



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:29 am GMT

PDB ID : 4QBZ
Title : Crystal structure of human TLR8 in complex with DS-802
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2014-05-09
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

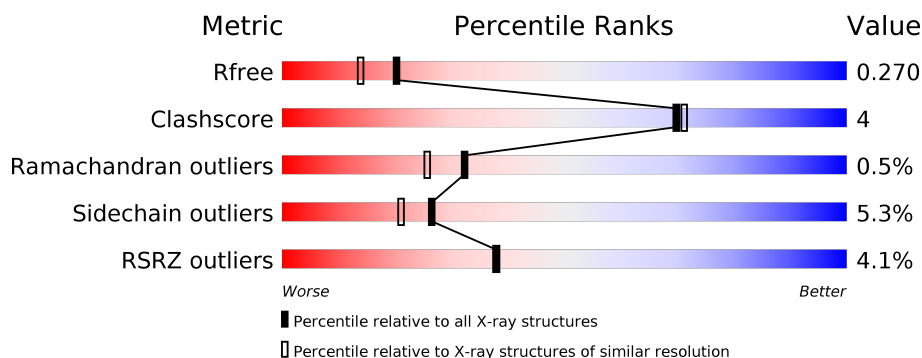
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	811	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>7%</div> </div> </div>
1	B	811	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>7%</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	901	-	-	-	X
2	NAG	A	907	-	-	-	X
2	NAG	A	910	-	-	-	X
2	NAG	B	906	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13074 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total	C	N	O	S	0	0	0
			6071	3882	1029	1141	19			
1	B	751	Total	C	N	O	S	0	1	0
			6062	3878	1031	1134	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
A	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
A	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	24	SER	-	EXPRESSION TAG	UNP Q9NR97
B	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
B	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
B	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
B	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
B	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
B	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	833	ARG	-	EXPRESSION TAG	UNP Q9NR97

- Molecule 2 is SUGAR (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		
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		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

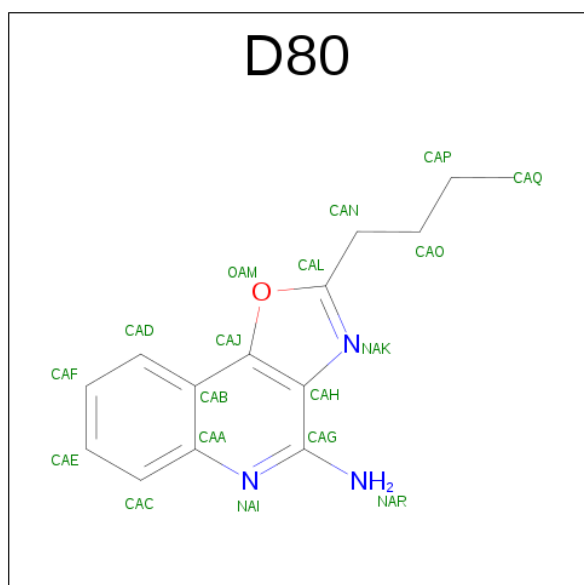
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-BUTYL[1,3]OXAZOLO[4,5-C]QUINOLIN-4-AMINE (three-letter code: D80) (formula: C₁₄H₁₅N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			18	14	3	1		
6	B	1	Total	C	N	O	0	0
			18	14	3	1		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	4	Total 50	C 28	N 2	O 20	0	0

