wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2017 – 06:42 AM EDT

PDB ID	:	2I37
Title	:	Crystal structure of a photoactivated rhodopsin
Authors	:	Lodowski, D.T.; Stenkamp, R.E.; Salom, D.; Le Trong, I.; Palczewski, K.
Deposited on	:	unknown
Resolution	:	4.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

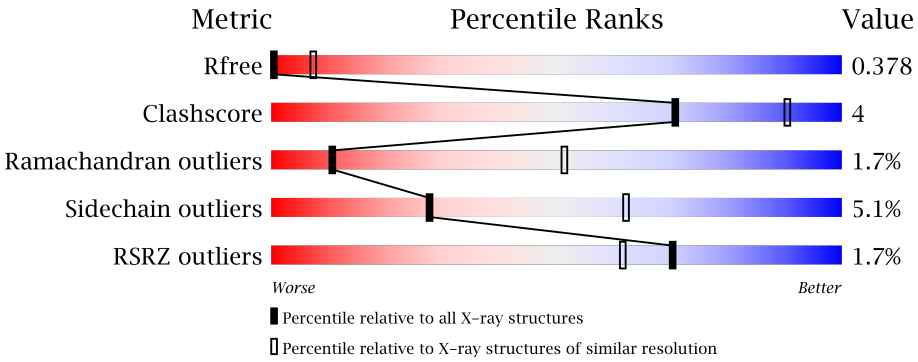
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 4.15 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	1166 (4.72-3.60)
Clashscore	112137	1018 (4.66-3.66)
Ramachandran outliers	110173	1021 (4.70-3.62)
Sidechain outliers	110143	1006 (4.70-3.62)
RSRZ outliers	101464	1178 (4.72-3.60)

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	349	.% 78% 13% • 9%
1	B	349	2% 77% 13% • 8%
1	C	349	.% 77% 13% • 9%

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
5	NDG	B	705	-	-	-	X

2 Entry composition

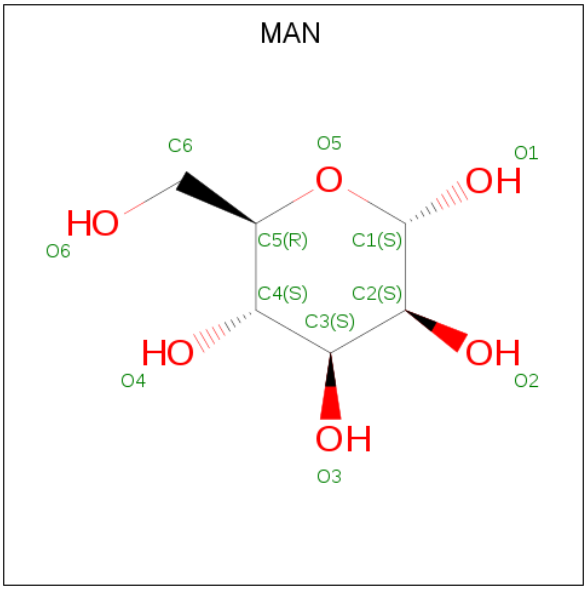
There are 5 unique types of molecules in this entry. The entry contains 7814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2518	1680	385	427	26			
1	B	320	Total	C	N	O	S	0	0	0
			2534	1689	387	432	26			
1	C	319	Total	C	N	O	S	0	0	0
			2525	1682	387	430	26			

- Molecule 2 is ALPHA-D-MANNOSE (three-letter code: MAN) (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			
2	C	1	Total	C	O		0	0
			11	6	5			

