W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 8, 2017 – 06:34 PM EST

PDB ID	:	4LXS
Title	:	Structure of the Toll - Spatzle complex, a molecular hub in Drosophila development and innate immunity (glycosylated form)
Authors	:	Stelter, M.; Parthier, C.; Breithaupt, C.; Stubbs, M.T.
Deposited on	:	unknown
Resolution	:	3.30 Å(reported)

The following versions of software and data (see references (i)) 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 3.30 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		12
Ramachandran outliers		1.2%
Sidechain outliers		7.2%
RSRZ outliers		0.8%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
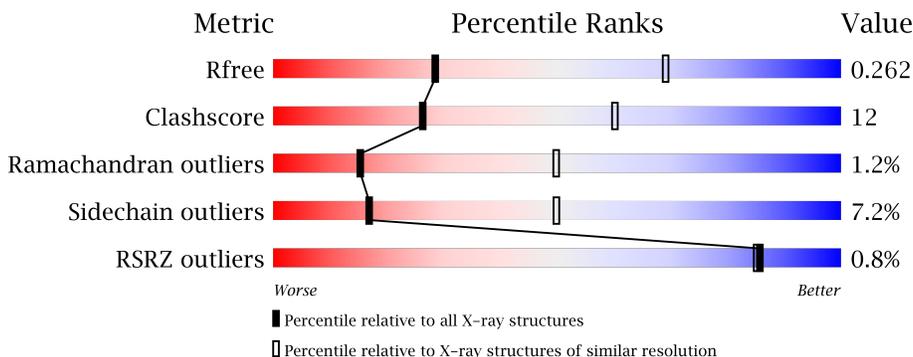
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	783	62% 30% · 5%
2	J	114	4% 36% 18% · 45%
2	K	114	46% 10% · 43%

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	NAG	A	2013	-	-	-	X
3	NAG	A	2023	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7311 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 Protein toll.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total 5977	C 3749	N 1080	O 1108	S 40	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	803	THR	-	EXPRESSION TAG	UNP P08953
A	804	GLY	-	EXPRESSION TAG	UNP P08953
A	805	HIS	-	EXPRESSION TAG	UNP P08953
A	806	HIS	-	EXPRESSION TAG	UNP P08953
A	807	HIS	-	EXPRESSION TAG	UNP P08953
A	808	HIS	-	EXPRESSION TAG	UNP P08953
A	809	HIS	-	EXPRESSION TAG	UNP P08953
A	810	HIS	-	EXPRESSION TAG	UNP P08953

- Molecule 2 is a protein called Protein spaetzle C-106.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	63	Total 506	C 317	N 88	O 94	S 7	0	0	0
2	K	65	Total 503	C 313	N 89	O 94	S 7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	107	LEU	-	EXPRESSION TAG	UNP P48607
J	108	GLU	-	EXPRESSION TAG	UNP P48607
J	109	HIS	-	EXPRESSION TAG	UNP P48607
J	110	HIS	-	EXPRESSION TAG	UNP P48607
J	111	HIS	-	EXPRESSION TAG	UNP P48607
J	112	HIS	-	EXPRESSION TAG	UNP P48607

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Chain	Residue	Modelled	Actual	Comment	Reference
J	113	HIS	-	EXPRESSION TAG	UNP P48607
J	114	HIS	-	EXPRESSION TAG	UNP P48607
K	107	LEU	-	EXPRESSION TAG	UNP P48607
K	108	GLU	-	EXPRESSION TAG	UNP P48607
K	109	HIS	-	EXPRESSION TAG	UNP P48607
K	110	HIS	-	EXPRESSION TAG	UNP P48607
K	111	HIS	-	EXPRESSION TAG	UNP P48607
K	112	HIS	-	EXPRESSION TAG	UNP P48607
K	113	HIS	-	EXPRESSION TAG	UNP P48607
K	114	HIS	-	EXPRESSION TAG	UNP P48607

