LINKER	UNP D3QK41
B	368	ASN	-	LINKER	UNP D3QK41
B	369	ASN	-	LINKER	UNP D3QK41
B	370	ASN	-	LINKER	UNP D3QK41

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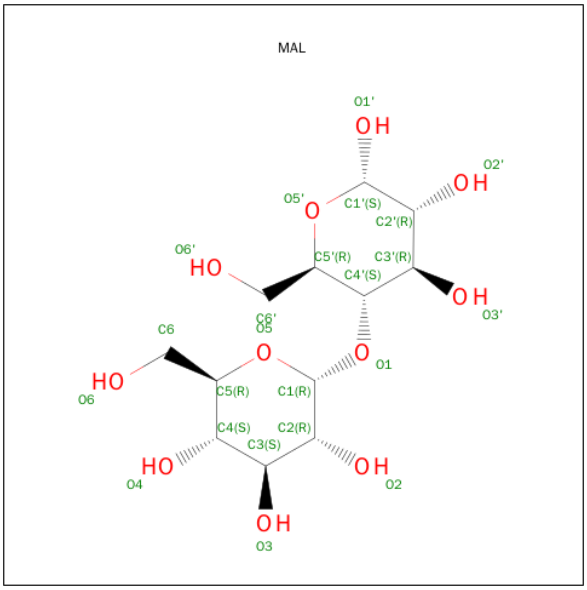
Chain	Residue	Modelled	Actual	Comment	Reference
B	371	ASN	-	LINKER	UNP D3QK41
B	372	ASN	-	LINKER	UNP D3QK41
B	373	ASN	-	LINKER	UNP D3QK41
B	374	ASN	-	LINKER	UNP D3QK41
B	375	ASN	-	LINKER	UNP D3QK41
B	376	ASN	-	LINKER	UNP D3QK41
B	377	ASN	-	LINKER	UNP D3QK41
B	378	ASN	-	LINKER	UNP D3QK41
B	379	ASN	-	LINKER	UNP D3QK41
B	380	ASN	-	LINKER	UNP D3QK41
B	381	ASN	-	LINKER	UNP D3QK41
B	382	ASN	-	LINKER	UNP D3QK41
B	383	ASN	-	LINKER	UNP D3QK41
B	384	ASN	-	LINKER	UNP D3QK41
B	385	ASN	-	LINKER	UNP D3QK41
B	386	ASN	-	LINKER	UNP D3QK41
B	1016	GLN	ARG	CONFLICT	UNP P25189

- Molecule 2 is SUGAR (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 water.

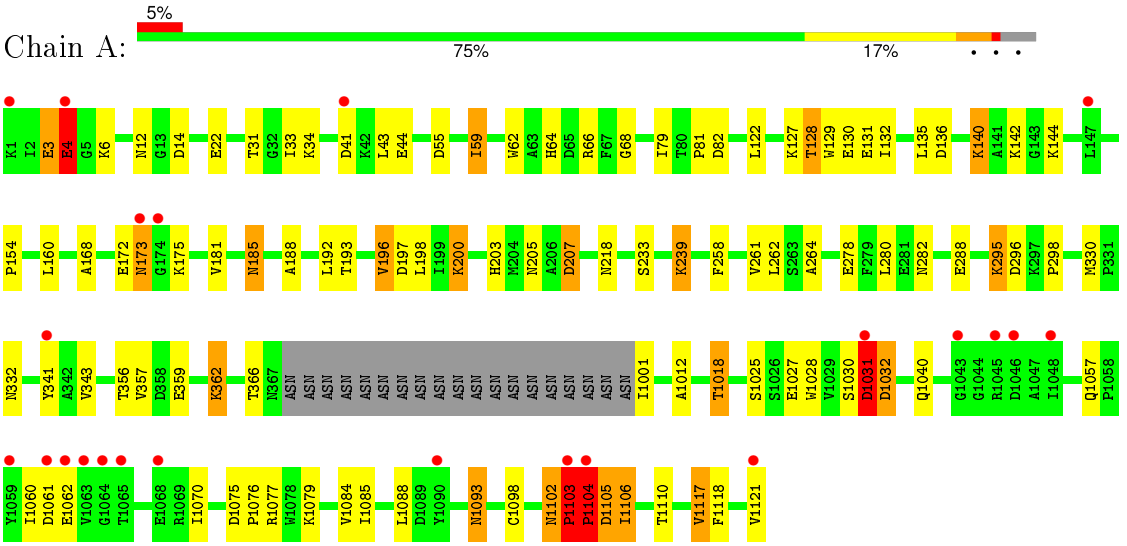
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	271	Total O 271 271	0	0
3	B	233	Total O 233 233	0	0

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.

