Full wwPDB X-ray Structure Validation Report (i)

Dec 15, 2016 – 03:13 PM EST

PDB ID	:	5KKB
Title	:	Structure of mouse Golgi alpha-1,2-mannosidase IA and Man9GlcNAc2-PA complex
Authors	:	Xiang, Y.; Moremen, K.W.
Deposited on	:	2016-06-21
Resolution	:	1.77 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:

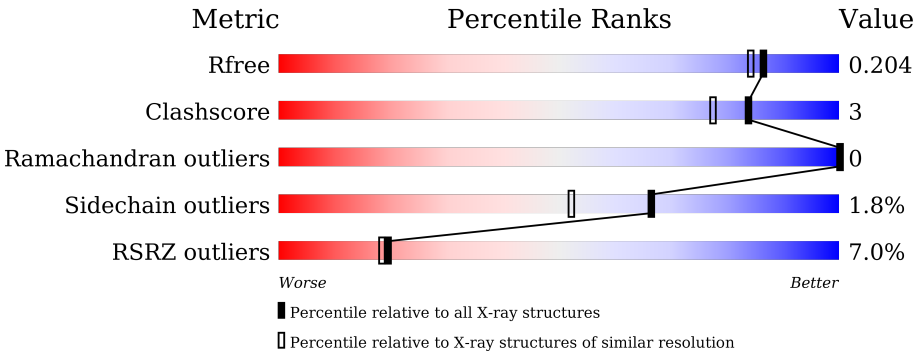
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.77 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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	469	6% 93% 7%
1	B	469	8% 92% 8%

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	MAN	A	703	-	-	-	X
6	1PS	A	712	-	-	-	X
6	1PS	B	711	-	-	X	X

2 Entry composition

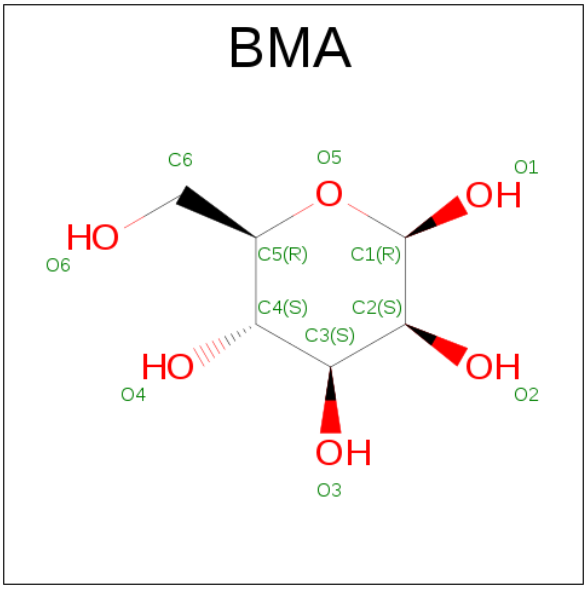
There are 8 unique types of molecules in this entry. The entry contains 8514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mannosyl-oligosaccharide 1,2-alpha-mannosidase IA.

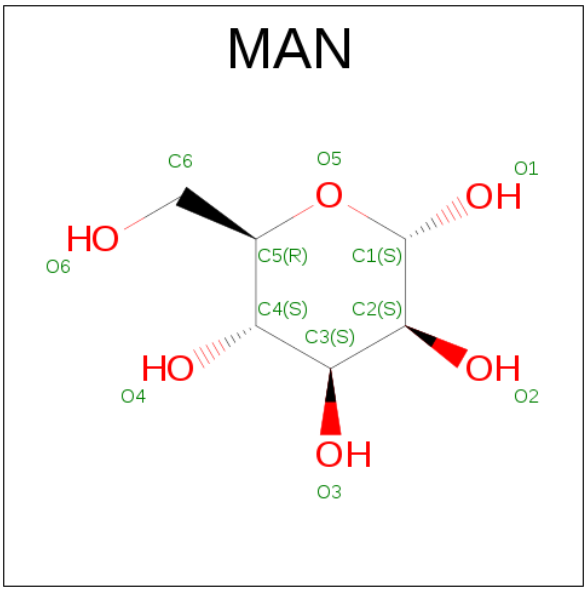
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	5	0
			3820	2468	645	689	18			
1	B	469	Total	C	N	O	S	0	6	0
			3815	2470	639	688	18			

