Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:46 AM GMT

PDB ID	:	2EAB
Title	:	Crystal structure of 1,2-a-L-fucosidase from Bifidobacterium bifidum (apo form)
Authors	:	Nagae, M.; Tsuchiya, A.; Katayama, T.; Yamamoto, K.; Wakatsuki, S.; Kato, R.
Deposited on	:	2007-01-31
Resolution	:	1.12 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:

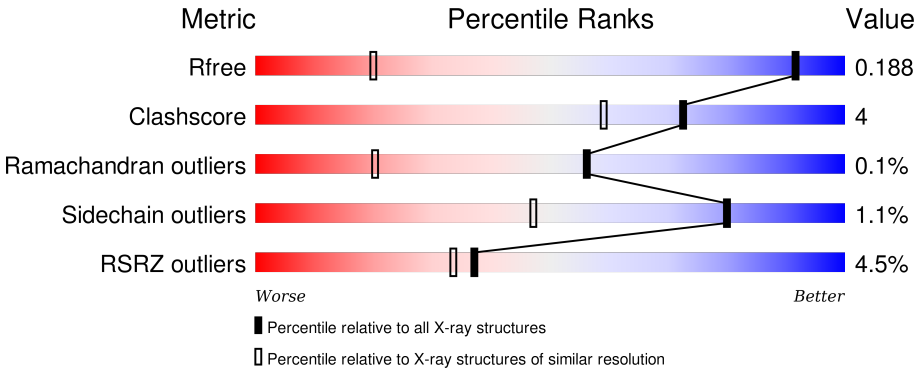
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.12 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	1158 (1.18-1.06)
Clashscore	102246	1215 (1.18-1.06)
Ramachandran outliers	100387	1162 (1.18-1.06)
Sidechain outliers	100360	1160 (1.18-1.06)
RSRZ outliers	91569	1161 (1.18-1.06)

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	899	5% 92% 6%
1	B	899	4% 91% 6%

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	EDO	A	4804	-	-	-	X
3	EDO	A	4805	-	-	-	X
3	EDO	A	4806	-	-	-	X
3	EDO	A	4807	-	-	-	X
3	EDO	A	4810	-	-	-	X
3	EDO	A	4812	-	-	X	X
3	EDO	B	4801	-	-	-	X
3	EDO	B	4802	-	X	X	X
3	EDO	B	4803	-	-	X	X
3	EDO	B	4808	-	X	X	X
3	EDO	B	4809	-	-	-	X
3	EDO	B	4811	-	-	X	X
4	TRS	A	5001	-	-	-	X
4	TRS	A	5002	-	-	-	X
4	TRS	B	5003	-	-	-	X
4	TRS	B	5004	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16940 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 Alpha-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	888	Total	C	N	O	S	0	0	0
			6760	4205	1168	1372	15			
1	B	881	Total	C	N	O	S	0	0	0
			6715	4181	1160	1359	15			

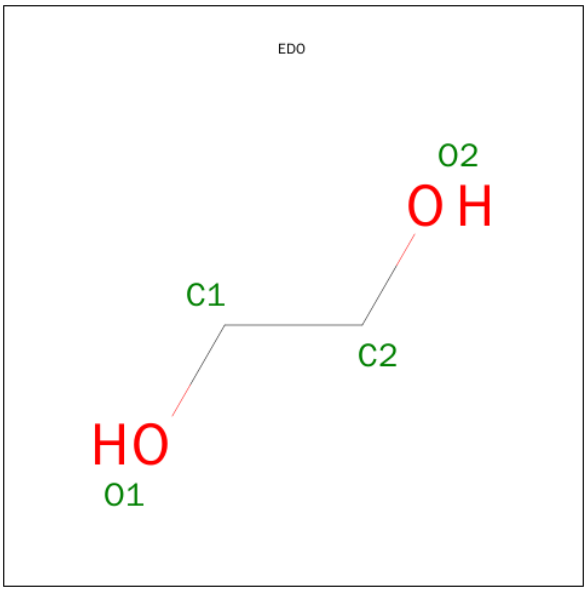
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP Q6JV24
B	0	MET	-	INITIATING METHIONINE	UNP Q6JV24

