



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:27 PM GMT

PDB ID : 4TVZ
Title : Crystal Structure of SCARB2 in Neural Condition (pH7.5)
Authors : Dang, M.H.; Wang, X.X.; Rao, Z.H.
Deposited on : 2014-06-29
Resolution : 3.01 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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-20026982
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-20026982

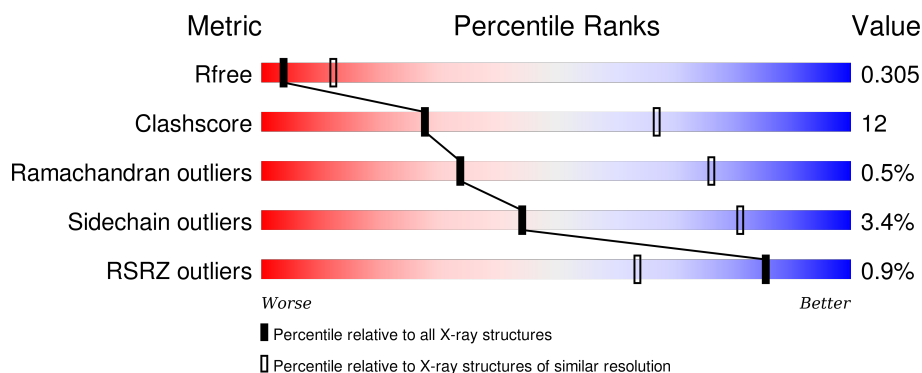
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	394	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>33%</div> <div>.</div> </div> </div>
1	B	394	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>..</div> </div> </div>

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
2	NAG	A	521	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6892 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 Scavenger receptor class B member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3148	2031	510	596	11			
1	B	394	Total	C	N	O	S	0	0	0
			3127	2019	505	592	11			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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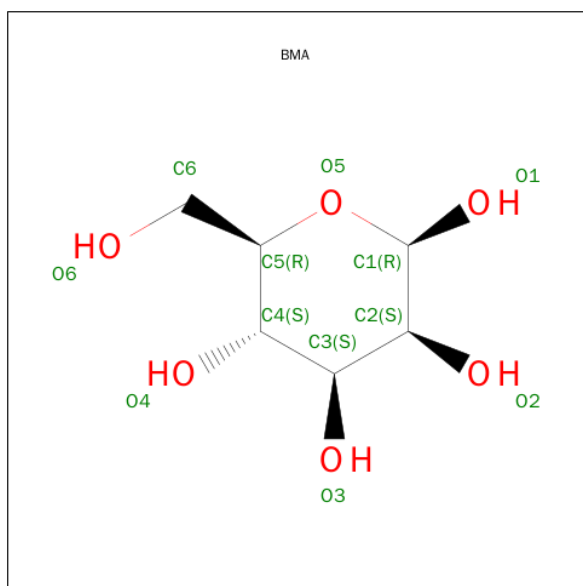
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

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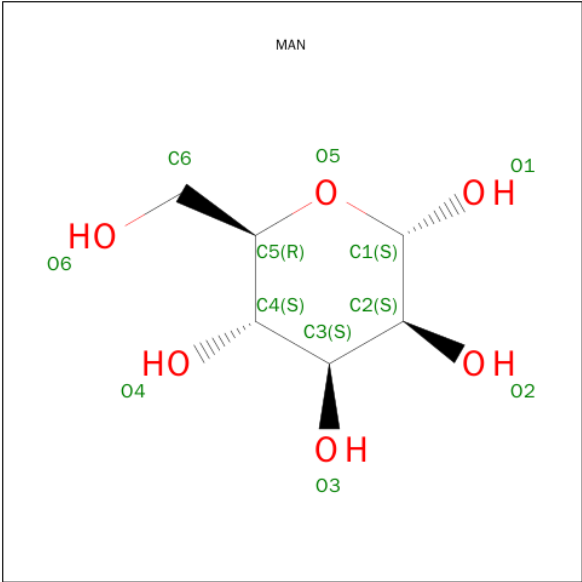
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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