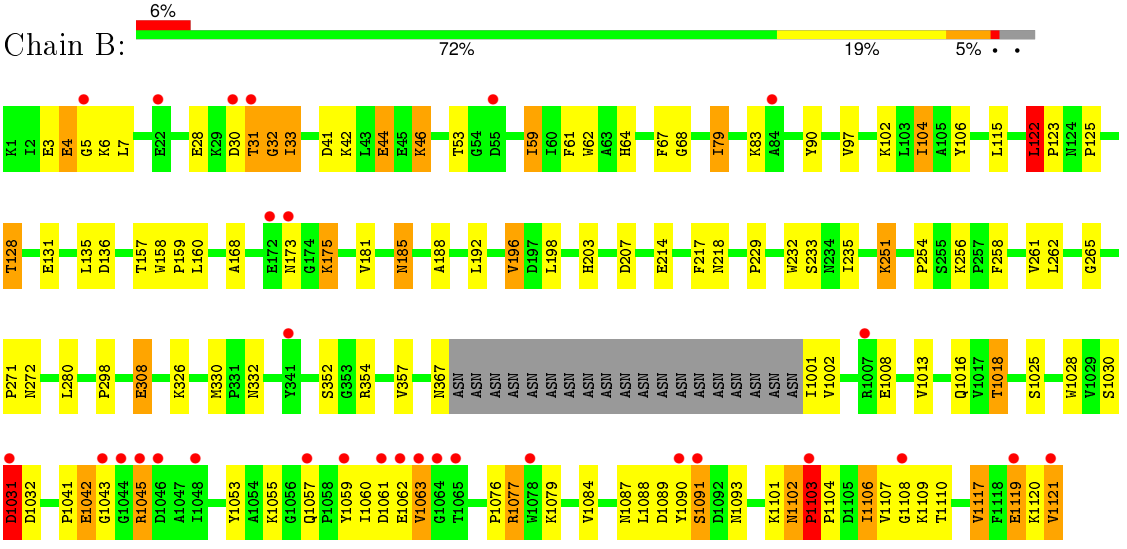
- Molecule 1: Maltose-binding periplasmic protein, Myelin protein P0

Chain A:



- Molecule 1: Maltose-binding periplasmic protein, Myelin protein P0

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.90Å 54.89Å 146.07Å 90.00° 98.54° 90.00°	Depositor
Resolution (Å)	19.96 – 2.10 19.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.10) 99.8 (19.96-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.183 , 0.252 0.185 , 0.252	Depositor DCC
R_{free} test set	2895 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 58.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 56887 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8212	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.93% 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	0.61	0/3930	0.69	3/5340 (0.1%)
1	B	0.59	0/3930	0.66	2/5340 (0.0%)
All	All	0.60	0/7860	0.67	5/10680 (0.0%)

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	5
1	B	0	3
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1104	PRO	N-CA-C	6.75	129.64	112.10
1	B	122	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	1032	ASP	N-CA-C	6.32	128.06	111.00
1	B	1103	PRO	C-N-CD	5.52	140.00	128.40
1	A	1103	PRO	C-N-CD	-5.33	108.86	120.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1031	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	1102	ASN	Peptide
1	A	1103	PRO	Peptide
1	A	1104	PRO	Peptide
1	A	3	GLU	Peptide
1	B	1031	ASP	Peptide
1	B	1102	ASN	Peptide
1	B	3	GLU	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	3831	0	3739	81	0
1	B	3831	0	3739	110	0
2	A	23	0	22	4	0
2	B	23	0	22	0	0
3	A	271	0	0	6	1
3	B	233	0	0	23	0
All	All	8212	0	7522	195	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 13.