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

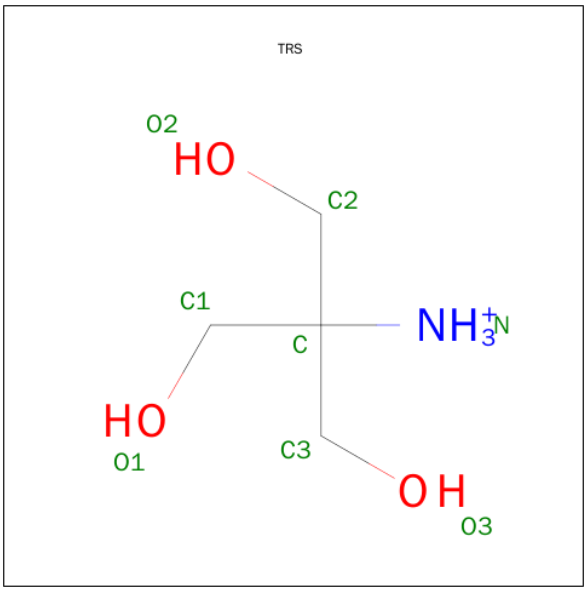
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	A	1	Total C N O 8 4 1 3	0	0
4	B	1	Total C N O 8 4 1 3	0	0
4	B	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is water.

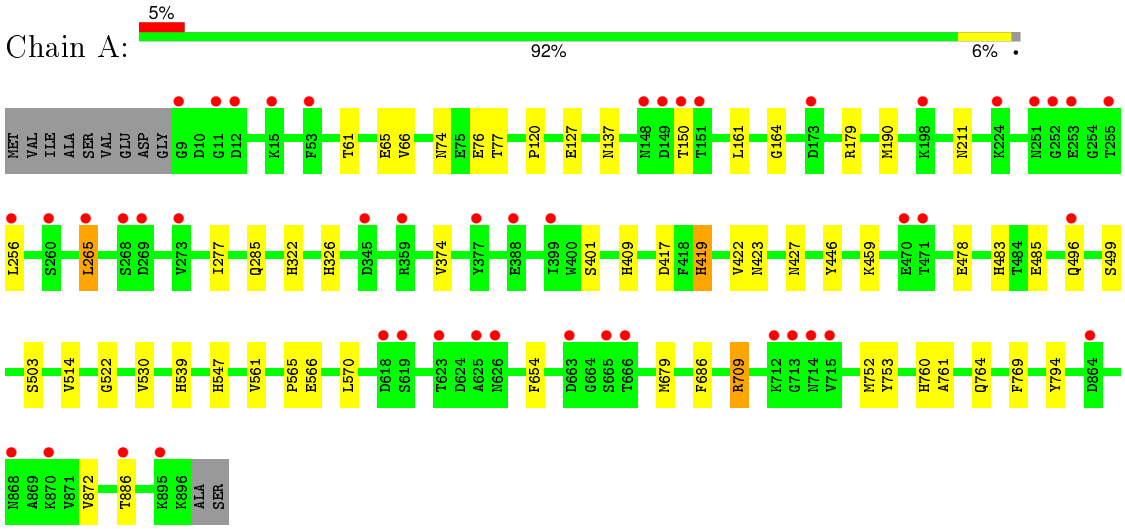
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1648	Total O 1648 1648	0	0
5	B	1735	Total O 1735 1735	0	0

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.