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

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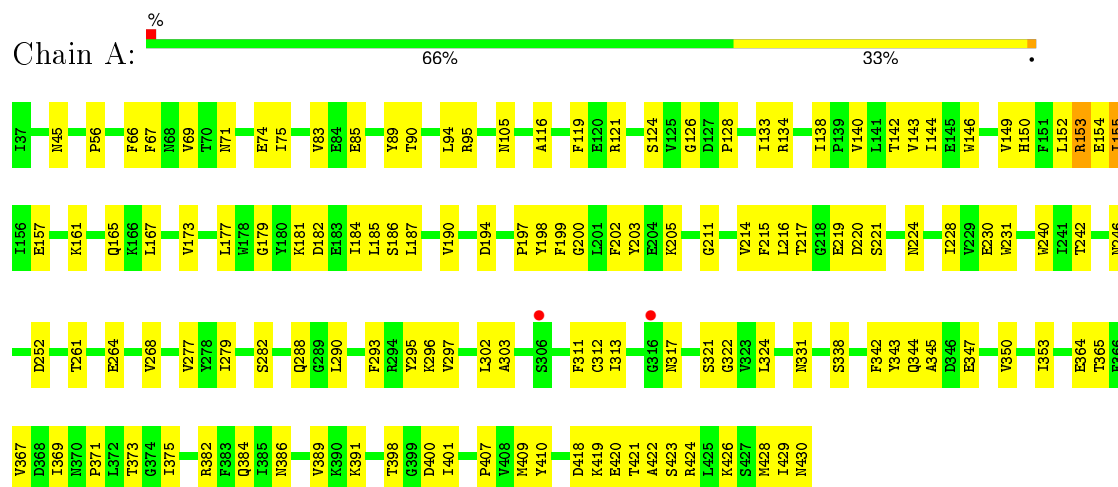
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

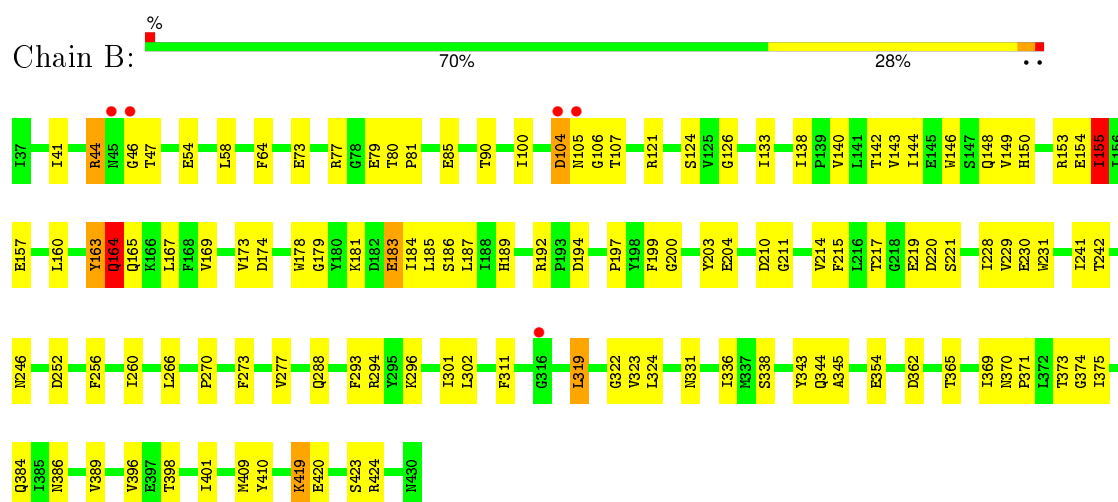
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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: Scavenger receptor class B member 2



• Molecule 1: Scavenger receptor class B member 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.96 Å 63.72 Å 219.93 Å 90.00° 99.75° 90.00°	Depositor
Resolution (Å)	34.88 – 3.01 49.26 – 3.01	Depositor EDS
% Data completeness (in resolution range)	69.6 (34.88-3.01) 69.6 (49.26-3.01)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.27 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.259 , 0.304 0.260 , 0.305	Depositor DCC
R_{free} test set	894 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.2	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 18219 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6892	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 41.99 % 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 2.1791e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BMA, NAG, 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	0.31	1/3231 (0.0%)	0.57	0/4401
1	B	0.28	0/3210	0.61	5/4376 (0.1%)
All	All	0.30	1/6441 (0.0%)	0.59	5/8777 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	GLU	CD-OE2	7.01	1.33	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	GLN	N-CA-C	6.06	127.35	111.00
1	B	319	LEU	CA-CB-CG	6.05	129.22	115.30
1	B	106	GLY	N-CA-C	-5.47	99.41	113.10
1	B	149	VAL	C-N-CA	-5.41	108.18	121.70
1	B	155	ILE	CG1-CB-CG2	-5.30	99.74	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	163	TYR	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	3148	0	2999	86	0
1	B	3127	0	2957	72	0
2	A	182	0	161	3	0
2	B	182	0	161	1	0
3	A	33	0	25	1	0
3	B	33	0	27	0	0
4	A	99	0	86	0	0
4	B	88	0	75	0	0
All	All	6892	0	6491	158	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 12.

