



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2017 – 06:36 PM EST

PDB ID : 4LXR  
Title : Structure of the Toll - Spatzle complex, a molecular hub in Drosophila development and innate immunity  
Authors : Stelter, M.; Parthier, C.; Breithaupt, C.; Stubbs, M.T.  
Deposited on : unknown  
Resolution : 2.20 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](mailto: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.

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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 : 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

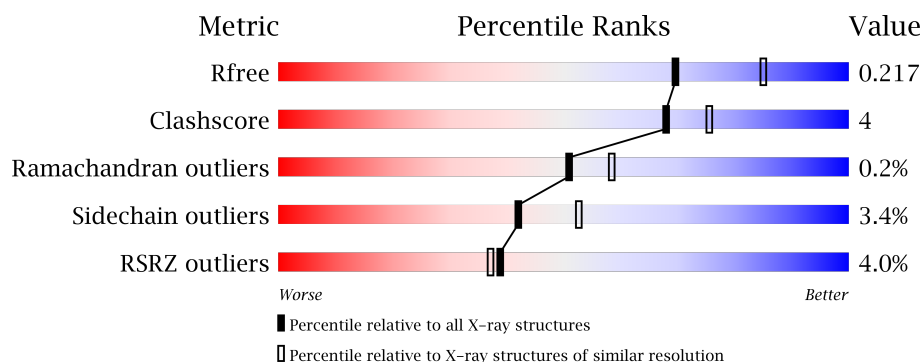
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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  $\geq 3$ , 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	783	<div> <div>3%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
2	J	114	<div> <div>8%</div> <div>48%</div> <div>7%</div> <div>•</div> <div>44%</div> </div>
2	K	114	<div> <div>5%</div> <div>52%</div> <div>5%</div> <div>•</div> <div>42%</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
3	NAG	A	2013	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7862 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
			Total	C	N	O	S			
1	A	755	6084	3811	1107	1125	41	0	4	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
			Total	C	N	O	S			
2	J	64	509	317	91	94	7	0	0	0
2	K	66	510	317	90	96	7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

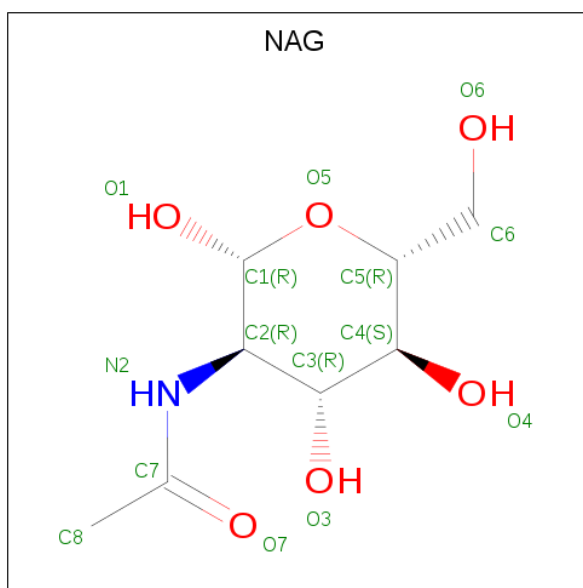
Chain	Residue	Modelled	Actual	Comment	Reference
J	107	LEU	-	EXPRESSION TAG	UNP P48607
J	108	GLU	-	EXPRESSION TAG	UNP P48607
J	109	HIS	-	EXPRESSION TAG	UNP P48607
J	110	HIS	-	EXPRESSION TAG	UNP P48607
J	111	HIS	-	EXPRESSION TAG	UNP P48607
J	112	HIS	-	EXPRESSION TAG	UNP P48607

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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		