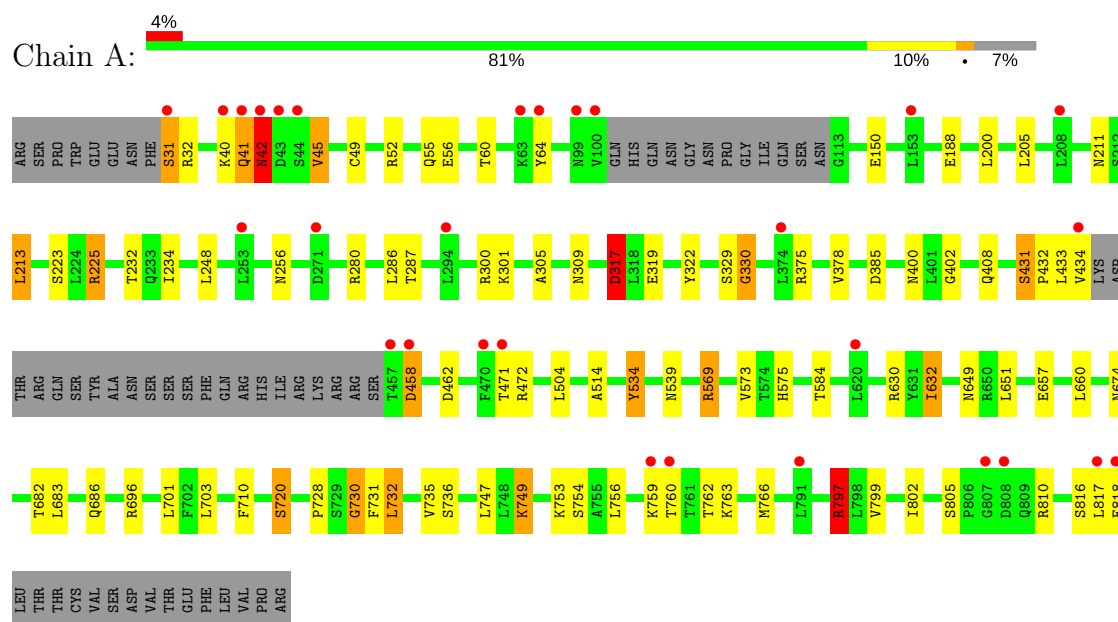
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	277	Total 277	O 277	0	0
8	B	229	Total 229	O 229	0	0