The worst 5 of 158 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD23	1:A:153:ARG:H	1.35	0.89
1:A:296:LYS:NZ	1:A:364:GLU:OE1	2.20	0.72
1:A:220:ASP:OD2	1:A:221:SER:N	2.25	0.70
1:B:165:GLN:HE21	1:B:184:ILE:HG12	1.56	0.69
1:B:220:ASP:OD2	1:B:221:SER:N	2.25	0.68

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	392/394 (100%)	381 (97%)	9 (2%)	2 (0%)	34	76
1	B	392/394 (100%)	383 (98%)	7 (2%)	2 (0%)	34	76
All	All	784/788 (100%)	764 (97%)	16 (2%)	4 (0%)	34	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	B	155	ILE
1	A	331	ASN
1	B	331	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/355 (96%)	335 (98%)	7 (2%)	63	89
1	B	336/355 (95%)	320 (95%)	16 (5%)	31	71
All	All	678/710 (96%)	655 (97%)	23 (3%)	44	81

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	ASP
1	B	153	ARG
1	B	396	VAL
1	B	150	HIS
1	B	164	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	GLN
1	B	165	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

49 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	NAG	A	501	1	14,14,15	0.69	1 (7%)	15,19,21	0.95	1 (6%)
2	NAG	A	502	1,2	14,14,15	0.39	0	15,19,21	0.46	0
2	NAG	A	503	3,2	14,14,15	0.55	0	15,19,21	0.37	0
3	BMA	A	504	2,4	11,11,12	0.68	0	15,15,17	0.84	0
4	MAN	A	505	3	11,11,12	0.69	0	15,15,17	1.50	3 (20%)
2	NAG	A	506	1,2	14,14,15	0.30	0	15,19,21	0.34	0
2	NAG	A	507	2	14,14,15	0.22	0	15,19,21	0.42	0
2	NAG	A	508	1	14,14,15	0.94	1 (7%)	15,19,21	1.07	1 (6%)
2	NAG	A	509	1,2	14,14,15	0.32	0	15,19,21	0.52	0
2	NAG	A	510	2	14,14,15	0.27	0	15,19,21	0.33	0
2	NAG	A	511	1	14,14,15	0.30	0	15,19,21	0.60	0
2	NAG	A	512	1,2	14,14,15	0.50	0	15,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	513	3,2	14,14,15	0.34	0	15,19,21	0.36	0
3	BMA	A	514	2,4	11,11,12	0.90	1 (9%)	15,15,17	0.84	0
4	MAN	A	515	3,4	11,11,12	1.01	1 (9%)	15,15,17	0.88	1 (6%)
4	MAN	A	516	4	11,11,12	0.74	0	15,15,17	0.96	1 (6%)
4	MAN	A	517	4	11,11,12	0.72	0	15,15,17	1.30	2 (13%)
4	MAN	A	518	4	11,11,12	1.34	2 (18%)	15,15,17	3.54	7 (46%)
4	MAN	A	519	4	11,11,12	0.82	0	15,15,17	1.10	2 (13%)
4	MAN	A	520	3	11,11,12	0.89	1 (9%)	15,15,17	0.91	0
2	NAG	A	521	1,2	14,14,15	0.19	0	15,19,21	0.96	1 (6%)
2	NAG	A	522	3,2	14,14,15	0.43	0	15,19,21	0.24	0
3	BMA	A	523	2,4	11,11,12	0.62	0	15,15,17	0.83	0
4	MAN	A	524	3	11,11,12	0.91	1 (9%)	15,15,17	0.95	1 (6%)
4	MAN	A	525	3	11,11,12	0.71	0	15,15,17	1.05	2 (13%)
2	NAG	B	501	1	14,14,15	0.83	1 (7%)	15,19,21	0.91	1 (6%)
2	NAG	B	502	1,2	14,14,15	0.40	0	15,19,21	0.38	0
2	NAG	B	503	3,2	14,14,15	0.29	0	15,19,21	0.26	0
3	BMA	B	504	2	11,11,12	0.89	1 (9%)	15,15,17	0.79	0
2	NAG	B	505	1,2	14,14,15	0.29	0	15,19,21	0.23	0
2	NAG	B	506	2	14,14,15	0.23	0	15,19,21	0.27	0
2	NAG	B	507	1	14,14,15	0.69	1 (7%)	15,19,21	0.97	1 (6%)
2	NAG	B	508	1,2	14,14,15	0.40	0	15,19,21	0.42	0
2	NAG	B	509	2	14,14,15	0.25	0	15,19,21	0.23	0
2	NAG	B	510	1	14,14,15	0.18	0	15,19,21	0.36	0
2	NAG	B	511	1,2	14,14,15	0.41	0	15,19,21	0.44	0
2	NAG	B	512	3,2	14,14,15	0.16	0	15,19,21	0.45	0
3	BMA	B	513	2,4	11,11,12	0.79	1 (9%)	15,15,17	0.92	0
4	MAN	B	514	3,4	11,11,12	1.12	1 (9%)	15,15,17	0.80	1 (6%)
4	MAN	B	515	4	11,11,12	0.96	1 (9%)	15,15,17	0.99	1 (6%)
4	MAN	B	516	4	11,11,12	0.85	1 (9%)	15,15,17	1.58	3 (20%)
4	MAN	B	517	4	11,11,12	1.33	2 (18%)	15,15,17	3.56	8 (53%)
4	MAN	B	518	4	11,11,12	0.85	1 (9%)	15,15,17	1.14	1 (6%)
4	MAN	B	519	3,4	11,11,12	0.79	0	15,15,17	0.90	1 (6%)
4	MAN	B	520	4	11,11,12	0.71	0	15,15,17	0.99	2 (13%)
2	NAG	B	521	1,2	14,14,15	0.16	0	15,19,21	0.91	2 (13%)
2	NAG	B	522	3,2	14,14,15	0.43	0	15,19,21	0.33	0
3	BMA	B	523	2,4	11,11,12	0.72	0	15,15,17	0.82	0
4	MAN	B	524	3	11,11,12	0.92	1 (9%)	15,15,17	0.88	1 (6%)