All (195) 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)
2:A:1122:MAL:O1	2:A:1122:MAL:C1	1.64	1.42
1:B:1104:PRO:O	3:B:484:HOH:O	1.52	1.23
1:B:30:ASP:HB2	3:B:478:HOH:O	1.45	1.16
1:B:367:ASN:C	3:B:496:HOH:O	1.84	1.14
1:B:1045:ARG:HG3	1:B:1045:ARG:HH11	0.97	1.07
1:A:12:ASN:ND2	1:A:14:ASP:OD1	1.89	1.04
1:B:79:ILE:HB	3:B:450:HOH:O	1.56	1.04
1:A:12:ASN:ND2	1:A:14:ASP:H	1.55	1.03
1:A:1001:ILE:N	3:A:486:HOH:O	1.96	0.97
1:A:1031:ASP:OD1	1:A:1031:ASP:O	1.81	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:SER:H	1:A:1102:ASN:HD21	1.02	0.95
1:A:41:ASP:HB3	3:A:1189:HOH:O	1.69	0.91
1:B:1045:ARG:HG3	1:B:1045:ARG:NH1	1.76	0.91
1:B:1119:GLU:H	1:B:1119:GLU:CD	1.76	0.87
1:B:64:HIS:HD2	1:B:261:VAL:H	1.19	0.86
1:A:79:ILE:HG22	1:A:81:PRO:HD3	1.59	0.85
1:B:1030:SER:H	1:B:1102:ASN:HD21	1.23	0.83
1:A:64:HIS:HD2	1:A:261:VAL:H	1.25	0.81
1:A:1030:SER:H	1:A:1102:ASN:ND2	1.79	0.79
1:B:1042:GLU:OE1	1:B:1093:ASN:HB3	1.84	0.78
1:A:59:ILE:CD1	1:A:264:ALA:HB1	2.14	0.77
1:A:12:ASN:ND2	1:A:14:ASP:CG	2.38	0.77
1:B:44:GLU:HG2	1:B:62:TRP:CZ2	2.20	0.77
2:A:1122:MAL:O1	2:A:1122:MAL:C2	2.33	0.76
1:B:1045:ARG:CG	1:B:1045:ARG:HH11	1.89	0.76
1:A:1093:ASN:HD21	1:A:1117:VAL:H	1.31	0.76
1:B:214:GLU:HA	3:B:475:HOH:O	1.87	0.74
1:B:44:GLU:HG3	1:B:62:TRP:CH2	2.22	0.74
1:B:1062:GLU:O	1:B:1063:VAL:HB	1.87	0.74
1:B:90:TYR:HE2	1:B:308:GLU:HG2	1.52	0.74
1:A:68:GLY:HA3	1:A:332:ASN:O	1.88	0.73
1:B:1001:ILE:N	3:B:449:HOH:O	2.20	0.73
1:A:12:ASN:HD21	1:A:14:ASP:CG	1.89	0.72
1:A:1031:ASP:OD1	1:A:1031:ASP:C	2.29	0.71
1:B:64:HIS:CD2	1:B:261:VAL:H	2.07	0.70
1:B:79:ILE:HG21	1:B:106:TYR:CE1	2.26	0.69
1:A:1030:SER:CB	1:A:1103:PRO:HD2	2.23	0.69
1:A:128:THR:HG22	1:A:131:GLU:H	1.58	0.69
1:A:1030:SER:O	1:A:1031:ASP:O	2.11	0.68
1:B:1060:ILE:HG21	3:B:1176:HOH:O	1.93	0.68
2:A:1122:MAL:C4'	2:A:1122:MAL:C1	2.70	0.68
1:B:157:THR:HG23	3:B:389:HOH:O	1.94	0.67
1:B:217:PHE:HB3	3:B:475:HOH:O	1.94	0.67
1:B:44:GLU:CG	1:B:62:TRP:CZ2	2.78	0.67
1:A:128:THR:HG21	3:A:439:HOH:O	1.94	0.66
1:B:79:ILE:CB	3:B:450:HOH:O	2.26	0.66
1:A:185:ASN:HD22	1:A:185:ASN:C	1.98	0.66
1:B:128:THR:HG21	3:B:1240:HOH:O	1.96	0.66