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
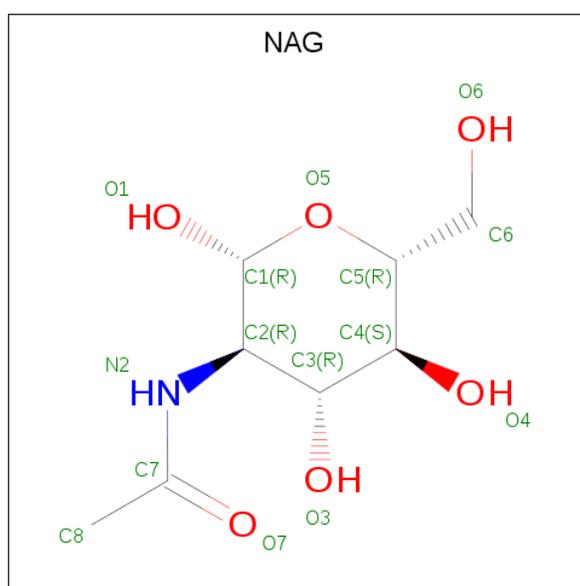
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).
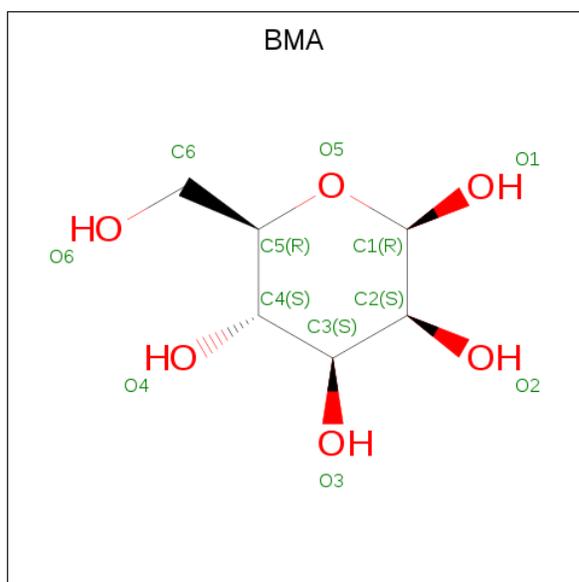
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).
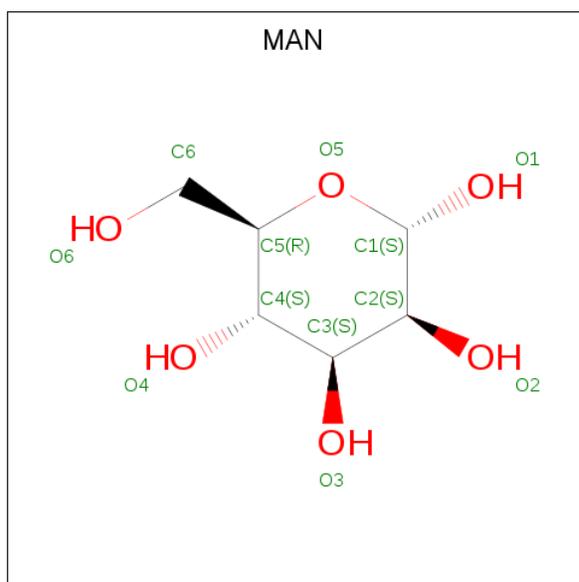
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 11	C 6	O 5	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).
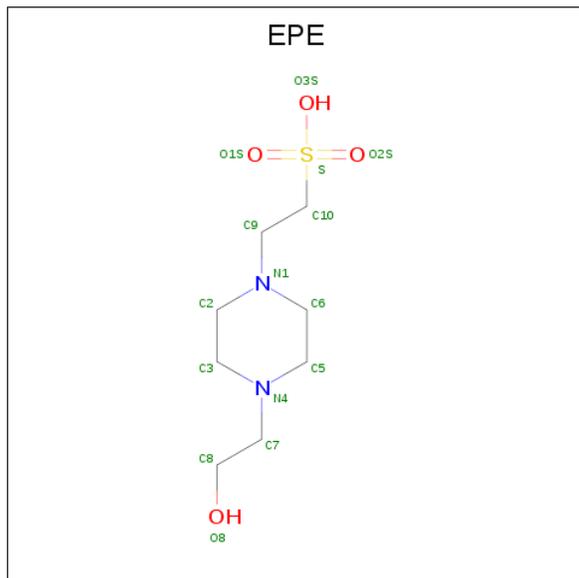
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	15	8	2	4	1	0	0