- Molecule 2 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



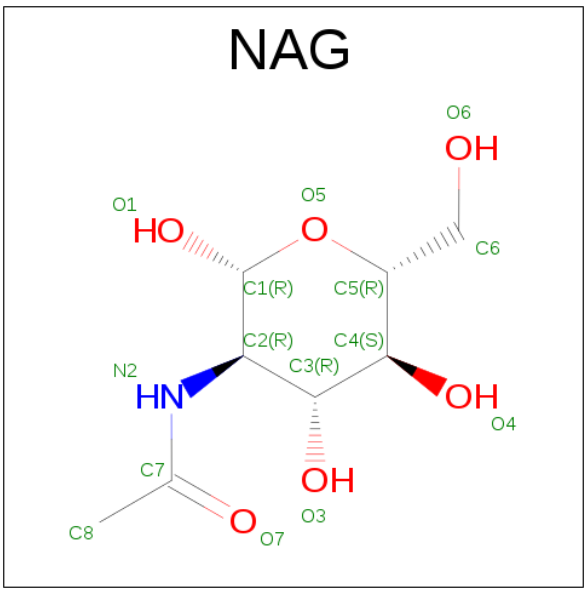
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

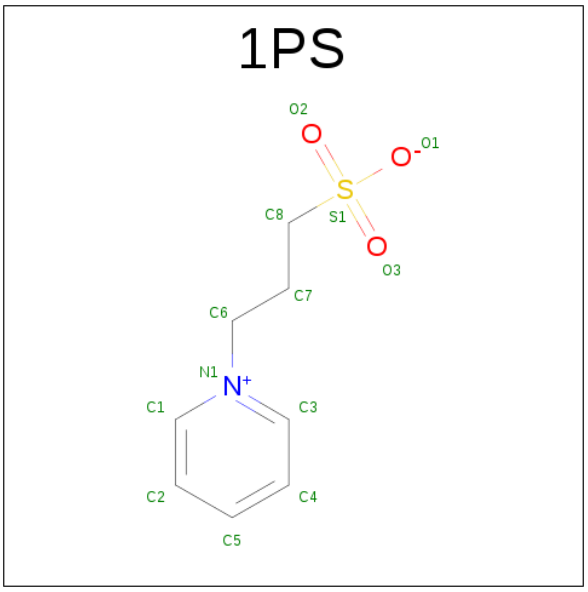


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 15 8 1 6	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 15 8 1 6	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is LANTHANUM (III) ION (three-letter code: LA) (formula: La).

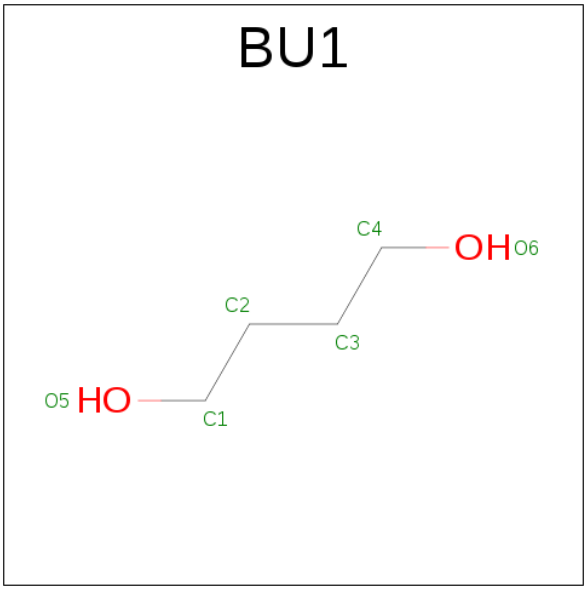
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total La 1 1	0	0
5	A	1	Total La 1 1	0	0

- Molecule 6 is 3-PYRIDINIUM-1-YLPROPANE-1-SULFONATE (three-letter code: 1PS) (formula: $C_8H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
6	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 7 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O		0	0
			6	4	2			

- Molecule 8 is water.