1:A:12:ASN:ND2	1:A:14:ASP:N	2.37	0.65
1:A:1106:ILE:H	1:A:1106:ILE:HD13	1.60	0.65
1:A:1030:SER:N	1:A:1102:ASN:HD21	1.86	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:HIS:HE1	1:A:330:MET:O	1.80	0.65
1:B:1101:LYS:HG2	1:B:1108:GLY:HA2	1.78	0.64
1:A:64:HIS:CD2	1:A:261:VAL:H	2.12	0.64
1:A:1025:SER:OG	1:A:1079:LYS:NZ	2.28	0.64
1:B:128:THR:HG22	1:B:131:GLU:H	1.63	0.64
1:A:1027:GLU:HG2	1:A:1104:PRO:HB2	1.81	0.63
1:A:59:ILE:HD11	1:A:264:ALA:HB1	1.80	0.63
1:B:79:ILE:HG21	1:B:106:TYR:CZ	2.34	0.62
1:A:1070:ILE:HD13	1:A:1085:ILE:HD13	1.79	0.62
1:B:185:ASN:HD22	1:B:185:ASN:C	2.02	0.62
1:B:30:ASP:CG	1:B:31:THR:H	2.02	0.62
1:B:1106:ILE:HD12	3:B:484:HOH:O	1.98	0.62
1:B:136:ASP:OD2	1:B:203:HIS:HD2	1.83	0.62
1:A:1060:ILE:HG22	1:A:1061:ASP:H	1.64	0.62
1:B:44:GLU:CG	1:B:62:TRP:CH2	2.83	0.61
1:B:1087:ASN:HB3	3:B:1174:HOH:O	2.01	0.60
1:A:1031:ASP:CG	1:A:1031:ASP:O	2.39	0.60
1:A:1030:SER:HB3	1:A:1103:PRO:HD2	1.84	0.60
1:B:31:THR:OG1	1:B:31:THR:O	2.19	0.59
1:B:4:GLU:H	1:B:271:PRO:HG2	1.67	0.59
1:B:1030:SER:N	1:B:1102:ASN:HD21	1.97	0.59
1:A:136:ASP:OD2	1:A:203:HIS:HD2	1.85	0.59
1:B:1002:VAL:CG2	1:B:1109:LYS:HG2	2.33	0.59
1:A:295:LYS:HD2	1:A:295:LYS:C	2.22	0.58
1:B:1109:LYS:N	3:B:473:HOH:O	2.37	0.58
1:B:1030:SER:HB3	1:B:1103:PRO:HD2	1.86	0.58
1:A:233:SER:OG	1:A:298:PRO:HD3	2.04	0.58
1:A:59:ILE:HD13	1:A:280:LEU:HD11	1.84	0.58
1:A:356:THR:HG23	1:A:1077:ARG:HD2	1.86	0.57
1:B:30:ASP:O	1:B:31:THR:C	2.42	0.57
1:B:64:HIS:HE1	1:B:330:MET:O	1.86	0.57
1:A:203:HIS:HE1	3:A:1286:HOH:O	1.86	0.57
1:B:1031:ASP:O	1:B:1032:ASP:HB2	2.05	0.56
1:B:168:ALA:O	1:B:181:VAL:HA	2.05	0.56
1:A:192:LEU:O	1:A:196:VAL:HG13	2.06	0.56
1:A:59:ILE:HD12	1:A:264:ALA:HB1	1.87	0.56
1:A:193:THR:OG1	1:A:357:VAL:HG21	2.06	0.56
1:B:122:LEU:CD1	1:B:125:PRO:HA	2.36	0.55
1:A:12:ASN:HD22	1:A:14:ASP:H	1.48	0.55
1:B:1055:LYS:NZ	3:B:1267:HOH:O	2.39	0.55
1:B:185:ASN:ND2	1:B:188:ALA:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:ILE:HG22	1:A:1061:ASP:N	2.22	0.54
1:B:90:TYR:CE2	1:B:308:GLU:HG2	2.38	0.54
1:B:59:ILE:HD12	1:B:280:LEU:HD11	1.88	0.54
1:B:41:ASP:O	1:B:46:LYS:NZ	2.40	0.54
1:B:30:ASP:CB	3:B:478:HOH:O	2.26	0.54