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 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: Protein toll
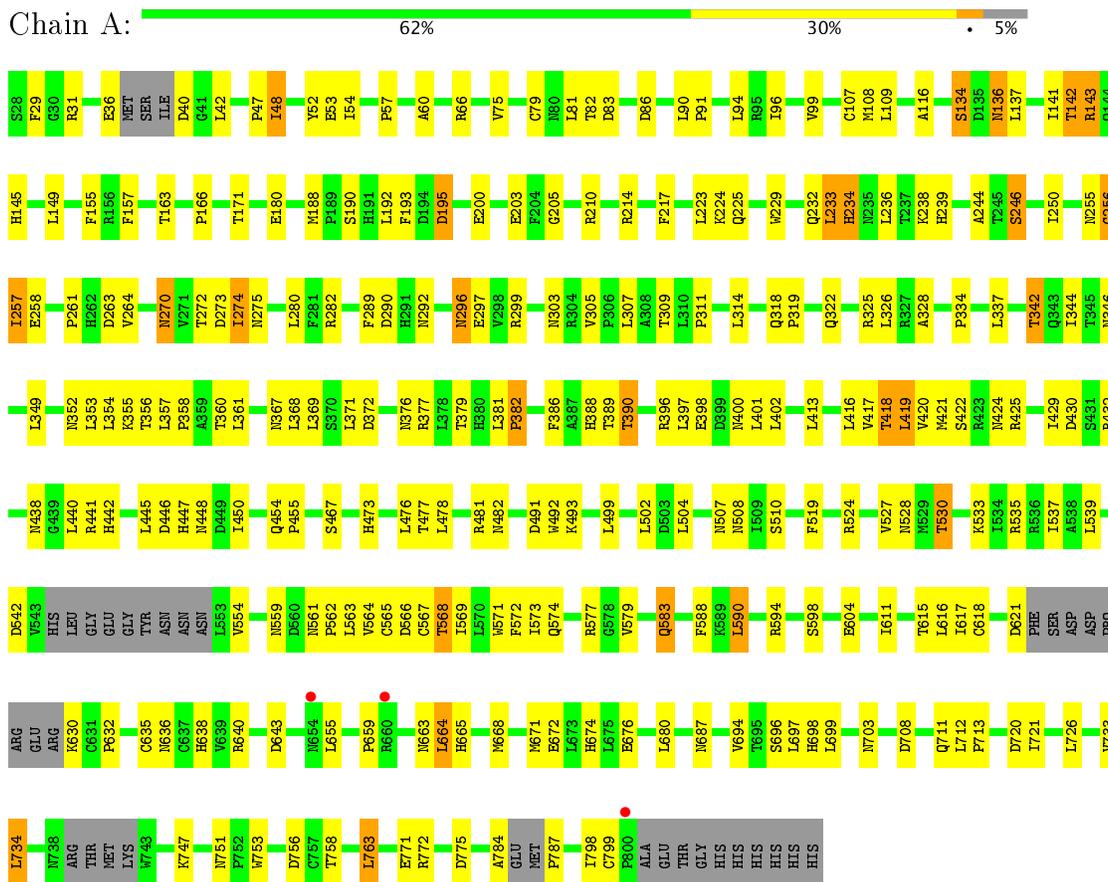
- Molecule 2: Protein spaetzle C-106

• Molecule 2: Protein spaetzle C-106

Chain K:
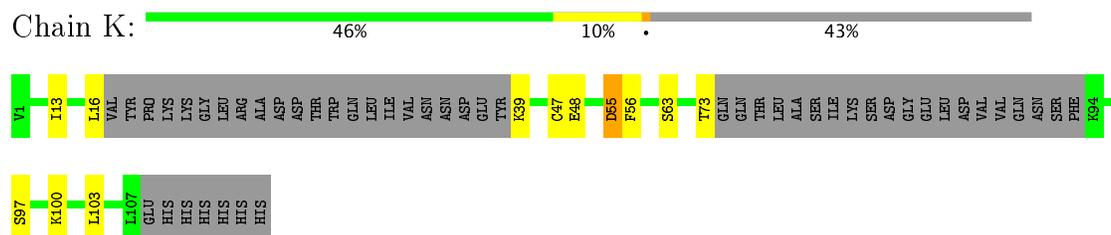
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	171.28Å 76.82Å 123.82Å 90.00° 126.29° 90.00°	Depositor
Resolution (Å)	33.95 – 3.30 33.95 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.6 (33.95-3.30) 93.7 (33.95-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.74 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.207 , 0.264 0.203 , 0.262	Depositor DCC
R_{free} test set	925 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	74.2	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 11.3	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	0.91	EDS
Total number of atoms	7311	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, EPE, BMA, 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	0.27	0/6091	0.50	0/8271
2	J	0.33	0/515	0.47	0/690
2	K	0.31	0/510	0.42	0/681
All	All	0.28	0/7116	0.49	0/9642

