



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:58 AM UTC

PDB ID : 5Y3M / pdb_00005y3m
Title : Crystal structure of bovine TLR9 in complex with two DNAs (CpG DNA and TCGTTT DNA)
Authors : Ohto, U.; Shimizu, T.
Deposited on : 2017-07-29
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

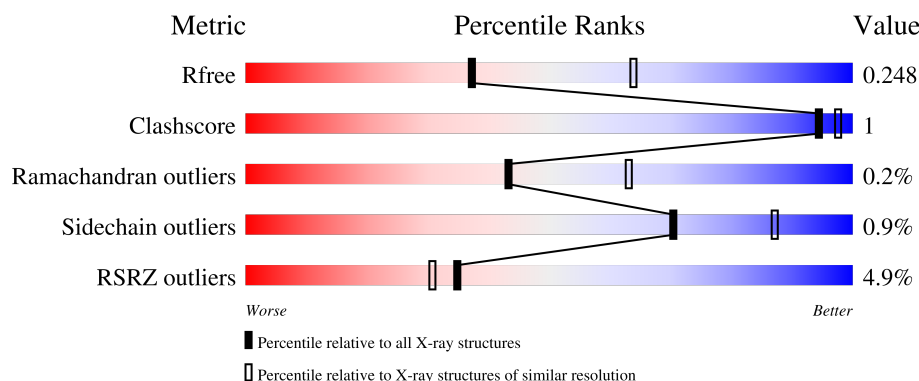
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	801	4% 88% • 8%
1	B	801	5% 88% • 9%
2	E	6	67% 33%
2	F	6	17% 50% 33% 17%
3	C	10	50% 10% 40%

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Mol	Chain	Length	Quality of chain
3	D	10	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12274 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 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			5802	3703	1031	1043	25			
1	B	732	Total	C	N	O	S	0	0	0
			5772	3685	1026	1038	23			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ARG	-	expression tag	UNP Q5I2M5
A	22	SER	-	expression tag	UNP Q5I2M5
A	23	PRO	-	expression tag	UNP Q5I2M5
A	24	TRP	-	expression tag	UNP Q5I2M5
A	816	GLU	CYS	conflict	UNP Q5I2M5
A	818	LEU	-	expression tag	UNP Q5I2M5
A	819	VAL	-	expression tag	UNP Q5I2M5
A	820	PRO	-	expression tag	UNP Q5I2M5
A	821	ARG	-	expression tag	UNP Q5I2M5
B	21	ARG	-	expression tag	UNP Q5I2M5
B	22	SER	-	expression tag	UNP Q5I2M5
B	23	PRO	-	expression tag	UNP Q5I2M5
B	24	TRP	-	expression tag	UNP Q5I2M5
B	816	GLU	CYS	conflict	UNP Q5I2M5
B	818	LEU	-	expression tag	UNP Q5I2M5
B	819	VAL	-	expression tag	UNP Q5I2M5
B	820	PRO	-	expression tag	UNP Q5I2M5
B	821	ARG	-	expression tag	UNP Q5I2M5

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			78	39	12	24	3			

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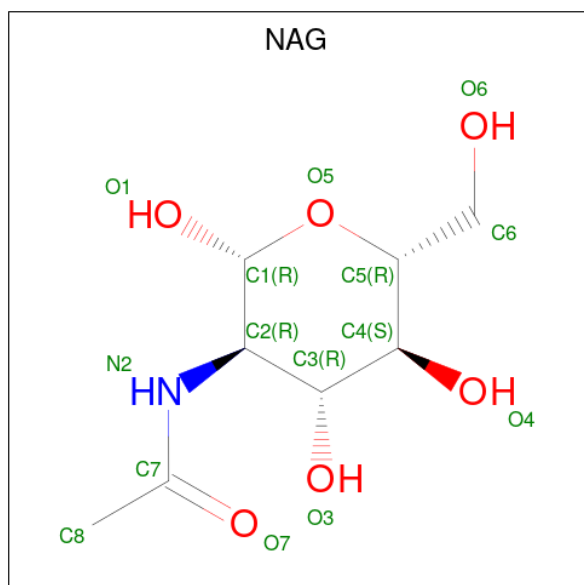
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	5	Total	C	N	O	P	0	0	0
			98	49	14	31	4			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*CP*GP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	6	Total	C	N	O	P	0	0	0
			125	59	22	38	6			
3	C	6	Total	C	N	O	P	0	0	0
			125	59	22	38	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