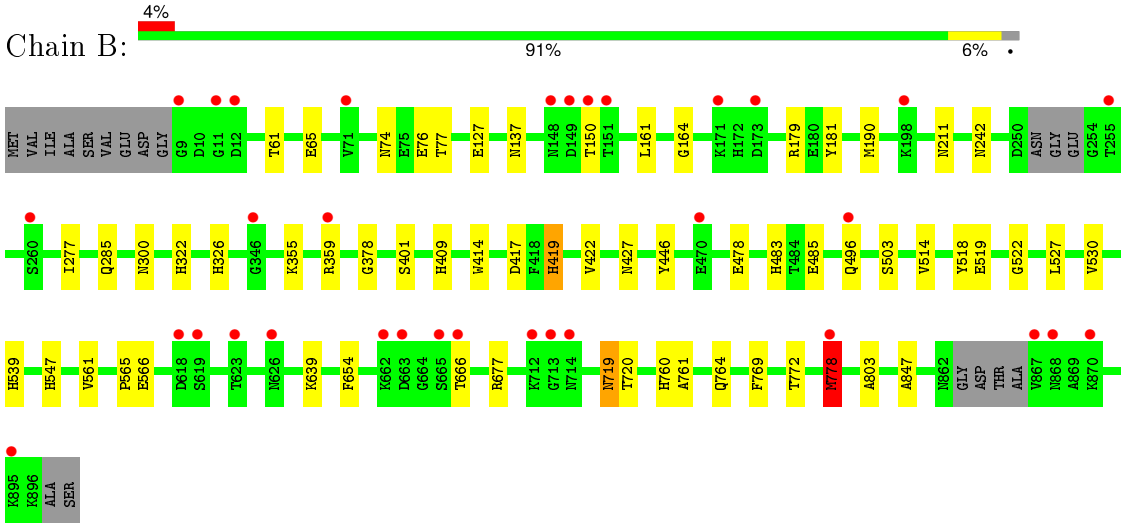
- Molecule 1: Alpha-fucosidase

Chain A:



- Molecule 1: Alpha-fucosidase

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	90.18Å 112.03Å 98.32Å 90.00° 94.74° 90.00°	Depositor
Resolution (Å)	35.05 – 1.12 35.05 – 1.12	Depositor EDS
% Data completeness (in resolution range)	91.6 (35.05-1.12) 91.6 (35.05-1.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.12Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.175 , 0.189 0.174 , 0.188	Depositor DCC
R_{free} test set	33894 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	8.9	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 676976 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16940	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CA, TRS, EDO

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	0.32	0/6906	0.54	0/9393
1	B	0.32	0/6859	0.55	2/9326 (0.0%)
All	All	0.32	0/13765	0.54	2/18719 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	778	MET	CA-CB-CG	5.58	122.78	113.30
1	B	778	MET	CB-CA-C	5.11	120.63	110.40

There are no chirality outliers.

There are no planarity outliers.

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	6760	0	6433	46	0
1	B	6715	0	6397	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	0	36	11	0
3	B	24	0	36	21	0
4	A	16	0	22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	22	0	0
5	A	1648	0	0	9	0
5	B	1735	0	0	8	0
All	All	16940	0	12946	111	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 4.