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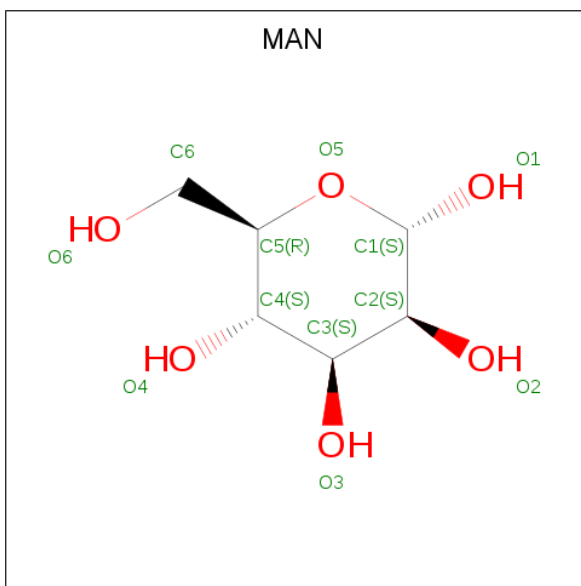
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



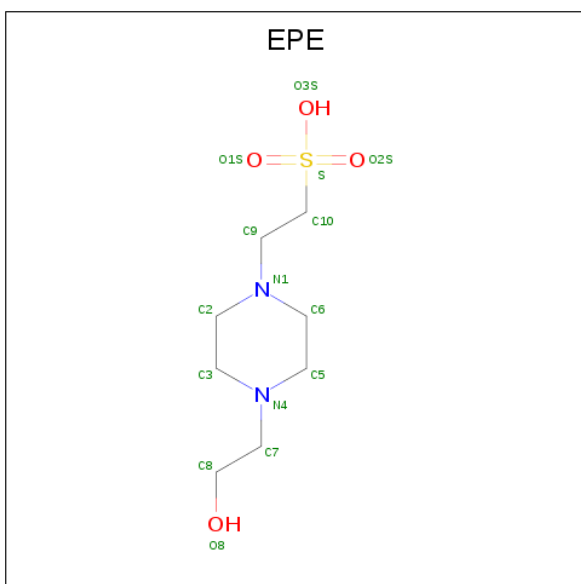
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

- 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	C	O	0	0
			11	6	5		

- 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
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is water.

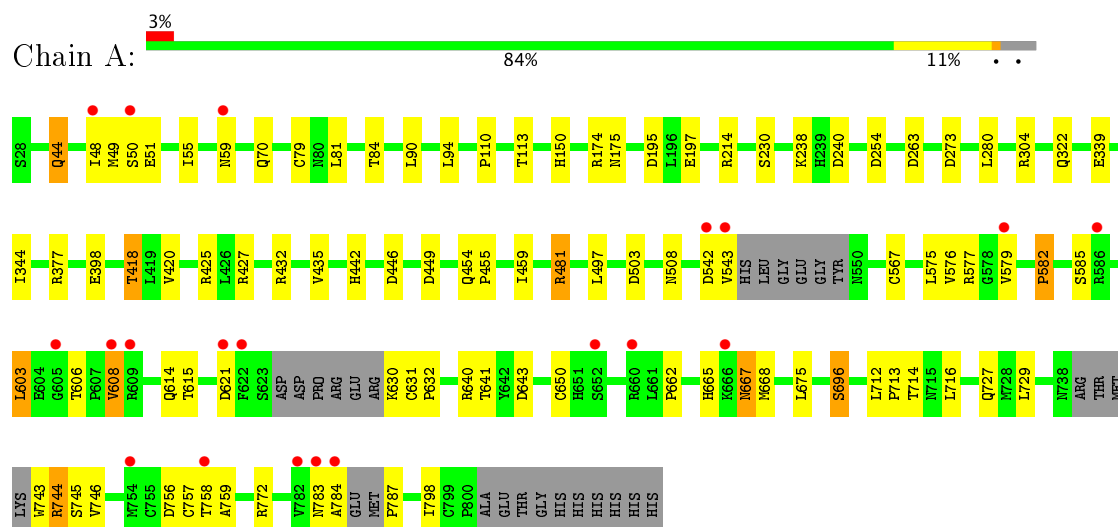
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	436	Total 436	O 436	0	0
7	J	32	Total 32	O 32	0	0
7	K	36	Total 36	O 36	0	0