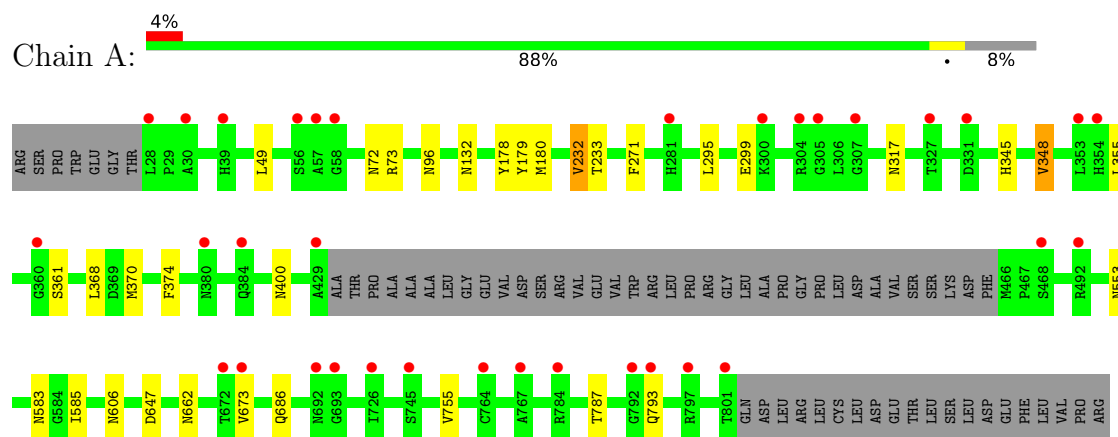
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	E	1	Total	O	0	0
			1	1		
5	F	3	Total	O	0	0
			3	3		
5	B	68	Total	O	0	0
			68	68		

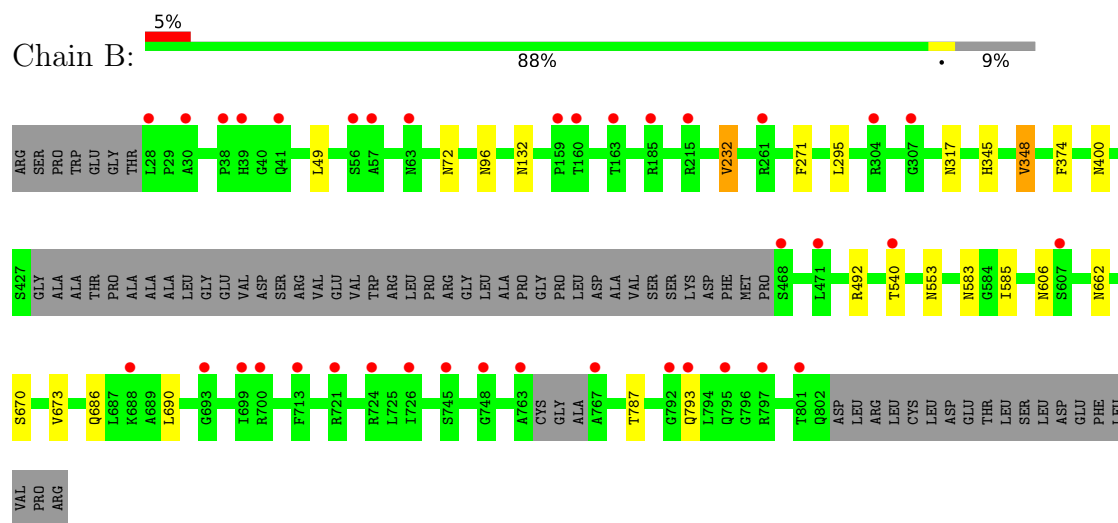
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