All (111) 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)
3:B:4808:EDO:C2	3:B:4808:EDO:C1	1.79	1.61
3:B:4811:EDO:C2	3:B:4811:EDO:C1	1.79	1.58
3:A:4812:EDO:C2	3:A:4812:EDO:O2	1.70	1.40
3:B:4802:EDO:C1	3:B:4802:EDO:C2	1.99	1.39
3:B:4803:EDO:C1	3:B:4803:EDO:O1	1.74	1.36
3:A:4805:EDO:C2	3:A:4805:EDO:O2	1.76	1.32
3:A:4806:EDO:O2	3:A:4806:EDO:C2	1.80	1.29
3:B:4809:EDO:O1	3:B:4809:EDO:C1	1.91	1.18
1:B:483:HIS:HD2	1:B:503:SER:H	1.12	0.96
1:A:483:HIS:HD2	1:A:503:SER:H	1.12	0.92
1:B:417:ASP:OD1	1:B:419:HIS:HD2	1.61	0.83
1:B:719:ASN:HD22	1:B:720:THR:H	1.23	0.83
1:A:137:ASN:HD22	1:A:211:ASN:HD22	1.28	0.81
1:A:417:ASP:OD1	1:A:419:HIS:HD2	1.63	0.81
1:B:242:ASN:HD21	1:B:300:ASN:HD22	1.31	0.79
1:B:137:ASN:HD22	1:B:211:ASN:HD22	1.28	0.79
3:B:4808:EDO:O1	3:B:4808:EDO:C2	2.33	0.77
3:B:4808:EDO:O2	3:B:4808:EDO:C1	2.32	0.77
1:B:483:HIS:CD2	1:B:503:SER:H	2.02	0.76
1:B:677:ARG:HE	1:B:719:ASN:HD21	1.31	0.75
1:A:686:PHE:CE1	3:A:4807:EDO:H12	2.25	0.71
1:A:74:ASN:HD21	1:A:401:SER:H	1.36	0.71
1:A:483:HIS:CD2	1:A:503:SER:H	2.02	0.71
1:B:74:ASN:HD21	1:B:401:SER:H	1.38	0.69
1:A:374:VAL:CG2	1:A:752:MET:HE2	2.24	0.68
1:B:565:PRO:HG2	3:B:4803:EDO:H11	1.75	0.68
1:B:847:ALA:HB2	5:B:6033:HOH:O	1.93	0.67
1:B:764:GLN:NE2	3:B:4802:EDO:O1	2.24	0.66
1:A:65:GLU:O	1:A:179:ARG:NH2	2.30	0.65
1:A:374:VAL:HG22	1:A:752:MET:HE2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4802:EDO:C2	3:B:4802:EDO:O1	2.45	0.63
1:A:423:ASN:HD21	3:A:4805:EDO:H12	1.64	0.62
1:B:65:GLU:O	1:B:179:ARG:NH2	2.33	0.62
1:A:161:LEU:O	1:A:326:HIS:HE1	1.83	0.61
1:B:539:HIS:HD2	5:B:5445:HOH:O	1.82	0.61
3:A:4812:EDO:O2	3:A:4812:EDO:C1	2.49	0.60
1:B:519:GLU:HA	3:B:4811:EDO:O2	2.01	0.60
1:A:539:HIS:HD2	5:A:5429:HOH:O	1.84	0.60
1:A:886:THR:HG23	5:A:5630:HOH:O	2.01	0.59
1:B:161:LEU:O	1:B:326:HIS:HE1	1.86	0.58
1:A:753:TYR:HA	5:A:6597:HOH:O	2.03	0.58
1:A:374:VAL:HG22	1:A:752:MET:CE	2.32	0.58
1:A:409:HIS:HE1	1:A:485:GLU:OE2	1.86	0.58
1:A:679:MET:HG2	1:A:709:ARG:HG2	1.87	0.57
3:B:4811:EDO:O1	3:B:4811:EDO:C2	2.51	0.57
1:B:285:GLN:HE22	1:B:446:TYR:HA	1.70	0.57
1:A:66:VAL:HG23	5:A:6580:HOH:O	2.04	0.57
1:A:483:HIS:HD2	1:A:503:SER:N	1.94	0.56
1:A:285:GLN:O	3:A:4810:EDO:H21	2.06	0.56
1:A:764:GLN:NE2	3:A:4806:EDO:O2	2.33	0.55
1:B:409:HIS:HE1	1:B:485:GLU:OE2	1.88	0.55
1:B:483:HIS:HD2	1:B:503:SER:N	1.94	0.54
1:A:285:GLN:HE22	1:A:446:TYR:HA	1.72	0.53
1:B:778:MET:HB2	1:B:803:ALA:O	2.08	0.53
1:A:561:VAL:HG13	5:A:6559:HOH:O	2.07	0.53
1:A:74:ASN:ND2	1:A:401:SER:H	2.06	0.52
1:A:137:ASN:ND2	1:A:211:ASN:HD22	2.03	0.52
1:B:74:ASN:ND2	1:B:401:SER:H	2.07	0.51