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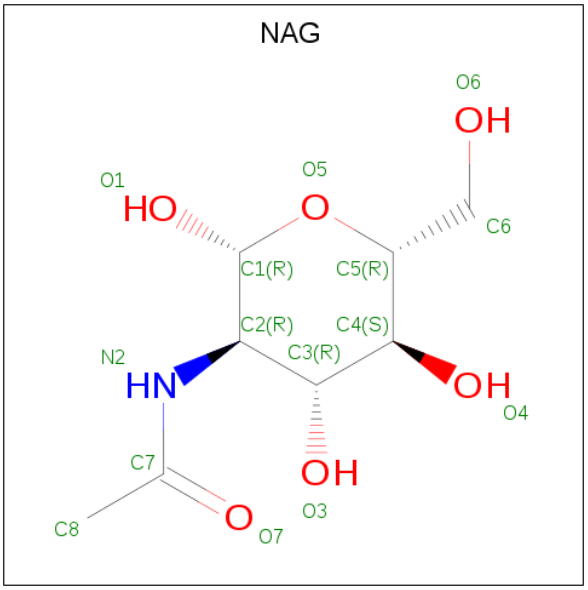
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 11 6 5	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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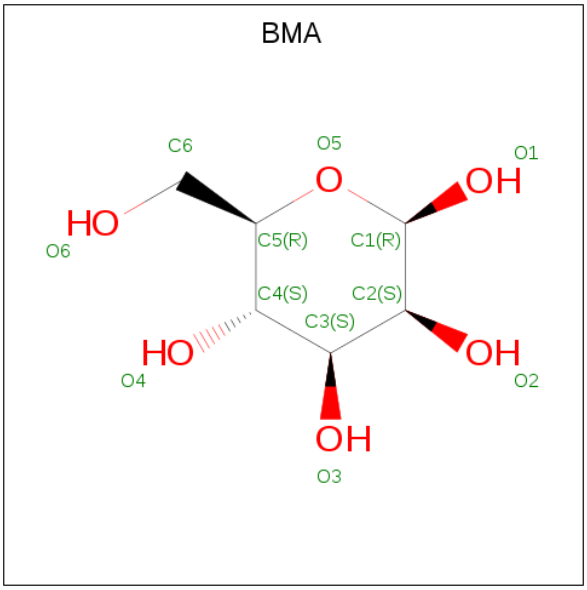
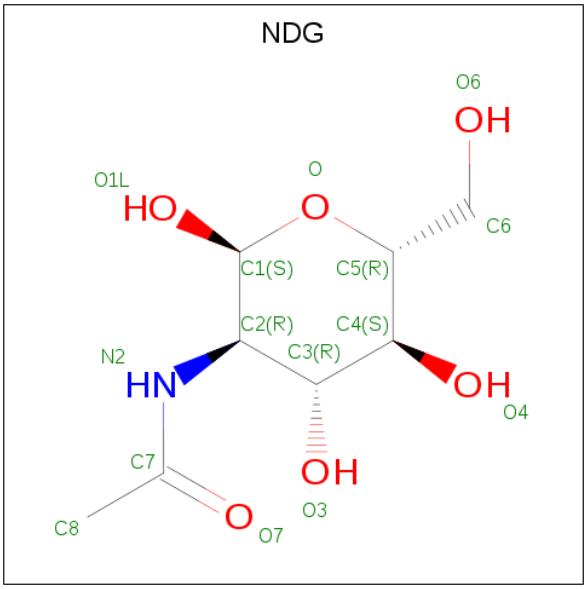
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 5 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



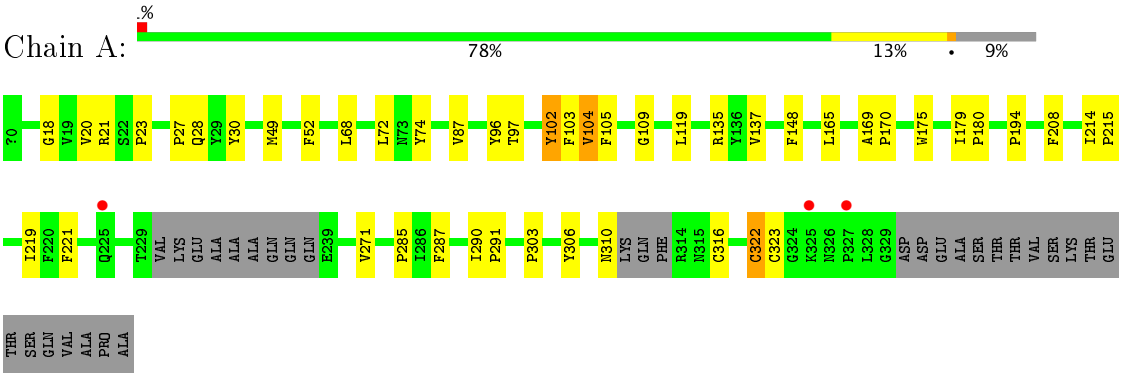
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