1:B:1109:LYS:HZ1	1:B:1110:THR:H	1.55	0.54
1:B:1030:SER:H	1:B:1102:ASN:ND2	2.00	0.54
1:B:42:LYS:HA	1:B:44:GLU:OE2	2.08	0.53
1:B:59:ILE:CD1	1:B:280:LEU:HD21	2.38	0.53
1:B:1018:THR:HB	1:B:1084:VAL:HG22	1.90	0.53
1:A:288:GLU:HG3	3:A:1281:HOH:O	2.07	0.53
1:A:359:GLU:OE2	1:A:1077:ARG:NH1	2.42	0.53
1:B:1002:VAL:HG23	1:B:1109:LYS:HG2	1.90	0.53
1:A:362:LYS:HZ3	1:A:366:THR:HG23	1.73	0.53
1:A:128:THR:HG23	1:A:130:GLU:H	1.74	0.53
1:B:352:SER:OG	1:B:354:ARG:HG3	2.09	0.53
1:A:140:LYS:HD2	1:A:144:LYS:O	2.09	0.53
1:A:197:ASP:HA	1:A:200:LYS:HG2	1.91	0.52
1:A:168:ALA:O	1:A:181:VAL:HA	2.09	0.52
1:A:362:LYS:NZ	1:A:366:THR:CG2	2.72	0.52
1:A:31:THR:HG22	1:A:33:ILE:HG12	1.91	0.52
1:B:1106:ILE:N	3:B:484:HOH:O	2.31	0.52
1:A:1018:THR:HB	1:A:1084:VAL:HG22	1.92	0.52
1:A:362:LYS:NZ	1:A:366:THR:HG23	2.25	0.51
1:A:122:LEU:HD21	1:A:135:LEU:HD21	1.92	0.51
1:B:46:LYS:HZ2	1:B:46:LYS:HB2	1.74	0.51
1:A:205:ASN:HB3	1:A:207:ASP:OD1	2.10	0.51
1:B:1041:PRO:O	1:B:1043:GLY:N	2.44	0.51
1:B:44:GLU:HG3	1:B:62:TRP:CZ3	2.45	0.51
1:B:1109:LYS:NZ	1:B:1110:THR:H	2.08	0.51
1:A:128:THR:HB	1:A:131:GLU:OE1	2.11	0.51
1:B:1031:ASP:O	1:B:1032:ASP:CB	2.58	0.50
1:A:154:PRO:CB	1:A:343:VAL:HG23	2.41	0.50
1:B:1103:PRO:O	1:B:1106:ILE:HG23	2.11	0.50
1:B:122:LEU:HD13	1:B:125:PRO:HA	1.93	0.50
2:A:1122:MAL:O1	2:A:1122:MAL:O5	2.26	0.50
1:A:12:ASN:HD21	1:A:14:ASP:H	1.48	0.49
1:A:1093:ASN:ND2	1:A:1117:VAL:HG13	2.28	0.49
1:A:22:GLU:OE1	1:A:295:LYS:NZ	2.46	0.49
1:A:295:LYS:HE2	1:A:296:ASP:HB2	1.94	0.49
1:B:1013:VAL:HG21	1:B:1090:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:GLY:O	1:B:33:ILE:HG22	2.13	0.48
1:B:53:THR:O	1:B:53:THR:HG22	2.14	0.48
1:B:59:ILE:HD11	1:B:61:PHE:CE1	2.49	0.48
1:A:1093:ASN:ND2	1:A:1117:VAL:H	2.03	0.48
1:B:1016:GLN:NE2	3:B:1224:HOH:O	2.46	0.47
1:B:1090:TYR:O	1:B:1091:SER:CB	2.61	0.47
1:B:28:GLU:O	1:B:32:GLY:HA2	2.14	0.47
1:B:7:LEU:HG	3:B:493:HOH:O	2.14	0.47
1:A:62:TRP:CD1	1:A:66:ARG:HG3	2.50	0.47
1:A:43:LEU:HD12	1:A:43:LEU:C	2.35	0.47
1:A:129:TRP:HA	1:A:132:ILE:HD12	1.97	0.47
1:B:68:GLY:HA3	1:B:332:ASN:O	2.15	0.47
1:B:30:ASP:CG	1:B:31:THR:N	2.67	0.47
1:A:362:LYS:HE2	1:A:362:LYS:HA	1.97	0.47