3:B:4808:EDO:H11	5:B:5049:HOH:O	2.11	0.51
3:B:4802:EDO:C1	3:B:4802:EDO:O2	2.56	0.50
1:B:478:GLU:OE1	1:B:539:HIS:HE1	1.95	0.50
1:B:419:HIS:HE1	5:B:5554:HOH:O	1.94	0.49
3:A:4812:EDO:C2	3:A:4812:EDO:HO2	2.13	0.49
1:A:419:HIS:HE1	5:A:5625:HOH:O	1.95	0.49
1:B:127:GLU:HA	1:B:496:GLN:CG	2.43	0.49
1:B:355:LYS:HG2	1:B:359:ARG:HE	1.76	0.49
1:A:127:GLU:HA	1:A:496:GLN:CG	2.43	0.49
1:B:417:ASP:OD1	1:B:419:HIS:CD2	2.53	0.49
1:B:561:VAL:HG13	5:B:6664:HOH:O	2.12	0.49
3:B:4808:EDO:C1	3:B:4808:EDO:HO2	2.24	0.48
1:B:639:LYS:HD3	5:B:5718:HOH:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASP:OD1	1:A:419:HIS:CD2	2.55	0.48
1:A:794:TYR:OH	1:A:872:VAL:HG11	2.14	0.48
1:B:566:GLU:HG2	5:B:5545:HOH:O	2.12	0.48
1:B:514:VAL:HG12	1:B:530:VAL:HG12	1.96	0.48
1:A:566:GLU:HG2	5:A:5512:HOH:O	2.14	0.47
1:A:256:LEU:HD11	1:A:265:LEU:HG	1.96	0.47
1:A:478:GLU:OE1	1:A:539:HIS:HE1	1.96	0.47
1:B:322:HIS:HD2	5:B:5097:HOH:O	1.97	0.47
1:A:514:VAL:HG12	1:A:530:VAL:HG12	1.96	0.46
1:A:459:LYS:HE3	5:A:6458:HOH:O	2.15	0.45
3:B:4803:EDO:C2	3:B:4803:EDO:O1	2.56	0.45
1:A:322:HIS:HD2	5:A:5080:HOH:O	1.98	0.45
1:A:374:VAL:HG21	1:A:752:MET:HE2	1.99	0.45
3:B:4811:EDO:H21	3:B:4811:EDO:C1	2.21	0.44
1:A:164:GLY:O	1:A:322:HIS:HE1	2.00	0.44
1:A:499:SER:HB3	1:A:570:LEU:HD11	2.00	0.43
1:A:190:MET:HB3	1:A:277:ILE:HB	2.00	0.43
1:B:565:PRO:HA	1:B:566:GLU:HA	1.78	0.43
3:B:4811:EDO:H22	3:B:4811:EDO:C1	2.21	0.42
1:B:565:PRO:CG	3:B:4803:EDO:H11	2.48	0.42
1:A:522:GLY:HA2	3:A:4812:EDO:H21	2.02	0.42
1:A:565:PRO:HA	1:A:566:GLU:HA	1.78	0.42
1:A:76:GLU:HG3	1:A:77:THR:HG23	2.00	0.42
1:B:164:GLY:O	1:B:322:HIS:HE1	2.02	0.42
1:B:76:GLU:HG3	1:B:77:THR:HG23	2.01	0.42
1:A:760:HIS:N	1:A:761:ALA:HA	2.35	0.41
1:B:179:ARG:HD2	1:B:181:TYR:OH	2.21	0.41
1:A:427:ASN:HA	1:A:769:PHE:CD2	2.56	0.41
1:B:719:ASN:ND2	1:B:720:THR:H	2.05	0.41
1:B:127:GLU:HA	1:B:496:GLN:HG2	2.02	0.41
1:B:414:TRP:CH2	3:B:4802:EDO:H12	2.56	0.41
1:B:760:HIS:N	1:B:761:ALA:HA	2.36	0.41
1:A:120:PRO:HB3	1:A:561:VAL:HG21	2.02	0.41
1:B:190:MET:HB3	1:B:277:ILE:HB	2.02	0.41
1:B:427:ASN:HA	1:B:769:PHE:CD2	2.56	0.41
1:B:518:TYR:CE1	1:B:527:LEU:HB2	2.56	0.41
1:B:677:ARG:HE	1:B:719:ASN:ND2	2.07	0.40
1:A:686:PHE:CZ	3:A:4807:EDO:H12	2.56	0.40
1:B:378:GLY:HA3	1:B:772:THR:OG1	2.21	0.40
1:B:522:GLY:HA2	3:B:4811:EDO:H11	2.04	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	886/899 (99%)	862 (97%)	23 (3%)	1 (0%)	56 20
1	B	875/899 (97%)	850 (97%)	24 (3%)	1 (0%)	56 20
All	All	1761/1798 (98%)	1712 (97%)	47 (3%)	2 (0%)	56 20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	VAL
1	B	422	VAL