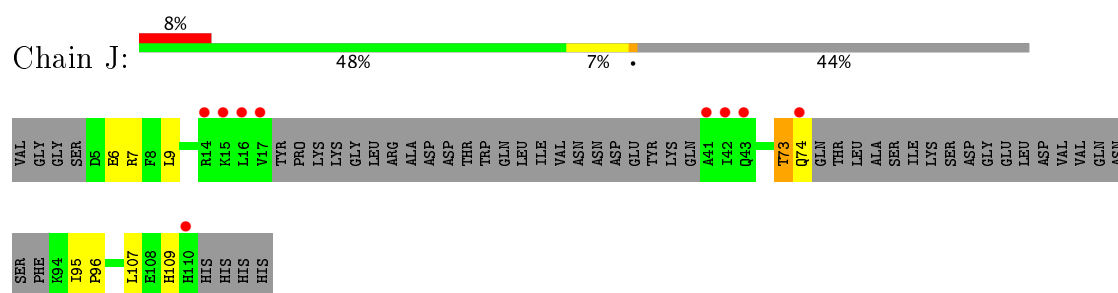
### 3 Residue-property plots [i](#)

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.

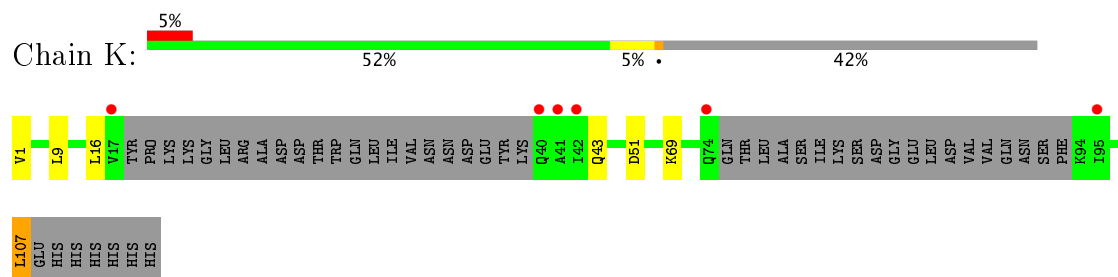
#### • Molecule 1: Protein toll



#### • Molecule 2: Protein spaetzle C-106



#### • Molecule 2: Protein spaetzle C-106



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.03Å 78.17Å 124.45Å 90.00° 126.30° 90.00°	Depositor
Resolution (Å)	42.68 – 2.20 45.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.68-2.20) 99.3 (45.75-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.176 , 0.218 0.174 , 0.217	Depositor DCC
$R_{free}$ test set	3364 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.40	0/6200	0.56	0/8416
2	J	0.39	0/518	0.50	0/694
2	K	0.38	0/517	0.52	0/692
All	All	0.40	0/7235	0.56	0/9802

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6084	0	6061	55	0
2	J	509	0	485	7	0
2	K	510	0	496	6	0
3	A	196	0	176	2	0
4	A	33	0	28	0	0
5	A	11	0	10	0	0
6	A	15	0	17	1	0
7	A	436	0	0	9	0
7	J	32	0	0	0	0
7	K	36	0	0	1	0
All	All	7862	0	7273	64	0