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 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.

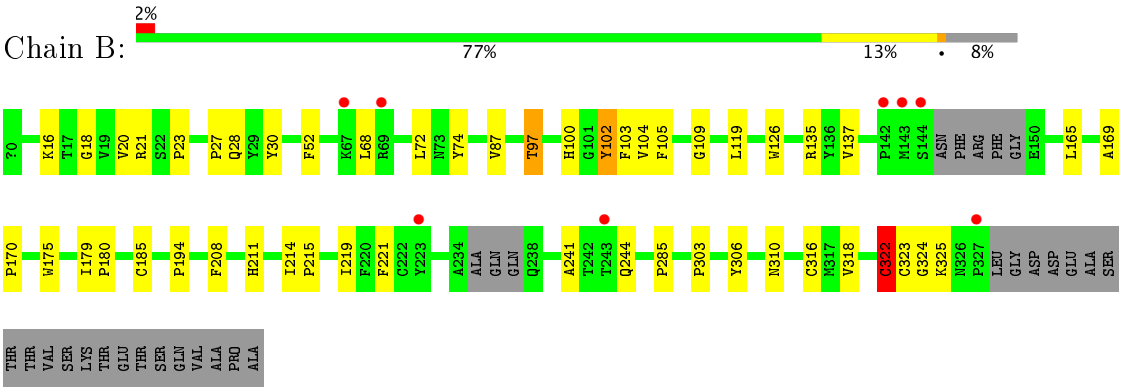
- Molecule 1: Rhodopsin

Chain A:



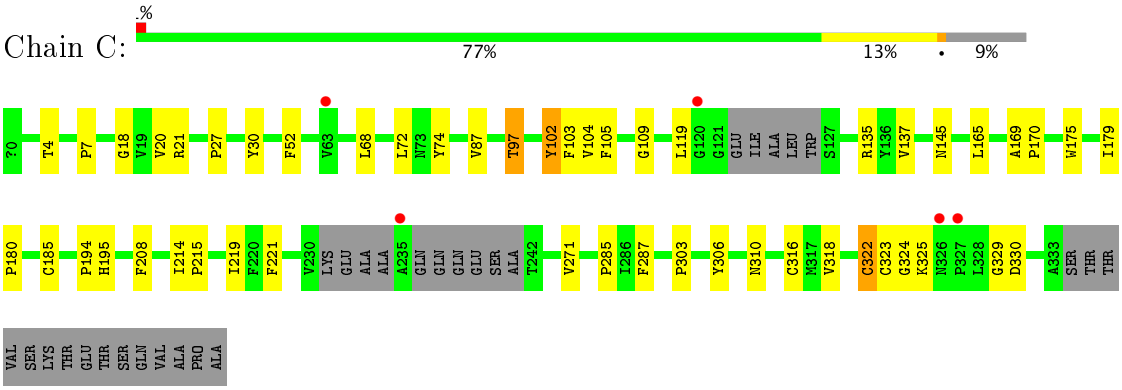
- Molecule 1: Rhodopsin

Chain B:



- Molecule 1: Rhodopsin

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	161.25Å 161.25Å 143.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.15 29.81 – 4.15	Depositor EDS
% Data completeness (in resolution range)	76.8 (30.00-4.15) 76.8 (29.81-4.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 4.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.377 , 0.382 0.376 , 0.378	Depositor DCC
R_{free} test set	645 reflections (5.46%)	DCC
Wilson B-factor (Å^2)	233.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7814	wwPDB-VP
Average B, all atoms (Å^2)	183.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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, 0.333 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, NDG, NAG, ACE, 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	0.37	0/2596	0.46	0/3538
1	B	0.39	0/2611	0.47	0/3558
1	C	0.37	0/2601	0.47	0/3541
All	All	0.38	0/7808	0.47	0/10637

There are no bond length outliers.