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	5977	0	5951	153	0
2	J	506	0	482	15	0
2	K	503	0	492	6	0
3	A	266	0	238	5	0
4	A	33	0	28	1	0
5	A	11	0	10	0	0
6	A	15	0	17	1	0
All	All	7311	0	7218	170	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 170 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:282:ARG:HH12	1:A:305:VAL:HB	1.39	0.87
1:A:640:ARG:NH2	1:A:643:ASP:OD2	2.17	0.76
1:A:270:ASN:N	1:A:270:ASN:OD1	2.25	0.70
1:A:617:ILE:HG22	1:A:640:ARG:HB3	1.73	0.70
1:A:256:GLY:HA2	1:A:280:LEU:HD13	1.74	0.70

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	735/783 (94%)	629 (86%)	96 (13%)	10 (1%)	13	46
2	J	57/114 (50%)	49 (86%)	8 (14%)	0	100	100
2	K	59/114 (52%)	54 (92%)	5 (8%)	0	100	100
All	All	851/1011 (84%)	732 (86%)	109 (13%)	10 (1%)	15	50

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	LEU
1	A	234	HIS
1	A	238	LYS
1	A	256	GLY
1	A	389	THR

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	691/723 (96%)	644 (93%)	47 (7%)	18	53
2	J	57/101 (56%)	52 (91%)	5 (9%)	12	40
2	K	56/101 (55%)	50 (89%)	6 (11%)	8	30
All	All	804/925 (87%)	746 (93%)	58 (7%)	17	50

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	LEU
1	A	499	LEU
2	K	47	CYS
1	A	425	ARG
1	A	445	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	HIS
1	A	636	ASN
1	A	424	ASN
1	A	145	HIS
1	A	526	HIS

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

24 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	#$|Z| > 2$
3	NAG	A	2001	1,3	14,14,15	0.46	0	15,19,21	0.53	0
3	NAG	A	2002	3,4	14,14,15	0.68	1 (7%)	15,19,21	0.90	0
4	BMA	A	2003	3,4	11,11,12	1.40	2 (18%)	13,15,17	1.87	4 (30%)
4	BMA	A	2004	5,4	11,11,12	1.10	1 (9%)	13,15,17	1.21	1 (7%)
5	MAN	A	2005	4	11,11,12	1.08	1 (9%)	13,15,17	1.44	2 (15%)
3	NAG	A	2006	1	14,14,15	0.29	0	15,19,21	0.39	0
3	NAG	A	2007	1	14,14,15	0.29	0	15,19,21	0.40	0
3	NAG	A	2008	1,3	14,14,15	0.39	0	15,19,21	0.76	0
3	NAG	A	2009	3	14,14,15	0.32	0	15,19,21	0.44	0
3	NAG	A	2010	1,3	14,14,15	0.48	0	15,19,21	0.48	0
3	NAG	A	2011	3,4	14,14,15	0.47	0	15,19,21	0.70	0
4	BMA	A	2012	3	11,11,12	0.71	0	13,15,17	0.67	0
3	NAG	A	2013	1,3	14,14,15	0.30	0	15,19,21	0.58	0
3	NAG	A	2014	3	14,14,15	0.40	0	15,19,21	0.56	0
3	NAG	A	2015	1,3	14,14,15	0.33	0	15,19,21	0.49	0
3	NAG	A	2016	3	14,14,15	0.64	0	15,19,21	0.86	1 (6%)
3	NAG	A	2017	1,3	14,14,15	0.39	0	15,19,21	0.43	0
3	NAG	A	2018	3	14,14,15	0.19	0	15,19,21	0.46	0
3	NAG	A	2019	1,3	14,14,15	0.70	1 (7%)	15,19,21	0.68	0
3	NAG	A	2020	3	14,14,15	0.40	0	15,19,21	0.57	0
3	NAG	A	2021	1	14,14,15	0.49	0	15,19,21	0.51	0
3	NAG	A	2022	1	14,14,15	1.43	2 (14%)	15,19,21	0.83	1 (6%)
3	NAG	A	2023	1	14,14,15	0.38	0	15,19,21	0.52	0
6	EPE	A	2024	-	15,15,15	0.81	1 (6%)	18,20,20	2.04	6 (33%)