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	704/712 (99%)	697 (99%)	7 (1%)	82 51
1	B	700/712 (98%)	692 (99%)	8 (1%)	80 47
All	All	1404/1424 (99%)	1389 (99%)	15 (1%)	80 47

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR
1	A	150	THR
1	A	265	LEU
1	A	419	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	547	HIS
1	A	654	PHE
1	A	709	ARG
1	B	61	THR
1	B	150	THR
1	B	419	HIS
1	B	547	HIS
1	B	654	PHE
1	B	666	THR
1	B	719	ASN
1	B	778	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	100	ASN
1	A	134	ASN
1	A	137	ASN
1	A	213	ASN
1	A	285	GLN
1	A	322	HIS
1	A	326	HIS
1	A	409	HIS
1	A	419	HIS
1	A	423	ASN
1	A	483	HIS
1	A	513	ASN
1	A	539	HIS
1	A	742	GLN
1	A	764	GLN
1	A	841	ASN
1	B	74	ASN
1	B	93	ASN
1	B	100	ASN
1	B	134	ASN
1	B	137	ASN
1	B	172	HIS
1	B	213	ASN
1	B	285	GLN
1	B	300	ASN
1	B	322	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	326	HIS
1	B	397	GLN
1	B	409	HIS
1	B	419	HIS
1	B	423	ASN
1	B	483	HIS
1	B	513	ASN
1	B	539	HIS
1	B	675	GLN
1	B	678	HIS
1	B	719	ASN
1	B	742	GLN
1	B	764	GLN
1	B	841	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

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\|>2$
3	EDO	A	4804	-	3,3,3	1.63	0	2,2,2	0.82	0
3	EDO	A	4805	-	3,3,3	4.10	2 (66%)	2,2,2	0.57	0
3	EDO	A	4806	-	3,3,3	4.35	1 (33%)	2,2,2	0.83	0
3	EDO	A	4807	-	3,3,3	1.39	0	2,2,2	0.84	0
3	EDO	A	4810	-	3,3,3	0.85	0	2,2,2	0.53	0
3	EDO	A	4812	-	3,3,3	3.16	1 (33%)	2,2,2	2.01	1 (50%)
4	TRS	A	5001	-	7,7,7	1.43	2 (28%)	9,9,9	1.55	1 (11%)
4	TRS	A	5002	-	7,7,7	1.49	2 (28%)	9,9,9	1.38	1 (11%)
3	EDO	B	4801	-	3,3,3	1.51	1 (33%)	2,2,2	0.70	0
3	EDO	B	4802	-	3,3,3	4.27	2 (66%)	2,2,2	2.88	2 (100%)
3	EDO	B	4803	-	3,3,3	3.57	1 (33%)	2,2,2	0.89	0
3	EDO	B	4808	-	3,3,3	3.20	3 (100%)	2,2,2	3.42	2 (100%)
3	EDO	B	4809	-	3,3,3	5.34	1 (33%)	2,2,2	1.03	0
3	EDO	B	4811	-	3,3,3	2.71	1 (33%)	2,2,2	2.83	1 (50%)
4	TRS	B	5003	-	7,7,7	1.45	2 (28%)	9,9,9	1.53	1 (11%)
4	TRS	B	5004	-	7,7,7	1.47	2 (28%)	9,9,9	1.51	1 (11%)