1:B:97:VAL:O	1:B:104:ILE:HD13	2.13	0.47
1:A:218:ASN:N	1:A:218:ASN:HD22	2.13	0.47
1:B:1119:GLU:CD	1:B:1119:GLU:N	2.56	0.46
1:B:128:THR:HB	1:B:131:GLU:OE1	2.15	0.46
1:A:185:ASN:ND2	1:A:188:ALA:H	2.13	0.46
1:B:192:LEU:O	1:B:196:VAL:HG13	2.15	0.46
1:B:1077:ARG:HA	1:B:1077:ARG:HD2	1.49	0.46
1:A:362:LYS:HZ2	1:A:366:THR:CG2	2.29	0.46
1:B:1045:ARG:NH1	1:B:1045:ARG:CG	2.58	0.46
1:B:123:PRO:HD2	3:B:1284:HOH:O	2.15	0.46
1:B:1103:PRO:O	1:B:1104:PRO:C	2.46	0.45
1:B:233:SER:OG	1:B:298:PRO:HD3	2.16	0.45
1:B:31:THR:O	1:B:33:ILE:N	2.43	0.45
1:B:1057:GLN:HG2	1:B:1059:TYR:CZ	2.52	0.45
1:B:67:PHE:HE2	1:B:265:GLY:HA3	1.82	0.45
1:B:1062:GLU:O	1:B:1063:VAL:CB	2.60	0.45
1:B:1041:PRO:C	1:B:1043:GLY:H	2.20	0.45
1:A:1093:ASN:HD22	1:A:1117:VAL:HG13	1.82	0.44
1:B:218:ASN:HD21	1:B:235:ILE:HG12	1.82	0.44
1:A:1075:ASP:HA	1:A:1076:PRO:HD2	1.88	0.44
1:B:79:ILE:HD11	3:B:1124:HOH:O	2.18	0.44
1:B:1108:GLY:C	3:B:473:HOH:O	2.56	0.44
1:A:185:ASN:C	1:A:185:ASN:ND2	2.69	0.43
1:B:1041:PRO:C	1:B:1043:GLY:N	2.71	0.43
1:B:251:LYS:HE3	3:B:1249:HOH:O	2.19	0.43
1:A:278:GLU:OE1	1:A:282:ASN:ND2	2.52	0.43
1:B:1102:ASN:HA	1:B:1103:PRO:HD3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.54	0.43
1:B:1120:LYS:O	1:B:1121:VAL:HG13	2.18	0.42
1:B:354:ARG:HD2	1:B:1028:TRP:CE3	2.54	0.42
1:B:158:TRP:N	1:B:159:PRO:CD	2.83	0.42
1:B:1101:LYS:HE2	1:B:1108:GLY:HA3	2.01	0.42
1:B:1089:ASP:C	1:B:1090:TYR:O	2.59	0.41
1:B:4:GLU:N	1:B:272:ASN:HD21	2.18	0.41
1:A:1012:ALA:HA	1:A:1118:PHE:O	2.19	0.41
1:A:127:LYS:HD2	1:A:127:LYS:HA	1.78	0.41
1:B:175:LYS:NZ	1:B:175:LYS:HB3	2.35	0.41
1:B:254:PRO:HB3	1:B:326:LYS:HD3	2.02	0.41
1:B:46:LYS:HB2	1:B:46:LYS:NZ	2.36	0.41
1:A:154:PRO:HB3	1:A:343:VAL:HG23	2.01	0.41
1:B:1120:LYS:HG3	1:B:1121:VAL:H	1.86	0.41
1:B:1093:ASN:OD1	1:B:1117:VAL:HG13	2.21	0.41
1:B:1053:TYR:CZ	1:B:1076:PRO:HG3	2.56	0.40
1:A:1102:ASN:HA	1:A:1103:PRO:HD3	1.57	0.40
1:A:239:LYS:HE2	3:A:451:HOH:O	2.21	0.40
1:B:1025:SER:OG	1:B:1079:LYS:NZ	2.55	0.40
1:A:3:GLU:HA	1:A:4:GLU:CB	2.52	0.40
1:A:1098:CYS:O	1:A:1110:THR:HA	2.21	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)
3:A:1156:HOH:O	3:A:1308:HOH:O[2_556]	2.13	0.07