There are no bond angle outliers.

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	2518	0	2491	20	0
1	B	2534	0	2513	23	0
1	C	2525	0	2494	22	0
2	A	11	0	10	0	0
2	B	11	0	9	0	0
2	C	22	0	19	0	0
3	A	56	0	49	1	0
3	B	56	0	50	2	0
3	C	42	0	37	4	0
4	B	11	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	12	0	0
5	C	14	0	12	0	0
All	All	7814	0	7705	63	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.

The worst 5 of 63 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:16:LYS:O	1:C:7:PRO:HA	1.94	0.67
1:B:322:CYS:O	1:B:323:CYS:SG	2.56	0.64
1:C:4:THR:CG2	3:C:505:NAG:H83	2.32	0.60
1:A:20:VAL:O	3:A:505:NAG:O5	2.23	0.55
1:B:219:ILE:O	1:B:219:ILE:HG22	2.07	0.55

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	312/349 (89%)	272 (87%)	35 (11%)	5 (2%)	11 52
1	B	314/349 (90%)	271 (86%)	38 (12%)	5 (2%)	11 52
1	C	312/349 (89%)	269 (86%)	37 (12%)	6 (2%)	9 49
All	All	938/1047 (90%)	812 (87%)	110 (12%)	16 (2%)	11 51

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	CYS

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Mol	Chain	Res	Type
1	A	18	GLY
1	A	323	CYS
1	B	18	GLY
1	C	18	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	271/296 (92%)	257 (95%)	14 (5%)	27	62
1	B	273/296 (92%)	259 (95%)	14 (5%)	28	62
1	C	272/296 (92%)	258 (95%)	14 (5%)	28	62
All	All	816/888 (92%)	774 (95%)	42 (5%)	28	62

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	103	PHE
1	B	175	TRP
1	C	208	PHE
1	B	104	VAL
1	B	135	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	ASN
1	B	151	ASN
1	C	151	ASN
1	A	315	ASN
1	C	73	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

18 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	MAN	A	503	3	11,11,12	0.55	0	13,15,17	1.46	1 (7%)
3	NAG	A	504	3,2	14,14,15	0.52	0	15,19,21	1.59	2 (13%)
3	NAG	A	505	1,3	14,14,15	0.59	0	15,19,21	1.56	3 (20%)
3	NAG	A	704	3	14,14,15	0.80	1 (7%)	15,19,21	1.56	2 (13%)
3	NAG	A	705	1,3	14,14,15	0.56	0	15,19,21	0.98	1 (6%)
3	NAG	B	501	4	14,14,15	0.63	0	15,19,21	1.02	1 (6%)
4	BMA	B	502	3,2	11,11,12	0.65	0	13,15,17	1.16	1 (7%)
2	MAN	B	503	3,4	11,11,12	0.84	0	13,15,17	1.90	3 (23%)
3	NAG	B	504	3,2	14,14,15	0.44	0	15,19,21	1.22	2 (13%)
3	NAG	B	505	1,3	14,14,15	0.66	0	15,19,21	1.18	1 (6%)
3	NAG	B	704	5	14,14,15	0.58	0	15,19,21	0.89	1 (6%)
5	NDG	B	705	1,3	14,14,15	0.59	0	15,19,21	1.54	3 (20%)
2	MAN	C	502	2	11,11,12	0.52	0	13,15,17	1.41	1 (7%)
2	MAN	C	503	3,2	11,11,12	0.54	0	13,15,17	2.75	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	504	3,2	14,14,15	0.62	0	15,19,21	0.86	0
3	NAG	C	505	1,3	14,14,15	0.46	0	15,19,21	0.85	0
3	NAG	C	704	5	14,14,15	0.71	0	15,19,21	1.30	3 (20%)
5	NDG	C	705	1,3	14,14,15	0.49	0	15,19,21	1.36	3 (20%)