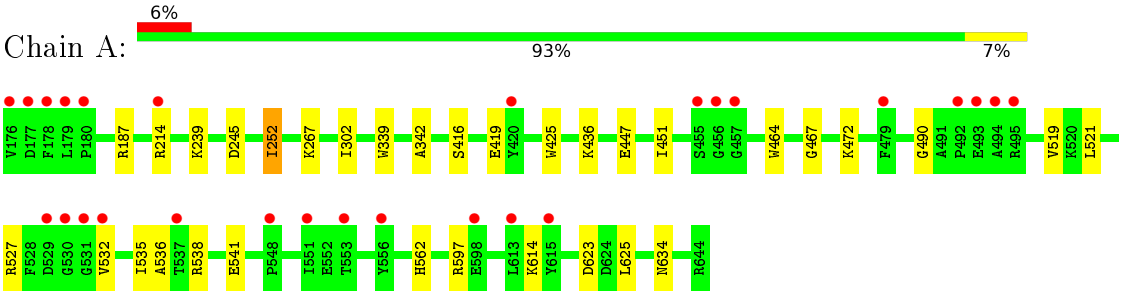
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	305	Total O 305 305	0	0
8	B	306	Total O 306 306	0	0

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.

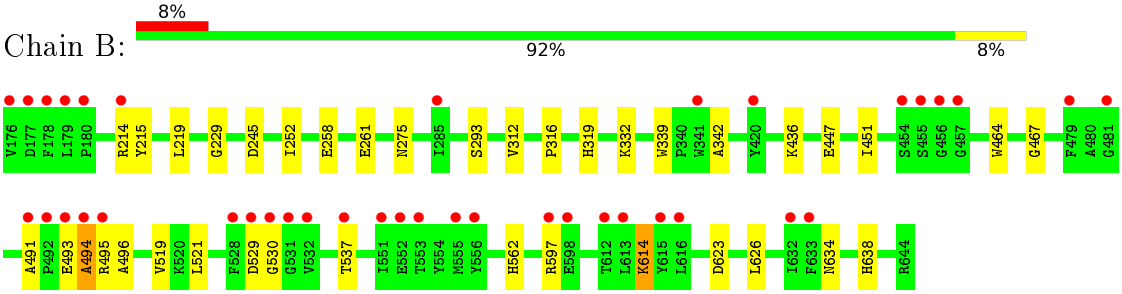
- Molecule 1: Mannosyl-oligosaccharide 1,2-alpha-mannosidase IA

Chain A:



- Molecule 1: Mannosyl-oligosaccharide 1,2-alpha-mannosidase IA

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.95Å 131.49Å 87.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 1.77 41.76 – 1.77	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.84-1.77) 91.3 (41.76-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 1.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.161 , 0.191 0.178 , 0.204	Depositor DCC
R_{free} test set	1915 reflections (1.97%)	DCC
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	1.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8514	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5266e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, LA, BU1, 1PS, MAN

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	0.38	0/3928	0.54	0/5315
1	B	0.38	0/3926	0.54	0/5315
All	All	0.38	0/7854	0.54	0/10630

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	494	ALA	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	3820	0	3731	17	0
1	B	3815	0	3735	24	0
2	A	11	0	8	0	0
2	B	11	0	8	0	0
3	A	77	0	63	0	0
3	B	77	0	63	0	0
4	A	29	0	27	0	0
4	B	29	0	27	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	13	0	11	2	0
6	B	13	0	11	7	0
7	B	6	0	10	1	0
8	A	305	0	0	3	0
8	B	306	0	0	2	0
All	All	8514	0	7694	46	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 3.