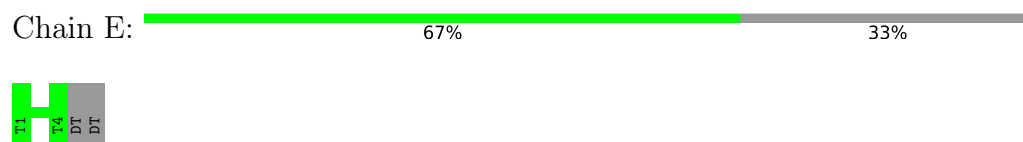
• Molecule 1: Toll-like receptor 9



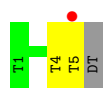
• Molecule 1: Toll-like receptor 9



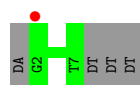
• Molecule 2: DNA (5'-D(*TP*CP*GP*T)-3')



- Molecule 2: DNA (5'-D(*TP*CP*GP*T)-3')



- Molecule 3: DNA (5'-D(P*GP*GP*CP*GP*TP*T)-3')



- Molecule 3: DNA (5'-D(P*GP*GP*CP*GP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.18Å 68.69Å 153.53Å 90.00° 100.64° 90.00°	Depositor
Resolution (Å)	48.96 – 2.50 48.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.96-2.50) 99.9 (48.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.225 , 0.244 0.229 , 0.248	Depositor DCC
R_{free} test set	3058 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.57	0/5938	0.79	0/8072
1	B	0.57	0/5906	0.77	0/8027
2	E	0.32	0/86	0.71	0/131
2	F	0.39	0/108	0.89	0/165
3	C	0.29	0/139	0.64	0/213
3	D	0.30	0/139	0.71	0/213
All	All	0.56	0/12316	0.78	0/16821

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 [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	5802	0	5840	19	0
1	B	5772	0	5810	12	0
2	E	78	0	48	0	0
2	F	98	0	60	1	0
3	C	125	0	69	1	0
3	D	125	0	69	0	0
4	A	70	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	70	0	65	0	0
5	A	62	0	0	0	0
5	B	68	0	0	0	0
5	E	1	0	0	0	0
5	F	3	0	0	0	0
All	All	12274	0	12026	32	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 1.

All (32) 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:662:ASN:HA	1:A:686:GLN:HE22	1.51	0.74
1:B:662:ASN:HA	1:B:686:GLN:HE22	1.52	0.73
2:F:4:DT:H2''	2:F:5:DT:H3'	1.79	0.64
1:A:73:ARG:NH2	3:C:4:DC:OP2	2.35	0.60
1:B:585:ILE:H	1:B:606:ASN:HD22	1.49	0.60
1:A:585:ILE:H	1:A:606:ASN:HD22	1.49	0.59
1:A:647:ASP:HA	1:A:673:VAL:CG1	2.35	0.56
1:A:295:LEU:H	1:A:317:ASN:HD22	1.54	0.55
1:A:553:ASN:H	1:A:583:ASN:HD21	1.55	0.54
1:B:96:ASN:HB2	1:B:132:ASN:HD21	1.73	0.54
1:B:295:LEU:H	1:B:317:ASN:HD22	1.54	0.53
1:A:96:ASN:HB2	1:A:132:ASN:HD21	1.74	0.53
1:B:553:ASN:H	1:B:583:ASN:HD21	1.56	0.52
1:A:368:LEU:HD21	1:A:370:MET:HE3	1.91	0.51
1:B:232:VAL:HG13	1:B:271:PHE:CD1	2.47	0.50
1:B:670:SER:O	1:B:673:VAL:HG22	2.11	0.49
1:A:374:PHE:H	1:A:400:ASN:HD22	1.60	0.49
1:B:374:PHE:H	1:B:400:ASN:HD22	1.60	0.48
1:A:232:VAL:HG13	1:A:271:PHE:CD1	2.48	0.48
1:A:179:TYR:CD1	1:A:180:MET:HG2	2.49	0.48
1:A:179:TYR:CE1	1:A:180:MET:HG2	2.50	0.47
1:A:583:ASN:HB2	1:A:606:ASN:HD21	1.81	0.46
1:B:583:ASN:HB2	1:B:606:ASN:HD21	1.81	0.46
1:B:49:LEU:H	1:B:72:ASN:HD22	1.65	0.45
1:B:345:HIS:HB3	1:B:348:VAL:HG22	1.98	0.44
1:A:49:LEU:H	1:A:72:ASN:HD22	1.65	0.44
1:A:178:TYR:CZ	1:A:180:MET:HB2	2.52	0.44
1:A:355:LEU:HD11	1:A:370:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:ASN:H	1:B:583:ASN:ND2	2.17	0.43
1:A:647:ASP:HA	1:A:673:VAL:HG11	1.99	0.42
1:A:345:HIS:HB3	1:A:348:VAL:HG22	2.03	0.41
1:A:553:ASN:H	1:A:583:ASN:ND2	2.17	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	734/801 (92%)	694 (95%)	38 (5%)	2 (0%)	36	55
1	B	726/801 (91%)	688 (95%)	37 (5%)	1 (0%)	48	68
All	All	1460/1602 (91%)	1382 (95%)	75 (5%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	SER
1	A	793	GLN
1	B	793	GLN