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	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	503	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	504	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	505	3	-	0/2/19/22	1/1/1/1
2	NAG	A	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	507	2	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	0/6/23/26	0/1/1/1
2	NAG	A	509	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	510	2	-	0/6/23/26	0/1/1/1
2	NAG	A	511	1	-	0/6/23/26	0/1/1/1
2	NAG	A	512	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	513	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	514	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	515	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	516	4	-	0/2/19/22	0/1/1/1
4	MAN	A	517	4	-	0/2/19/22	1/1/1/1
4	MAN	A	518	4	-	0/2/19/22	1/1/1/1
4	MAN	A	519	4	-	0/2/19/22	0/1/1/1
4	MAN	A	520	3	-	0/2/19/22	0/1/1/1
2	NAG	A	521	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	522	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	523	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	524	3	-	0/2/19/22	0/1/1/1
4	MAN	A	525	3	-	0/2/19/22	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	503	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	504	2	-	0/2/19/22	0/1/1/1
2	NAG	B	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	506	2	-	0/6/23/26	0/1/1/1
2	NAG	B	507	1	-	0/6/23/26	0/1/1/1
2	NAG	B	508	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	509	2	-	0/6/23/26	0/1/1/1
2	NAG	B	510	1	-	0/6/23/26	0/1/1/1
2	NAG	B	511	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	512	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	513	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	514	3,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	515	4	-	0/2/19/22	0/1/1/1
4	MAN	B	516	4	-	0/2/19/22	1/1/1/1
4	MAN	B	517	4	-	0/2/19/22	1/1/1/1
4	MAN	B	518	4	-	0/2/19/22	0/1/1/1
4	MAN	B	519	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	520	4	-	0/2/19/22	0/1/1/1
2	NAG	B	521	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	522	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	523	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	524	3	-	0/2/19/22	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	514	MAN	O5-C1	-3.03	1.38	1.43
4	A	515	MAN	O5-C1	-2.83	1.39	1.43
4	B	517	MAN	O5-C1	-2.74	1.39	1.43
4	B	515	MAN	O5-C1	-2.62	1.39	1.43
4	B	524	MAN	O5-C1	-2.52	1.39	1.43

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	518	MAN	O5-C1-C2	-10.87	93.51	110.89
4	B	517	MAN	O5-C1-C2	-10.72	93.76	110.89
4	B	517	MAN	C3-C4-C5	-3.86	103.35	110.23
4	A	518	MAN	O5-C5-C4	-3.62	104.13	110.13
4	A	518	MAN	C3-C4-C5	-3.57	103.87	110.23

There are no chirality outliers.

There are no torsion outliers.