All (46) 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:623:ASP:H	7:B:713:BU1:H22	1.31	0.96
6:B:711:1PS:H2	8:B:943:HOH:O	1.84	0.77
1:A:267:LYS:HG2	1:A:302:ILE:HG12	1.73	0.69
1:B:316:PRO:HD3	6:B:711:1PS:O1	1.98	0.64
1:B:530:GLY:O	8:B:801:HOH:O	2.16	0.63
1:A:519:VAL:HG23	1:A:521:LEU:H	1.72	0.53
1:B:252[B]:ILE:HD11	1:B:614:LYS:HG3	1.90	0.53
1:B:519:VAL:HG23	1:B:521:LEU:H	1.74	0.52
1:B:219:LEU:HD13	1:B:229:GLY:HA3	1.91	0.52
1:B:562:HIS:NE2	1:B:623:ASP:OD2	2.43	0.51
1:B:275:ASN:OD1	1:B:332:LYS:HD2	2.12	0.50
1:B:319:HIS:ND1	6:B:711:1PS:H5	2.26	0.50
6:A:712:1PS:H4	8:A:901:HOH:O	2.11	0.49
1:B:464:TRP:CE2	1:B:467:GLY:HA2	2.48	0.49
1:B:447:GLU:HG2	1:B:451:ILE:HD12	1.95	0.49
1:A:464:TRP:CE2	1:A:467:GLY:HA2	2.48	0.49
1:A:252:ILE:HD11	1:A:625:LEU:HG	1.95	0.48
1:B:494:ALA:HA	1:B:496:ALA:H	1.78	0.48
1:B:252[A]:ILE:CD1	1:B:626:LEU:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:GLU:HA	1:B:494:ALA:HA	1.60	0.47
1:B:214:ARG:HG2	1:B:215:TYR:CZ	2.49	0.47
1:A:562:HIS:NE2	1:A:623:ASP:OD2	2.47	0.47
6:B:711:1PS:O1	6:B:711:1PS:H61	2.14	0.46
1:B:562:HIS:CE1	1:B:623:ASP:OD2	2.69	0.46
1:B:339:TRP:HB2	1:B:342:ALA:HB2	1.97	0.46
1:A:532:VAL:HB	1:A:535:ILE:HD13	1.98	0.45
1:B:312:VAL:HG13	6:B:711:1PS:O3	2.17	0.45
1:A:267:LYS:HE2	1:A:302:ILE:HG21	1.98	0.45
1:A:536:ALA:HB1	1:A:541[A]:GLU:HG3	1.99	0.44
1:B:258:GLU:O	1:B:261:GLU:HG2	2.18	0.44
6:A:712:1PS:H61	8:A:845:HOH:O	2.17	0.44
1:B:493:GLU:HB2	1:B:496:ALA:HB2	1.99	0.44
1:A:447:GLU:HG2	1:A:451:ILE:HD12	1.99	0.43
1:A:472:LYS:HD3	1:A:527:ARG:CZ	2.48	0.43
6:B:711:1PS:H71	6:B:711:1PS:H3	1.77	0.43
1:A:425:TRP:HH2	1:A:490:GLY:HA3	1.85	0.42
1:B:319:HIS:HB2	6:B:711:1PS:H5	2.01	0.42
1:B:436:LYS:NZ	1:B:491:ALA:HB3	2.35	0.42
1:A:562:HIS:CE1	1:A:623:ASP:OD2	2.72	0.42
1:A:416:SER:HA	1:A:419:GLU:HB3	2.02	0.41
1:B:562:HIS:HE2	1:B:623:ASP:CG	2.22	0.41
1:A:425:TRP:CD1	1:A:436:LYS:HB2	2.56	0.41
1:A:339:TRP:HB2	1:A:342:ALA:HB2	2.03	0.41
1:A:538:ARG:O	1:A:541[A]:GLU:HG2	2.21	0.41
1:A:239:LYS:NZ	8:A:805:HOH:O	2.43	0.40
1:B:293[B]:SER:OG	1:B:638:HIS:HB3	2.21	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	472/469 (101%)	459 (97%)	13 (3%)	0	100	100
1	B	473/469 (101%)	460 (97%)	13 (3%)	0	100	100
All	All	945/938 (101%)	919 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	397/392 (101%)	390 (98%)	7 (2%)	66	52
1	B	398/392 (102%)	391 (98%)	7 (2%)	66	52
All	All	795/784 (101%)	781 (98%)	14 (2%)	66	52

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	214	ARG
1	A	245	ASP
1	A	252	ILE
1	A	597	ARG
1	A	614	LYS
1	A	634	ASN
1	B	245	ASP
1	B	495	ARG
1	B	529	ASP
1	B	537	THR
1	B	597	ARG
1	B	614	LYS
1	B	634	ASN