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	659/712 (93%)	653 (99%)	6 (1%)	70	87
1	B	657/712 (92%)	651 (99%)	6 (1%)	70	87
All	All	1316/1424 (92%)	1304 (99%)	12 (1%)	70	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	A	233	THR
1	A	299	GLU
1	A	348	VAL
1	A	755	VAL
1	A	787	THR
1	B	232	VAL
1	B	348	VAL
1	B	492	ARG
1	B	540	THR
1	B	690	LEU
1	B	787	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	39	HIS
1	A	41	GLN
1	A	72	ASN
1	A	132	ASN
1	A	317	ASN
1	A	400	ASN
1	A	406	GLN
1	A	424	ASN
1	A	535	HIS
1	A	582	HIS
1	A	583	ASN
1	A	591	GLN
1	A	606	ASN
1	A	630	GLN
1	A	648	ASN
1	A	686	GLN
1	A	776	GLN

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Mol	Chain	Res	Type
1	B	37	GLN
1	B	39	HIS
1	B	72	ASN
1	B	78	HIS
1	B	132	ASN
1	B	317	ASN
1	B	400	ASN
1	B	424	ASN
1	B	472	ASN
1	B	555	GLN
1	B	582	HIS
1	B	583	ASN
1	B	591	GLN
1	B	606	ASN
1	B	630	GLN
1	B	648	ASN
1	B	662	ASN
1	B	686	GLN
1	B	776	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	$\# Z > 2$
4	NAG	B	1001	1	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
4	NAG	A	1001	1	14,14,15	0.31	0	17,19,21	0.82	0
4	NAG	A	1003	1	14,14,15	0.39	0	17,19,21	1.02	0
4	NAG	A	1000	1	14,14,15	0.50	0	17,19,21	1.30	1 (5%)
4	NAG	B	1004	1	14,14,15	0.39	0	17,19,21	0.84	0
4	NAG	B	1000	1	14,14,15	0.46	0	17,19,21	1.10	1 (5%)
4	NAG	A	1002	1	14,14,15	0.36	0	17,19,21	0.86	0
4	NAG	A	1004	1	14,14,15	0.52	0	17,19,21	0.95	0
4	NAG	B	1002	1	14,14,15	0.32	0	17,19,21	0.85	0
4	NAG	B	1003	1	14,14,15	0.32	0	17,19,21	0.96	1 (5%)