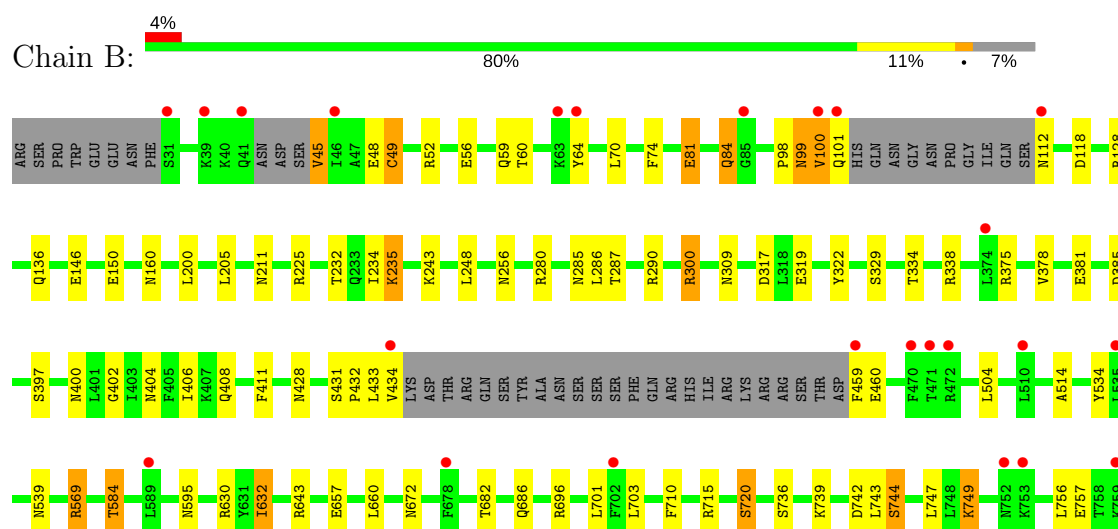
3 Residue-property plots

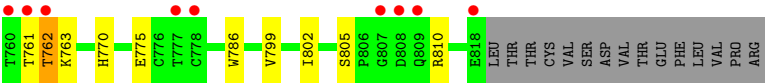
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.15Å 156.72Å 86.16Å 90.00° 77.10° 90.00°	Depositor
Resolution (Å)	26.38 – 2.00 26.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (26.38-2.00) 99.1 (26.36-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.209 , 0.264 0.218 , 0.270	Depositor DCC
R_{free} test set	6265 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13074	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, D80, 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	0.51	0/6196	0.92	9/8404 (0.1%)
1	B	0.47	0/6186	0.90	6/8387 (0.1%)
All	All	0.49	0/12382	0.91	15/16791 (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	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	569	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	643	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	630	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	290	ARG	NE-CZ-NH2	-5.82	117.39	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	458	ASP	Peptide
1	B	99	ASN	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	6071	0	6055	48	1
1	B	6062	0	6055	58	0
2	A	84	0	78	1	0
2	B	70	0	65	1	0
3	A	61	0	52	1	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	A	39	0	34	2	0
5	B	39	0	34	0	0
6	A	18	0	15	0	0
6	B	18	0	15	0	0
7	B	50	0	43	0	0
8	A	277	0	0	1	1
8	B	229	0	0	2	0
All	All	13074	0	12496	104	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 104 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:818:GLU:N	1:A:818:GLU:OE1	1.88	1.05
1:A:433:LEU:HD23	1:A:434:VAL:N	1.95	0.82
1:B:99:ASN:HB3	1:B:100:VAL:HG23	1.64	0.80
1:B:317:ASP:OD2	1:B:319:GLU:OE1	2.03	0.76
1:A:31:SER:OG	1:A:32:ARG:N	2.18	0.75

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:LYS:NZ	8:A:1277:HOH:O[1_556]	2.02	0.18

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	748/811 (92%)	698 (93%)	46 (6%)	4 (0%)	32	26
1	B	744/811 (92%)	693 (93%)	48 (6%)	3 (0%)	38	33
All	All	1492/1622 (92%)	1391 (93%)	94 (6%)	7 (0%)	32	26

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	B	762	THR
1	B	100	VAL
1	A	330	GLY
1	B	378	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	701/755 (93%)	663 (95%)	38 (5%)	26	20
1	B	699/755 (93%)	663 (95%)	36 (5%)	27	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1400/1510 (93%)	1326 (95%)	74 (5%)	26 21

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	760	THR
1	B	52	ARG
1	B	720	SER
1	A	766	MET
1	A	817	LEU

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	59	GLN
1	B	84	GLN
1	B	428	ASN
1	A	674	ASN
1	B	285	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 ⓘ

19 carbohydrates 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
3	NAG	A	902	1,3	14,14,15	0.82	0	15,19,21	1.47	4 (26%)
3	NAG	A	903	3	14,14,15	0.61	0	15,19,21	1.58	3 (20%)
3	BMA	A	904	3	11,11,12	0.45	0	13,15,17	1.84	3 (23%)
3	BMA	A	905	3	11,11,12	0.29	0	13,15,17	2.66	7 (53%)
3	MAN	A	906	3	11,11,12	0.77	0	14,15,17	3.85	8 (57%)
4	NAG	A	908	1,4	14,14,15	1.03	1 (7%)	15,19,21	1.92	5 (33%)
4	NAG	A	909	4	14,14,15	0.51	0	15,19,21	1.78	4 (26%)
5	NAG	A	912	1,5	14,14,15	0.59	0	15,19,21	1.71	3 (20%)
5	NAG	A	913	5	14,14,15	0.95	1 (7%)	15,19,21	2.36	6 (40%)
5	BMA	A	914	5	11,11,12	0.46	0	13,15,17	2.20	6 (46%)
7	NAG	B	902	1,7	14,14,15	0.63	0	15,19,21	1.95	7 (46%)
7	NAG	B	903	7	14,14,15	0.91	1 (7%)	15,19,21	1.45	2 (13%)
7	BMA	B	904	7	11,11,12	0.49	0	13,15,17	2.13	5 (38%)
7	MAN	B	905	7	11,11,12	0.52	0	13,15,17	2.96	7 (53%)
4	NAG	B	907	1,4	14,14,15	0.79	1 (7%)	15,19,21	2.14	5 (33%)
4	NAG	B	908	4	14,14,15	0.60	0	15,19,21	2.85	6 (40%)
5	NAG	B	911	1,5	14,14,15	0.78	0	15,19,21	1.52	1 (6%)
5	NAG	B	912	5	14,14,15	0.74	0	15,19,21	1.58	3 (20%)
5	BMA	B	913	5	11,11,12	0.55	0	13,15,17	2.08	4 (30%)