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	BMA	A	701	3,4	11,11,12	0.90	1 (9%)	15,15,17	1.02	0
3	MAN	A	702	3,2	11,11,12	0.79	1 (9%)	15,15,17	1.05	1 (6%)
3	MAN	A	703	3	11,11,12	0.80	0	15,15,17	0.97	1 (6%)
3	MAN	A	704	3	11,11,12	0.86	0	15,15,17	0.96	0
3	MAN	A	705	3	11,11,12	0.84	0	15,15,17	0.88	0
4	NAG	A	706	2	15,15,15	0.23	0	17,21,21	0.21	0
3	MAN	A	707	3,2	11,11,12	0.78	0	15,15,17	1.04	1 (6%)
3	MAN	A	708	3	11,11,12	0.90	0	15,15,17	0.96	2 (13%)
3	MAN	A	709	3,5	11,11,12	1.05	1 (9%)	15,15,17	1.80	4 (26%)
4	NAG	A	710	1	14,14,15	0.22	0	15,19,21	0.44	0
6	1PS	A	712	-	13,13,13	1.49	3 (23%)	16,17,17	2.76	3 (18%)
2	BMA	B	701	3,4	11,11,12	1.03	1 (9%)	15,15,17	1.17	2 (13%)
3	MAN	B	702	3,2	11,11,12	0.65	0	15,15,17	0.99	1 (6%)
3	MAN	B	703	3	11,11,12	0.81	0	15,15,17	0.98	2 (13%)
3	MAN	B	704	3	11,11,12	0.84	0	15,15,17	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	B	705	3	11,11,12	0.73	0	15,15,17	0.88	1 (6%)
4	NAG	B	706	2	15,15,15	0.26	0	17,21,21	0.38	0
3	MAN	B	707	3,2	11,11,12	1.04	0	15,15,17	0.92	1 (6%)
3	MAN	B	708	3	11,11,12	1.11	1 (9%)	15,15,17	1.08	2 (13%)
3	MAN	B	709	3,5	11,11,12	1.18	1 (9%)	15,15,17	1.83	4 (26%)
4	NAG	B	710	1	14,14,15	0.18	0	15,19,21	0.45	0
6	1PS	B	711	-	13,13,13	1.33	2 (15%)	16,17,17	2.75	7 (43%)
7	BU1	B	713	-	5,5,5	0.32	0	4,4,4	0.62	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	BMA	A	701	3,4	-	0/2/19/22	0/1/1/1
3	MAN	A	702	3,2	-	0/2/19/22	0/1/1/1
3	MAN	A	703	3	-	0/2/19/22	0/1/1/1
3	MAN	A	704	3	-	0/2/19/22	0/1/1/1
3	MAN	A	705	3	-	0/2/19/22	0/1/1/1
4	NAG	A	706	2	-	0/6/26/26	0/1/1/1
3	MAN	A	707	3,2	-	0/2/19/22	0/1/1/1
3	MAN	A	708	3	-	0/2/19/22	0/1/1/1
3	MAN	A	709	3,5	-	0/2/19/22	0/1/1/1
4	NAG	A	710	1	-	0/6/23/26	0/1/1/1
6	1PS	A	712	-	-	0/7/7/7	0/1/1/1
2	BMA	B	701	3,4	-	0/2/19/22	0/1/1/1
3	MAN	B	702	3,2	-	0/2/19/22	0/1/1/1
3	MAN	B	703	3	-	0/2/19/22	0/1/1/1
3	MAN	B	704	3	-	0/2/19/22	0/1/1/1
3	MAN	B	705	3	-	0/2/19/22	0/1/1/1
4	NAG	B	706	2	-	0/6/26/26	0/1/1/1
3	MAN	B	707	3,2	-	0/2/19/22	0/1/1/1
3	MAN	B	708	3	-	0/2/19/22	0/1/1/1
3	MAN	B	709	3,5	-	0/2/19/22	0/1/1/1
4	NAG	B	710	1	-	0/6/23/26	0/1/1/1
6	1PS	B	711	-	-	0/7/7/7	0/1/1/1
7	BU1	B	713	-	-	0/3/3/3	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	MAN	O5-C1	-2.05	1.40	1.43
2	A	701	BMA	C1-C2	2.02	1.57	1.52
6	A	712	1PS	O2-S1	2.21	1.51	1.45
2	B	701	BMA	C1-C2	2.24	1.57	1.52
6	B	711	1PS	O2-S1	2.32	1.51	1.45
3	B	709	MAN	O5-C5	2.39	1.48	1.43
6	A	712	1PS	O3-S1	2.47	1.52	1.45
3	A	709	MAN	O5-C5	2.48	1.48	1.43
3	B	708	MAN	C2-C3	2.48	1.55	1.52
6	B	711	1PS	C8-S1	2.90	1.81	1.77
6	A	712	1PS	C8-S1	3.33	1.82	1.77