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
3	EDO	A	4804	-	-	0/1/1/1	0/0/0/0
3	EDO	A	4805	-	-	0/1/1/1	0/0/0/0
3	EDO	A	4806	-	-	0/1/1/1	0/0/0/0
3	EDO	A	4807	-	-	0/1/1/1	0/0/0/0
3	EDO	A	4810	-	-	0/1/1/1	0/0/0/0
3	EDO	A	4812	-	-	0/1/1/1	0/0/0/0
4	TRS	A	5001	-	-	0/9/9/9	0/0/0/0
4	TRS	A	5002	-	-	0/9/9/9	0/0/0/0
3	EDO	B	4801	-	-	0/1/1/1	0/0/0/0
3	EDO	B	4802	-	-	0/1/1/1	0/0/0/0
3	EDO	B	4803	-	-	0/1/1/1	0/0/0/0
3	EDO	B	4808	-	-	0/1/1/1	0/0/0/0
3	EDO	B	4809	-	-	0/1/1/1	0/0/0/0
3	EDO	B	4811	-	-	0/1/1/1	0/0/0/0
4	TRS	B	5003	-	-	0/9/9/9	0/0/0/0
4	TRS	B	5004	-	-	0/9/9/9	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5002	TRS	C-N	-2.81	1.46	1.50
4	B	5004	TRS	C-N	-2.78	1.46	1.50
4	A	5001	TRS	O2-C2	-2.62	1.33	1.42
4	B	5003	TRS	O2-C2	-2.61	1.33	1.42
4	B	5003	TRS	C-N	-2.58	1.46	1.50
4	A	5001	TRS	C-N	-2.56	1.46	1.50
4	A	5002	TRS	O2-C2	-2.55	1.33	1.42
4	B	5004	TRS	O2-C2	-2.52	1.34	1.42
3	B	4802	EDO	O1-C1	2.03	1.53	1.42
3	B	4808	EDO	O1-C1	2.34	1.54	1.42
3	B	4801	EDO	O2-C2	2.36	1.54	1.42
3	B	4808	EDO	O2-C2	2.48	1.55	1.42
3	A	4805	EDO	C2-C1	3.20	1.71	1.47
3	B	4811	EDO	C2-C1	4.33	1.79	1.47
3	B	4808	EDO	C2-C1	4.38	1.79	1.47
3	A	4812	EDO	O2-C2	5.26	1.70	1.42
3	B	4803	EDO	O1-C1	5.94	1.74	1.42
3	A	4805	EDO	O2-C2	6.34	1.76	1.42
3	B	4802	EDO	C2-C1	7.09	1.99	1.47
3	A	4806	EDO	O2-C2	7.19	1.80	1.42
3	B	4809	EDO	O1-C1	9.17	1.91	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	4802	EDO	O1-C1-C2	-3.47	87.68	112.54
3	B	4808	EDO	O2-C2-C1	-3.44	87.87	112.54
3	B	4808	EDO	O1-C1-C2	-3.40	88.18	112.54
3	A	4812	EDO	O1-C1-C2	-2.17	97.00	112.54
3	B	4802	EDO	O2-C2-C1	-2.14	97.18	112.54
3	B	4811	EDO	O2-C2-C1	3.50	137.60	112.54
4	A	5002	TRS	O2-C2-C	4.03	119.34	111.18
4	B	5003	TRS	O2-C2-C	4.28	119.84	111.18
4	B	5004	TRS	O2-C2-C	4.29	119.86	111.18
4	A	5001	TRS	O2-C2-C	4.33	119.94	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4805	EDO	2	0
3	A	4806	EDO	2	0
3	A	4807	EDO	2	0
3	A	4810	EDO	1	0
3	A	4812	EDO	4	0
3	B	4802	EDO	5	0
3	B	4803	EDO	4	0
3	B	4808	EDO	5	0
3	B	4809	EDO	1	0
3	B	4811	EDO	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	888/899 (98%)	0.57	47 (5%)	30	27	5, 9, 18, 26	0
1	B	881/899 (97%)	0.49	33 (3%)	45	41	5, 9, 17, 24	0
All	All	1769/1798 (98%)	0.53	80 (4%)	37	33	5, 9, 17, 26	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	GLY	7.5
1	A	149	ASP	7.4
1	B	150	THR	7.3
1	B	9	GLY	7.1