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	516	MAN	C1-C2-C3-C4-C5-O5
4	A	517	MAN	C1-C2-C3-C4-C5-O5
4	A	505	MAN	C1-C2-C3-C4-C5-O5
4	A	518	MAN	C1-C2-C3-C4-C5-O5
4	B	517	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
2	A	512	NAG	2	0
3	A	514	BMA	1	0
2	B	521	NAG	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	394/394 (100%)	-0.30	2 (0%) 91 76	10, 28, 57, 99	0
1	B	394/394 (100%)	-0.11	5 (1%) 79 53	20, 41, 70, 95	0
All	All	788/788 (100%)	-0.21	7 (0%) 85 64	10, 35, 65, 99	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ASP	3.6
1	B	105	ASN	3.5
1	B	316	GLY	3.5
1	B	46	GLY	3.0
1	A	316	GLY	2.9

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	521	14/15	0.91	0.21	4.05	24,29,42,53	0
2	NAG	A	511	14/15	0.79	0.22	1.82	58,76,97,97	0
2	NAG	B	521	14/15	0.90	0.21	0.99	29,39,46,47	0
2	NAG	A	508	14/15	0.73	0.28	0.63	61,71,77,80	0
2	NAG	A	509	14/15	0.92	0.20	0.62	34,38,54,59	0
2	NAG	B	508	14/15	0.90	0.21	0.40	37,48,62,69	0
2	NAG	B	507	14/15	0.83	0.29	0.06	65,72,87,96	0
2	NAG	A	506	14/15	0.91	0.18	-0.57	30,43,52,54	0
2	NAG	A	512	14/15	0.95	0.16	-0.64	15,29,37,44	0
2	NAG	B	502	14/15	0.91	0.18	-0.69	29,38,46,52	0
2	NAG	B	511	14/15	0.92	0.16	-0.86	36,50,57,61	0
2	NAG	A	502	14/15	0.94	0.17	-0.94	15,24,32,34	0
2	NAG	B	505	14/15	0.94	0.18	-1.85	42,53,71,85	0
2	NAG	B	522	14/15	0.94	0.18	-	26,46,54,60	0
4	MAN	B	517	11/12	0.83	0.24	-	50,70,80,82	0
4	MAN	A	524	11/12	0.81	0.22	-	57,77,90,91	0
2	NAG	A	513	14/15	0.93	0.16	-	35,48,61,67	0
3	BMA	A	523	11/12	0.89	0.15	-	51,64,74,75	0
4	MAN	B	516	11/12	0.82	0.23	-	83,89,95,101	0
4	MAN	A	525	11/12	0.70	0.31	-	81,86,96,112	0
3	BMA	A	514	11/12	0.90	0.15	-	66,73,91,100	0
3	BMA	B	513	11/12	0.89	0.17	-	61,68,78,82	0
2	NAG	B	501	14/15	0.73	0.39	-	73,94,113,117	0
4	MAN	B	519	11/12	0.88	0.20	-	87,98,104,104	0
4	MAN	B	514	11/12	0.87	0.17	-	66,73,89,90	0
4	MAN	A	516	11/12	0.84	0.22	-	72,79,89,92	0
2	NAG	A	507	14/15	0.84	0.31	-	60,82,91,98	0
2	NAG	A	522	14/15	0.94	0.17	-	19,33,40,48	0
4	MAN	A	518	11/12	0.63	0.34	-	70,74,87,97	0
4	MAN	A	517	11/12	0.77	0.29	-	80,88,98,108	0
2	NAG	B	509	14/15	0.82	0.24	-	73,86,95,99	0
4	MAN	A	520	11/12	0.68	0.28	-	108,117,123,126	0
2	NAG	B	510	14/15	0.84	0.23	-	78,80,85,86	0
2	NAG	B	512	14/15	0.93	0.18	-	41,52,68,77	0
4	MAN	A	515	11/12	0.80	0.18	-	63,76,84,91	0
2	NAG	A	501	14/15	0.68	0.43	-	94,106,112,117	0
4	MAN	A	505	11/12	0.63	0.22	-	68,83,92,92	0
3	BMA	B	523	11/12	0.81	0.24	-	69,77,83,89	0
2	NAG	B	506	14/15	0.81	0.30	-	83,89,104,121	0
2	NAG	A	503	14/15	0.93	0.23	-	26,37,57,64	0
3	BMA	A	504	11/12	0.86	0.24	-	70,83,103,106	0
4	MAN	B	518	11/12	0.82	0.31	-	96,102,109,132	0
4	MAN	A	519	11/12	0.78	0.27	-	56,73,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MAN	B	515	11/12	0.82	0.20	-	76,87,98,98	0
4	MAN	B	524	11/12	0.78	0.31	-	83,88,94,100	0
4	MAN	B	520	11/12	0.54	0.42	-	94,115,126,128	0
2	NAG	B	503	14/15	0.91	0.22	-	39,59,69,90	0
3	BMA	B	504	11/12	0.83	0.29	-	75,86,95,106	0
2	NAG	A	510	14/15	0.80	0.28	-	64,72,82,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.