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	711	1PS	O1-S1-O2	-4.83	100.58	111.26
6	A	712	1PS	O3-S1-O2	-3.98	102.72	113.96
3	A	707	MAN	O2-C2-C3	-2.95	104.25	110.19
3	A	702	MAN	O2-C2-C3	-2.72	104.70	110.19
3	B	709	MAN	O2-C2-C3	-2.70	104.75	110.19
3	B	708	MAN	O2-C2-C3	-2.68	104.79	110.19
3	B	702	MAN	O2-C2-C3	-2.41	105.33	110.19
3	B	707	MAN	O2-C2-C3	-2.37	105.40	110.19
6	B	711	1PS	C7-C8-S1	-2.35	109.31	113.15
6	B	711	1PS	C7-C6-N1	-2.22	105.27	111.61
2	B	701	BMA	O2-C2-C3	-2.19	105.77	110.19
3	B	705	MAN	O2-C2-C3	-2.17	105.81	110.19
3	A	708	MAN	O2-C2-C3	-2.13	105.90	110.19
6	B	711	1PS	O1-S1-O3	-2.12	106.58	111.26
3	B	703	MAN	O2-C2-C3	-2.08	105.99	110.19
3	A	709	MAN	C1-C2-C3	2.09	112.09	109.55
3	A	709	MAN	O5-C1-C2	2.15	114.33	110.89
2	B	701	BMA	O2-C2-C1	2.23	113.70	109.23
6	B	711	1PS	C1-C2-C5	2.30	122.27	118.85
3	A	708	MAN	C1-O5-C5	2.37	115.62	112.14
3	B	708	MAN	C1-O5-C5	2.50	115.82	112.14
3	B	703	MAN	C1-O5-C5	2.54	115.87	112.14
3	A	703	MAN	C1-O5-C5	2.59	115.95	112.14
3	B	709	MAN	O5-C1-C2	2.60	115.05	110.89
3	B	709	MAN	O5-C5-C6	2.64	112.99	107.34
3	A	709	MAN	O5-C5-C6	2.75	113.22	107.34
6	B	711	1PS	O1-S1-C8	5.03	115.45	104.99
3	B	709	MAN	C1-O5-C5	5.03	119.54	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	709	MAN	C1-O5-C5	5.04	119.55	112.14
6	A	712	1PS	O2-S1-C8	5.86	111.01	106.87
6	B	711	1PS	O2-S1-C8	7.05	111.85	106.87
6	A	712	1PS	O3-S1-C8	8.05	112.56	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	712	1PS	2	0
6	B	711	1PS	7	0
7	B	713	BU1	1	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	469/469 (100%)	0.34	27 (5%)	26	24	14, 25, 50, 114	1 (0%)
1	B	469/469 (100%)	0.52	39 (8%)	14	13	14, 26, 51, 116	0
All	All	938/938 (100%)	0.43	66 (7%)	19	18	14, 26, 51, 116	1 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	ALA	13.1
1	A	531	GLY	11.3
1	A	532	VAL	9.8
1	B	531	GLY	8.6
1	A	494	ALA	8.5
1	B	532	VAL	7.1
1	B	177	ASP	6.0
1	B	494	ALA	5.6
1	B	492	PRO	5.3
1	B	178	PHE	5.2
1	B	493	GLU	5.1
1	A	530	GLY	4.9
1	A	179	LEU	4.8
1	B	179	LEU	4.7
1	A	492	PRO	4.6
1	A	177	ASP	4.3
1	A	176	VAL	4.0
1	A	493	GLU	4.0