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	NAG	A	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	903	3	-	0/6/23/26	0/1/1/1
3	BMA	A	904	3	-	0/2/19/22	0/1/1/1
3	BMA	A	905	3	-	0/2/19/22	0/1/1/1
3	MAN	A	906	3	-	0/2/18/22	0/1/1/1
4	NAG	A	908	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	909	4	-	0/6/23/26	0/1/1/1
5	NAG	A	912	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	913	5	-	0/6/23/26	0/1/1/1
5	BMA	A	914	5	-	0/2/19/22	0/1/1/1
7	NAG	B	902	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	903	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	B	904	7	-	0/2/19/22	0/1/1/1
7	MAN	B	905	7	-	0/2/19/22	0/1/1/1
4	NAG	B	907	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	908	4	-	0/6/23/26	0/1/1/1
5	NAG	B	911	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	912	5	-	0/6/23/26	0/1/1/1
5	BMA	B	913	5	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	908	NAG	O5-C1	-2.67	1.39	1.43
5	A	913	NAG	C8-C7	-2.22	1.45	1.50
4	B	907	NAG	O5-C1	-2.21	1.40	1.43
7	B	903	NAG	O5-C1	-2.14	1.40	1.43

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	906	MAN	C2-C3-C4	-8.95	98.89	110.59
7	B	905	MAN	O3-C3-C2	-6.06	99.00	110.02
3	A	906	MAN	C3-C4-C5	-5.53	104.38	109.91
7	B	905	MAN	O5-C1-C2	-5.48	102.20	110.79
3	A	906	MAN	C1-C2-C3	-5.37	101.92	111.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	906	MAN	1	0
5	A	913	NAG	2	0

5.6 Ligand geometry

13 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	901	1	14,14,15	0.64	0	15,19,21	1.56	3 (20%)
2	NAG	A	907	1	14,14,15	0.46	0	15,19,21	1.17	2 (13%)
2	NAG	A	910	1	14,14,15	0.76	0	15,19,21	1.85	3 (20%)
2	NAG	A	911	1	14,14,15	0.42	0	15,19,21	2.78	4 (26%)
2	NAG	A	915	1	14,14,15	0.90	1 (7%)	15,19,21	3.07	6 (40%)
2	NAG	A	916	1	14,14,15	0.62	0	15,19,21	3.00	6 (40%)
6	D80	A	917	-	16,20,20	0.95	1 (6%)	15,28,28	1.19	2 (13%)
6	D80	B	901	-	16,20,20	1.08	1 (6%)	15,28,28	0.83	0
2	NAG	B	906	1	14,14,15	0.42	0	15,19,21	2.45	9 (60%)
2	NAG	B	909	1	14,14,15	0.54	0	15,19,21	2.15	5 (33%)
2	NAG	B	910	1	14,14,15	0.37	0	15,19,21	1.87	2 (13%)
2	NAG	B	914	1	14,14,15	0.73	0	15,19,21	2.38	8 (53%)
2	NAG	B	915	1	14,14,15	0.52	0	15,19,21	3.48	6 (40%)

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	901	1	-	0/6/23/26	0/1/1/1
2	NAG	A	907	1	-	0/6/23/26	0/1/1/1
2	NAG	A	910	1	-	0/6/23/26	0/1/1/1
2	NAG	A	911	1	-	0/6/23/26	0/1/1/1
2	NAG	A	915	1	-	0/6/23/26	0/1/1/1
2	NAG	A	916	1	-	0/6/23/26	0/1/1/1
6	D80	A	917	-	-	0/3/4/4	0/2/3/3
6	D80	B	901	-	-	0/3/4/4	0/2/3/3
2	NAG	B	906	1	-	0/6/23/26	0/1/1/1
2	NAG	B	909	1	-	0/6/23/26	0/1/1/1
2	NAG	B	910	1	-	0/6/23/26	0/1/1/1
2	NAG	B	914	1	-	0/6/23/26	0/1/1/1
2	NAG	B	915	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	917	D80	CAB-CAJ	-2.35	1.38	1.41
2	A	915	NAG	O5-C1	-2.10	1.40	1.43
6	B	901	D80	CAC-CAA	-2.04	1.38	1.41