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	MAN	A	503	3	-	0/2/19/22	1/1/1/1
3	NAG	A	504	3,2	-	1/6/23/26	0/1/1/1
3	NAG	A	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	704	3	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1,3	-	1/6/23/26	0/1/1/1
3	NAG	B	501	4	-	0/6/23/26	0/1/1/1
4	BMA	B	502	3,2	-	0/2/19/22	0/1/1/1
2	MAN	B	503	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	504	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	704	5	-	0/6/23/26	0/1/1/1
5	NDG	B	705	1,3	-	0/6/23/26	0/1/1/1
2	MAN	C	502	2	-	0/2/19/22	0/1/1/1
2	MAN	C	503	3,2	-	0/2/19/22	0/1/1/1
3	NAG	C	504	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	704	5	-	0/6/23/26	0/1/1/1
5	NDG	C	705	1,3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	NAG	C1-C2	2.26	1.55	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	504	NAG	O5-C1-C2	-4.13	105.72	111.47
5	B	705	NDG	O-C1-C2	-3.47	106.64	111.47
3	A	504	NAG	C2-N2-C7	-3.34	118.07	122.94
3	A	505	NAG	O5-C1-C2	-2.41	108.11	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	504	NAG	C3-C4-C5	-2.23	106.29	110.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	705	NAG	O7-C7-N2-C2
3	A	504	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	NAG	1	0
3	B	505	NAG	2	0
3	C	505	NAG	4	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	317/349 (90%)	-0.24	3 (0%)	84	77	183, 183, 183, 183	0
1	B	319/349 (91%)	-0.13	8 (2%)	58	47	183, 183, 183, 183	0
1	C	318/349 (91%)	-0.29	5 (1%)	72	63	183, 183, 183, 183	0
All	All	954/1047 (91%)	-0.22	16 (1%)	70	61	183, 183, 183, 183	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	PRO	4.5
1	C	235	ALA	4.3
1	B	143	MET	3.5
1	B	144	SER	3.4
1	B	327	PRO	3.3

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, 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
5	NDG	B	705	14/15	0.61	0.69	3.44	183,183,183,183	0
5	NDG	C	705	14/15	0.76	0.30	0.71	183,183,183,183	0
3	NAG	A	505	14/15	0.92	0.22	-0.49	183,183,183,183	0
3	NAG	A	705	14/15	0.89	0.24	-0.57	183,183,183,183	0
3	NAG	C	505	14/15	0.94	0.22	-0.68	183,183,183,183	0
3	NAG	B	505	14/15	0.95	0.13	-1.02	183,183,183,183	0
2	MAN	C	502	11/12	0.92	0.11	-	183,183,183,183	0
3	NAG	B	704	14/15	0.60	0.57	-	183,183,183,183	0
3	NAG	A	704	14/15	0.62	0.45	-	183,183,183,183	0
3	NAG	C	704	14/15	0.75	0.62	-	183,183,183,183	0
3	NAG	A	504	14/15	0.83	0.19	-	183,183,183,183	0
2	MAN	C	503	11/12	0.84	0.16	-	183,183,183,183	0
2	MAN	A	503	11/12	0.71	0.31	-	183,183,183,183	0
3	NAG	C	504	14/15	0.95	0.16	-	183,183,183,183	0
2	MAN	B	503	11/12	0.91	0.13	-	183,183,183,183	0
4	BMA	B	502	11/12	0.72	0.23	-	183,183,183,183	0
3	NAG	B	504	14/15	0.96	0.09	-	183,183,183,183	0
3	NAG	B	501	14/15	0.76	0.34	-	183,183,183,183	1

6.5 Other polymers (i)

There are no such residues in this entry.