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	484/507 (96%)	466 (96%)	11 (2%)	7 (1%)	14 7
1	B	484/507 (96%)	456 (94%)	20 (4%)	8 (2%)	11 5
All	All	968/1014 (96%)	922 (95%)	31 (3%)	15 (2%)	13 7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	ASP
1	A	1104	PRO
1	A	1105	ASP
1	B	31	THR
1	B	1061	ASP
1	B	1063	VAL
1	A	4	GLU
1	B	4	GLU
1	B	1008	GLU
1	B	1031	ASP
1	B	1042	GLU
1	A	1028	TRP
1	A	1032	ASP
1	A	173	ASN
1	B	32	GLY

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	402/421 (96%)	366 (91%)	36 (9%)	12 8
1	B	402/421 (96%)	364 (90%)	38 (10%)	11 7
All	All	804/842 (96%)	730 (91%)	74 (9%)	11 7

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU

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Mol	Chain	Res	Type
1	A	6	LYS
1	A	34	LYS
1	A	44	GLU
1	A	55	ASP
1	A	59	ILE
1	A	82	ASP
1	A	128	THR
1	A	140	LYS
1	A	142	LYS
1	A	160	LEU
1	A	172	GLU
1	A	173	ASN
1	A	175	LYS
1	A	185	ASN
1	A	196	VAL
1	A	198	LEU
1	A	200	LYS
1	A	207	ASP
1	A	239	LYS
1	A	258	PHE
1	A	262	LEU
1	A	295	LYS
1	A	341	TYR
1	A	362	LYS
1	A	1018	THR
1	A	1031	ASP
1	A	1040	GLN
1	A	1057	GLN
1	A	1062	GLU
1	A	1088	LEU
1	A	1093	ASN
1	A	1105	ASP
1	A	1106	ILE
1	A	1117	VAL
1	A	1121	VAL
1	B	6	LYS
1	B	33	ILE
1	B	44	GLU
1	B	46	LYS
1	B	59	ILE
1	B	79	ILE
1	B	83	LYS

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Mol	Chain	Res	Type
1	B	102	LYS
1	B	104	ILE
1	B	115	LEU
1	B	122	LEU
1	B	128	THR
1	B	135	LEU
1	B	160	LEU
1	B	173	ASN
1	B	175	LYS
1	B	185	ASN
1	B	196	VAL
1	B	198	LEU
1	B	207	ASP
1	B	251	LYS
1	B	256	LYS
1	B	258	PHE
1	B	262	LEU
1	B	308	GLU
1	B	357	VAL
1	B	1018	THR
1	B	1031	ASP
1	B	1045	ARG
1	B	1077	ARG
1	B	1088	LEU
1	B	1091	SER
1	B	1103	PRO
1	B	1106	ILE
1	B	1107	VAL
1	B	1117	VAL
1	B	1119	GLU
1	B	1121	VAL

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

Mol	Chain	Res	Type
1	A	12	ASN
1	A	18	ASN
1	A	49	GLN
1	A	64	HIS
1	A	185	ASN
1	A	203	HIS
1	A	218	ASN

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	1052	HIS
1	A	1087	ASN
1	A	1093	ASN
1	A	1102	ASN
1	B	49	GLN
1	B	64	HIS
1	B	185	ASN
1	B	203	HIS
1	B	218	ASN
1	B	1052	HIS
1	B	1102	ASN

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

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	1122	-	24,24,24	1.73	1 (4%)	35,35,35	2.16	10 (28%)
2	MAL	B	1122	-	24,24,24	1.08	1 (4%)	35,35,35	1.54	6 (17%)