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
4	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1000	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1000	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1000	NAG	C4-C3-C2	3.46	116.09	111.02
4	B	1001	NAG	C2-N2-C7	2.33	126.03	122.90
4	B	1000	NAG	C2-N2-C7	2.24	125.90	122.90
4	B	1003	NAG	O5-C1-C2	-2.09	108.06	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1000	NAG	O5-C5-C6-O6
4	A	1001	NAG	O5-C5-C6-O6
4	A	1002	NAG	O5-C5-C6-O6
4	B	1003	NAG	O5-C5-C6-O6
4	B	1003	NAG	C4-C5-C6-O6
4	A	1001	NAG	C4-C5-C6-O6
4	A	1000	NAG	C4-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	B	1000	NAG	C1-C2-N2-C7
4	B	1001	NAG	C3-C2-N2-C7
4	B	1001	NAG	C1-C2-N2-C7
4	B	1000	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	738/801 (92%)	0.42	34 (4%) 37 33	16, 32, 50, 65	0
1	B	732/801 (91%)	0.44	37 (5%) 33 29	17, 31, 55, 71	0
2	E	4/6 (66%)	-0.30	0 100 100	30, 31, 33, 34	0
2	F	5/6 (83%)	-0.07	1 (20%) 3 2	24, 28, 39, 62	0
3	C	6/10 (60%)	0.10	0 100 100	38, 41, 46, 53	0
3	D	6/10 (60%)	0.68	1 (16%) 4 3	42, 44, 65, 83	0
All	All	1491/1634 (91%)	0.43	73 (4%) 35 31	16, 31, 53, 83	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	468	SER	5.6
1	A	57	ALA	4.7
1	A	793	GLN	4.4
1	A	58	GLY	4.3
1	B	57	ALA	4.3
1	B	767	ALA	4.3
1	A	764	CYS	4.2
1	A	56	SER	4.2
1	B	792	GLY	3.9
1	A	354	HIS	3.8
1	A	300	LYS	3.5
1	B	763	ALA	3.5
1	A	792	GLY	3.3
1	A	30	ALA	3.3
1	A	692	ASN	3.3
1	A	801	THR	3.2
1	B	793	GLN	3.1
1	B	159	PRO	3.0
1	A	281	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	724	ARG	3.0
1	A	693	GLY	2.9
3	D	2	DG	2.9
1	B	28	LEU	2.9
1	A	797	ARG	2.8
1	A	327	THR	2.8
1	B	163	THR	2.7
1	B	304	ARG	2.7
1	A	305	GLY	2.6
1	A	673	VAL	2.6
1	A	307	GLY	2.6
1	A	767	ALA	2.6
1	B	693	GLY	2.5
1	B	30	ALA	2.5
1	A	331	ASP	2.5
1	A	28	LEU	2.5
1	B	797	ARG	2.5
1	A	429	ALA	2.5
1	B	700	ARG	2.4
1	B	471	LEU	2.4
1	A	39	HIS	2.4
1	B	307	GLY	2.4
1	B	38	PRO	2.3
1	B	713	PHE	2.3
1	A	672	THR	2.3
1	B	726	ILE	2.3
1	B	39	HIS	2.2
1	B	721	ARG	2.2
2	F	5	DT	2.2
1	B	56	SER	2.2
1	B	261	ARG	2.2
1	B	185	ARG	2.2
1	A	353	LEU	2.1
1	B	699	ILE	2.1
1	B	607	SER	2.1
1	B	41	GLN	2.1
1	B	63	ASN	2.1
1	B	160	THR	2.1
1	B	801	THR	2.1
1	A	492	ARG	2.1
1	B	215	ARG	2.1
1	A	380	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	784	ARG	2.1
1	A	360	GLY	2.0
1	B	540	THR	2.0
1	A	384	GLN	2.0
1	B	795	GLN	2.0
1	A	304	ARG	2.0
1	B	688	LYS	2.0
1	B	748	GLY	2.0
1	A	726	ILE	2.0
1	A	468	SER	2.0
1	A	745	SER	2.0
1	B	745	SER	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	1001	14/15	0.68	0.18	54,58,59,60	0
4	NAG	A	1004	14/15	0.77	0.15	40,42,43,43	0
4	NAG	A	1003	14/15	0.77	0.14	39,41,41,42	0
4	NAG	B	1002	14/15	0.78	0.15	48,50,51,51	0
4	NAG	B	1004	14/15	0.80	0.14	39,41,42,42	0
4	NAG	B	1003	14/15	0.81	0.14	35,37,39,39	0
4	NAG	B	1000	14/15	0.85	0.11	33,33,33,33	0
4	NAG	A	1000	14/15	0.87	0.11	38,39,40,40	0
4	NAG	A	1001	14/15	0.88	0.11	31,32,33,34	0
4	NAG	A	1002	14/15	0.89	0.10	40,41,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.