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	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2002	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	2003	3,4	-	0/2/19/22	0/1/1/1
4	BMA	A	2004	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	2005	4	-	0/2/19/22	0/1/1/1
3	NAG	A	2006	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2007	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2008	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2009	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2010	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2011	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	2012	3	-	0/2/19/22	0/1/1/1
3	NAG	A	2013	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2014	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2015	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2016	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2017	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2018	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2019	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2020	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2021	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2022	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2023	1	-	0/6/23/26	0/1/1/1
6	EPE	A	2024	-	-	0/9/19/19	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2022	NAG	O5-C1	-4.64	1.36	1.43
3	A	2002	NAG	O5-C1	-2.17	1.40	1.43
4	A	2003	BMA	C4-C5	2.09	1.57	1.53
3	A	2022	NAG	C1-C2	2.32	1.55	1.52
3	A	2019	NAG	C1-C2	2.38	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2003	BMA	C1-C2-C3	-4.22	104.30	109.65
4	A	2003	BMA	O2-C2-C3	-2.13	105.98	110.17
4	A	2004	BMA	O3-C3-C2	2.12	113.88	110.02
6	A	2024	EPE	O1S-S-C10	2.17	108.66	106.79
3	A	2022	NAG	C4-C3-C2	2.17	114.20	111.02

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There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2004	BMA	1	0
3	A	2008	NAG	1	0
3	A	2009	NAG	1	0
3	A	2010	NAG	1	0
3	A	2011	NAG	1	0
3	A	2015	NAG	1	0
3	A	2023	NAG	1	0
6	A	2024	EPE	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 ⓘ

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	747/783 (95%)	-0.34	3 (0%)	92	92	4, 27, 58, 87	0
2	J	63/114 (55%)	0.09	4 (6%)	21	20	11, 33, 64, 71	0
2	K	65/114 (57%)	-0.05	0	100	100	10, 37, 60, 76	0
All	All	875/1011 (86%)	-0.28	7 (0%)	86	85	4, 28, 59, 87	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	660	ARG	5.0
2	J	13	ILE	3.4
2	J	14	ARG	3.3
1	A	654	ASN	2.5
2	J	15	LYS	2.2

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, 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(Å²)	Q<0.9
3	NAG	A	2013	14/15	0.90	0.18	2.66	25,40,55,66	0
3	NAG	A	2022	14/15	0.87	0.26	1.14	33,50,54,63	0
3	NAG	A	2023	14/15	0.86	0.41	1.01	39,60,70,84	0
3	NAG	A	2010	14/15	0.94	0.20	0.25	20,36,45,46	0
6	EPE	A	2024	15/15	0.92	0.23	0.08	25,33,45,47	0
3	NAG	A	2015	14/15	0.91	0.15	-0.41	34,42,49,51	0
3	NAG	A	2008	14/15	0.91	0.16	-0.49	26,37,53,61	0
3	NAG	A	2001	14/15	0.95	0.14	-0.98	16,22,31,31	0
3	NAG	A	2007	14/15	0.95	0.13	-1.13	28,33,43,49	0
3	NAG	A	2021	14/15	0.83	0.29	-	55,65,80,83	0
4	BMA	A	2004	11/12	0.93	0.14	-	30,38,43,43	0
3	NAG	A	2011	14/15	0.94	0.17	-	36,47,66,66	0
3	NAG	A	2020	14/15	0.90	0.32	-	49,60,63,66	0
3	NAG	A	2018	14/15	0.91	0.22	-	39,54,64,68	0
3	NAG	A	2014	14/15	0.80	0.37	-	47,73,81,83	0
4	BMA	A	2012	11/12	0.78	0.16	-	51,62,70,71	0
3	NAG	A	2017	14/15	0.92	0.19	-	47,55,66,69	0
5	MAN	A	2005	11/12	0.93	0.18	-	29,31,39,46	0
3	NAG	A	2016	14/15	0.88	0.25	-	48,59,70,75	0
3	NAG	A	2009	14/15	0.84	0.24	-	56,61,68,78	0
3	NAG	A	2006	14/15	0.82	0.21	-	36,59,66,75	0
4	BMA	A	2003	11/12	0.87	0.12	-	15,25,35,36	0
3	NAG	A	2019	14/15	0.94	0.35	-	44,49,59,61	0
3	NAG	A	2002	14/15	0.94	0.13	-	23,30,46,49	0

6.5 Other polymers (i)

There are no such residues in this entry.