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	1122	-	-	0/8/48/48	0/2/2/2
2	MAL	B	1122	-	-	0/8/48/48	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1122	MAL	O1-C1	4.61	1.54	1.41
2	A	1122	MAL	O1-C1	8.23	1.64	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1122	MAL	O1-C1-O5	-6.26	94.83	110.68
2	A	1122	MAL	O1-C1-C2	-5.38	95.01	108.10
2	B	1122	MAL	O1-C1-O5	-4.47	99.36	110.68
2	B	1122	MAL	O1-C1-C2	-2.66	101.63	108.10
2	A	1122	MAL	O3'-C3'-C2'	-2.45	104.82	110.34
2	B	1122	MAL	O3-C3-C2	-2.22	105.35	110.34
2	A	1122	MAL	O2'-C2'-C3'	-2.03	105.77	110.34
2	A	1122	MAL	C1'-O5'-C5'	2.12	117.40	113.47
2	A	1122	MAL	C1'-C2'-C3'	2.34	113.91	110.43
2	B	1122	MAL	C1-O1-C4'	2.50	124.54	118.01
2	A	1122	MAL	C1-O1-C4'	2.54	124.64	118.01
2	B	1122	MAL	O5-C1-C2	2.91	116.24	110.28
2	B	1122	MAL	C1-O5-C5	3.08	119.72	113.75
2	A	1122	MAL	C1-O5-C5	3.62	120.78	113.75
2	A	1122	MAL	O5'-C1'-C2'	3.95	116.10	109.80
2	A	1122	MAL	O5-C1-C2	4.25	118.99	110.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1122	MAL	4	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, 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	488/507 (96%)	0.14	23 (4%)	35	44	14, 26, 43, 66	2 (0%)
1	B	488/507 (96%)	0.31	30 (6%)	25	33	15, 28, 49, 68	2 (0%)
All	All	976/1014 (96%)	0.23	53 (5%)	29	38	14, 27, 48, 68	4 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1063	VAL	10.1
1	A	1063	VAL	7.2
1	B	1121	VAL	6.6
1	B	1044	GLY	6.4
1	B	31	THR	6.0
1	B	1062	GLU	5.4
1	A	1062	GLU	5.3
1	A	1121	VAL	5.3
1	A	1064	GLY	4.9
1	A	341	TYR	4.7
1	B	1045	ARG	4.6
1	B	1061	ASP	4.3
1	B	173	ASN	4.2
1	A	173	ASN	4.1
1	B	84	ALA	4.0
1	B	1064	GLY	4.0
1	B	30	ASP	3.7
1	B	1119	GLU	3.6
1	B	1108	GLY	3.5
1	B	1031	ASP	3.5
1	A	1031	ASP	3.3
1	B	1057	GLN	3.3
1	A	1045	ARG	3.3
1	B	1048	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	1090	TYR	3.1
1	B	1046	ASP	3.0
1	A	1	LYS	3.0
1	B	172	GLU	3.0
1	B	1091	SER	3.0
1	B	1043	GLY	2.9
1	A	4	GLU	2.9
1	B	55	ASP	2.8
1	A	1090	TYR	2.7
1	A	1043	GLY	2.7
1	A	1046	ASP	2.6
1	A	174	GLY	2.6
1	B	1059	TYR	2.5
1	B	341	TYR	2.5
1	B	1103	PRO	2.5
1	A	1104	PRO	2.4
1	A	1048	ILE	2.4
1	B	1078	TRP	2.3
1	A	1103	PRO	2.3
1	A	147	LEU	2.3
1	A	41	ASP	2.3
1	A	1061	ASP	2.2
1	A	1065	THR	2.2
1	A	1068	GLU	2.1
1	B	5	GLY	2.1
1	B	1065	THR	2.1
1	B	1007	ARG	2.1
1	B	22	GLU	2.0
1	A	1059	TYR	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

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	B	1122	23/23	0.95	0.10	-0.55	14,17,20,22	0
2	MAL	A	1122	23/23	0.94	0.10	-0.78	13,17,21,23	0

6.5 Other polymers

There are no such residues in this entry.