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	916	NAG	C1-O5-C5	-6.70	102.93	112.17
2	A	915	NAG	O3-C3-C4	-6.06	97.17	110.36
2	A	915	NAG	O5-C1-C2	-5.31	104.08	111.47
2	A	916	NAG	O5-C1-C2	-5.19	104.25	111.47
2	B	909	NAG	C6-C5-C4	-4.35	102.81	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	916	NAG	1	0
2	B	909	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	754/811 (92%)	-0.00	29 (3%) 41 41	20, 34, 59, 90	0
1	B	751/811 (92%)	0.10	33 (4%) 35 35	22, 38, 68, 96	0
All	All	1505/1622 (92%)	0.05	62 (4%) 38 38	20, 36, 63, 96	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	LEU	6.3
1	B	760	THR	6.2
1	B	100	VAL	6.0
1	A	100	VAL	5.4
1	B	459	PHE	5.3

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](#)

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(Å ²)	Q<0.9
3	NAG	A	903	14/15	0.95	0.12	0.20	27,33,39,48	0
7	NAG	B	903	14/15	0.92	0.10	-0.24	29,35,42,44	0
7	NAG	B	902	14/15	0.94	0.10	-0.65	28,31,37,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	907	14/15	0.96	0.09	-0.98	24,26,30,32	0
4	NAG	A	908	14/15	0.96	0.08	-1.05	22,25,30,32	0
5	NAG	B	911	14/15	0.95	0.07	-1.73	24,28,29,30	0
3	NAG	A	902	14/15	0.96	0.08	-1.78	23,26,30,38	0
5	NAG	A	912	14/15	0.97	0.06	-2.00	20,23,27,27	0
4	NAG	A	909	14/15	0.90	0.17	-	36,44,54,55	0
5	NAG	A	913	14/15	0.93	0.12	-	25,30,38,38	0
5	BMA	A	914	11/12	0.87	0.20	-	42,47,50,61	0
3	MAN	A	906	11/12	0.76	0.29	-	44,63,72,94	0
5	BMA	B	913	11/12	0.85	0.21	-	44,51,61,63	0
4	NAG	B	908	14/15	0.87	0.22	-	40,51,56,56	0
3	BMA	A	905	11/12	0.90	0.27	-	59,65,68,70	0
5	NAG	B	912	14/15	0.93	0.12	-	31,33,39,45	0
7	MAN	B	905	11/12	0.61	0.24	-	58,67,77,79	0
3	BMA	A	904	11/12	0.95	0.23	-	42,46,51,55	0
7	BMA	B	904	11/12	0.89	0.20	-	41,46,48,52	0

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, 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	910	14/15	0.94	0.19	7.55	45,56,60,67	0
2	NAG	B	906	14/15	0.88	0.19	4.83	33,43,46,57	0
2	NAG	A	901	14/15	0.79	0.27	3.81	48,57,63,66	0
2	NAG	A	907	14/15	0.94	0.15	2.91	33,39,44,47	0
2	NAG	A	915	14/15	0.91	0.13	0.97	33,43,48,50	0
2	NAG	B	914	14/15	0.94	0.12	0.79	27,40,53,55	0
6	D80	B	901	18/18	0.96	0.09	-0.51	21,24,28,30	0
6	D80	A	917	18/18	0.96	0.08	-1.09	21,25,28,28	0
2	NAG	B	910	14/15	0.87	0.27	-	55,62,65,66	0
2	NAG	A	911	14/15	0.86	0.29	-	57,62,68,71	0
2	NAG	A	916	14/15	0.91	0.23	-	45,51,63,67	0
2	NAG	B	909	14/15	0.91	0.18	-	41,54,64,67	0
2	NAG	B	915	14/15	0.87	0.19	-	48,54,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.