1	A	150	THR	5.7
1	B	149	ASP	5.6
1	A	11	GLY	5.0
1	B	11	GLY	4.9
1	A	714	ASN	4.7
1	A	148	ASN	4.6
1	B	714	ASN	4.6
1	A	251	ASN	4.5
1	B	148	ASN	4.4
1	A	868	ASN	4.1
1	A	252	GLY	4.1
1	A	260	SER	3.8
1	A	864	ASP	3.8
1	B	663	ASP	3.8
1	B	868	ASN	3.7
1	B	260	SER	3.6
1	B	662	LYS	3.6
1	B	359	ARG	3.5
1	B	618	ASP	3.4
1	A	359	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	255	THR	3.4
1	A	173	ASP	3.4
1	A	253	GLU	3.4
1	B	173	ASP	3.3
1	A	12	ASP	3.3
1	A	663	ASP	3.3
1	A	345	ASP	3.1
1	A	198	LYS	3.0
1	A	256	LEU	3.0
1	B	666	THR	2.9
1	A	618	ASP	2.8
1	A	626	ASN	2.8
1	B	151	THR	2.7
1	B	470	GLU	2.7
1	A	471	THR	2.7
1	A	619	SER	2.6
1	B	867	VAL	2.6
1	A	713	GLY	2.6
1	B	496	GLN	2.6
1	B	346	GLY	2.6
1	B	626	ASN	2.6
1	A	273	VAL	2.6
1	B	870	LYS	2.6
1	A	665	SER	2.5
1	A	496	GLN	2.5
1	A	151	THR	2.5
1	B	623	THR	2.5
1	A	268	SER	2.5
1	A	269	ASP	2.5
1	B	778	MET	2.5
1	A	470	GLU	2.5
1	B	12	ASP	2.5
1	A	623	THR	2.4
1	A	53	PHE	2.4
1	B	71	VAL	2.3
1	A	895	LYS	2.3
1	A	715	VAL	2.3
1	B	712	LYS	2.3
1	A	224	LYS	2.3
1	A	666	THR	2.2
1	B	255	THR	2.2
1	B	895	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	619	SER	2.2
1	B	198	LYS	2.2
1	A	625	ALA	2.2
1	A	15	LYS	2.2
1	B	665	SER	2.1
1	A	399	ILE	2.1
1	A	712	LYS	2.1
1	A	870	LYS	2.1
1	B	171	LYS	2.1
1	A	388	GLU	2.1
1	B	713	GLY	2.0
1	A	886	THR	2.0
1	A	265	LEU	2.0
1	A	377	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 (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
3	EDO	B	4808	4/4	0.48	0.50	48.72	37,38,40,41	0
3	EDO	A	4807	4/4	0.28	0.58	36.48	37,37,42,43	0
4	TRS	B	5003	8/8	0.76	0.32	34.32	23,27,27,27	0
3	EDO	B	4802	4/4	0.47	0.44	33.27	30,30,33,35	0
4	TRS	B	5004	8/8	0.82	0.33	32.55	19,24,24,24	0
3	EDO	A	4806	4/4	0.46	0.45	26.51	34,36,36,36	0
4	TRS	A	5002	8/8	0.81	0.32	24.59	21,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	TRS	A	5001	8/8	0.83	0.30	21.90	24,27,27,27	0
3	EDO	A	4812	4/4	0.54	0.48	20.76	40,41,41,42	0
3	EDO	A	4804	4/4	0.63	0.38	19.81	27,29,30,30	0
3	EDO	B	4803	4/4	0.64	0.35	18.99	24,25,25,28	0
3	EDO	B	4811	4/4	0.62	0.43	18.97	36,38,39,40	0
3	EDO	B	4809	4/4	0.63	0.43	18.53	37,38,40,40	0
3	EDO	A	4810	4/4	0.60	0.40	16.69	37,37,41,42	0
3	EDO	B	4801	4/4	0.47	0.40	7.81	38,38,39,40	0
3	EDO	A	4805	4/4	0.54	0.37	6.56	39,40,40,40	0
2	CA	B	899	1/1	1.00	0.05	-2.72	7,7,7,7	0
2	CA	A	899	1/1	1.00	0.03	-3.22	8,8,8,8	0

6.5 Other polymers

There are no such residues in this entry.