1	A	456	GLY	3.6
1	B	556	TYR	3.5
1	A	178	PHE	3.4
1	B	528	PHE	3.4
1	B	176	VAL	3.3
1	A	455	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	457	GLY	3.1
1	B	530	GLY	3.1
1	B	633	PHE	3.0
1	B	180	PRO	3.0
1	A	598	GLU	2.9
1	B	598	GLU	2.9
1	B	341	TRP	2.8
1	A	180	PRO	2.8
1	B	456	GLY	2.8
1	B	597	ARG	2.7
1	B	455	SER	2.7
1	A	548	PRO	2.7
1	B	613	LEU	2.7
1	A	556	TYR	2.7
1	B	615	TYR	2.7
1	A	551	ILE	2.6
1	A	615	TYR	2.6
1	B	479	PHE	2.6
1	B	537	THR	2.6
1	A	537	THR	2.5
1	A	613	LEU	2.5
1	B	529	ASP	2.5
1	B	555[A]	MET	2.5
1	A	457	GLY	2.5
1	B	285	ILE	2.5
1	B	616	LEU	2.5
1	A	214	ARG	2.4
1	A	495	ARG	2.4
1	B	214	ARG	2.4
1	B	420	TYR	2.4
1	A	420	TYR	2.3
1	A	553	THR	2.3
1	A	529	ASP	2.3
1	A	479	PHE	2.3
1	B	553	THR	2.2
1	B	551	ILE	2.2
1	B	632	ILE	2.1
1	B	454	SER	2.1
1	B	612	THR	2.1
1	B	552	GLU	2.1
1	B	481	GLY	2.1
1	B	495	ARG	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
6	1PS	B	711	13/13	0.69	0.43	41.53	30,37,55,57	13
6	1PS	A	712	13/13	0.52	0.44	25.95	30,43,59,61	13
3	MAN	A	703	11/12	0.90	0.15	4.13	32,39,44,44	0
3	MAN	A	708	11/12	0.97	0.15	1.26	12,15,18,18	0
3	MAN	B	703	11/12	0.89	0.12	1.08	31,37,41,45	0
3	MAN	A	709	11/12	0.94	0.18	0.75	10,15,21,24	0
3	MAN	B	708	11/12	0.98	0.14	0.52	13,15,17,18	0
3	MAN	B	709	11/12	0.93	0.16	0.15	12,16,20,23	0
7	BU1	B	713	6/6	0.87	0.12	-0.28	38,44,48,55	0
3	MAN	A	707	11/12	0.96	0.08	-1.16	13,17,26,32	0
3	MAN	B	707	11/12	0.97	0.07	-1.23	16,18,29,29	0
5	LA	B	712	1/1	1.00	0.14	-1.24	11,11,11,11	1
5	LA	A	711	1/1	1.00	0.13	-1.38	11,11,11,11	1
3	MAN	B	702	11/12	0.94	0.12	-	29,33,43,45	0
4	NAG	A	710	14/15	0.88	0.19	-	39,51,57,60	0
3	MAN	B	705	11/12	0.86	0.20	-	63,69,71,72	0
4	NAG	B	710	14/15	0.86	0.20	-	37,52,59,62	0
3	MAN	B	704	11/12	0.83	0.15	-	52,58,61,62	0
4	NAG	B	706	15/15	0.85	0.17	-	25,38,57,66	0
3	MAN	A	705	11/12	0.77	0.22	-	64,66,71,75	0
2	BMA	A	701	11/12	0.96	0.06	-	18,22,27,28	0
4	NAG	A	706	15/15	0.90	0.14	-	27,40,65,67	0
3	MAN	A	702	11/12	0.94	0.12	-	27,31,39,41	0
3	MAN	A	704	11/12	0.87	0.15	-	49,58,61,64	0
2	BMA	B	701	11/12	0.98	0.06	-	17,20,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.