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

All (64) 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:339:GLU:OE1	7:A:2479:HOH:O	2.04	0.74
1:A:481:ARG:NH2	3:A:2009:NAG:O6	2.23	0.72
1:A:743:TRP:HE1	1:A:745:SER:HB2	1.55	0.71
1:A:377:ARG:NH2	7:A:2399:HOH:O	2.23	0.71
1:A:44:GLN:HG2	1:A:55:ILE:HG12	1.77	0.67
1:A:48:ILE:HD12	2:K:16:LEU:HD21	1.77	0.66
1:A:51:GLU:OE2	7:A:2511:HOH:O	2.12	0.66
2:J:73:THR:HG22	2:J:95:ILE:HG22	1.79	0.65
1:A:759:ALA:HB3	1:A:798:ILE:HD11	1.79	0.64
1:A:174[A]:ARG:NH1	1:A:197:GLU:OE1	2.30	0.64
1:A:614:GLN:HB2	1:A:640:ARG:HD3	1.78	0.64
2:J:74:GLN:H	2:K:43:GLN:HG2	1.63	0.63
1:A:783:ASN:ND2	7:A:2501:HOH:O	2.32	0.62
1:A:79:CYS:HB3	1:A:81:LEU:HD13	1.82	0.61
1:A:665:HIS:HB2	1:A:668:MET:HG2	1.83	0.60
1:A:743:TRP:HA	1:A:772:ARG:HH12	1.67	0.59
1:A:543:VAL:HA	1:A:582:PRO:HB3	1.85	0.58
2:J:6:GLU:OE2	2:K:69:LYS:NZ	2.39	0.55
1:A:280:LEU:HD23	1:A:304:ARG:HB2	1.89	0.54
1:A:667:ASN:O	1:A:667:ASN:ND2	2.42	0.53
1:A:214:ARG:NH1	1:A:240:ASP:OD1	2.43	0.52
7:A:2306:HOH:O	2:J:109:HIS:HE1	1.93	0.51
1:A:696:SER:HB2	7:A:2517:HOH:O	2.11	0.51
1:A:576:VAL:HG11	1:A:608:VAL:HG12	1.93	0.50
1:A:784:ALA:HB3	1:A:787:PRO:N	2.27	0.50
2:K:51:ASP:OD1	7:K:216:HOH:O	2.20	0.50
1:A:713:PRO:HG2	1:A:716:LEU:HD13	1.94	0.49
3:A:2009:NAG:H83	7:A:2466:HOH:O	2.13	0.49
1:A:150:HIS:HE1	7:A:2489:HOH:O	1.95	0.48
1:A:481:ARG:NH1	1:A:503:ASP:OD2	2.45	0.48
1:A:418:THR:HB	1:A:442:HIS:HB2	1.94	0.48
1:A:398:GLU:HB3	1:A:420:VAL:HG12	1.97	0.47
1:A:650:CYS:HB2	1:A:675:LEU:HD23	1.97	0.47
1:A:174[A]:ARG:HG2	1:A:195:ASP:O	2.14	0.47
1:A:432:ARG:O	1:A:435:VAL:HG12	2.16	0.46
1:A:743:TRP:C	1:A:744:ARG:HG2	2.36	0.46
1:A:425:ARG:NH2	1:A:449:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:GLN:HG3	7:A:2451:HOH:O	2.16	0.46
1:A:50:SER:HB2	1:A:70:GLN:HE22	1.81	0.45
1:A:603:LEU:HD11	1:A:615:THR:HG21	1.97	0.45
1:A:744:ARG:H	1:A:772:ARG:NH1	2.15	0.44
1:A:446:ASP:N	1:A:446:ASP:OD1	2.49	0.44
1:A:712:LEU:HA	1:A:713:PRO:HD2	1.90	0.44
1:A:110:PRO:O	1:A:113:THR:HB	2.18	0.43
1:A:582:PRO:HG2	1:A:585:SER:HB3	2.00	0.43
1:A:238:LYS:HB2	1:A:263:ASP:O	2.18	0.43
1:A:322:GLN:HA	1:A:344:ILE:HA	2.00	0.42
1:A:454:GLN:HG2	1:A:459:ILE:HD11	2.00	0.42
1:A:454:GLN:HA	1:A:455:PRO:HD2	1.94	0.42
1:A:48:ILE:O	1:A:51:GLU:HG2	2.19	0.42
1:A:756:ASP:OD1	1:A:758:THR:HG22	2.19	0.42
1:A:567:CYS:HB2	1:A:641:THR:HG23	2.02	0.41
1:A:640:ARG:HD2	1:A:643:ASP:OD1	2.21	0.41
1:A:630:LYS:HA	1:A:662:PRO:HB3	2.01	0.41
2:J:7:ARG:HD2	2:K:107:LEU:HD13	2.01	0.41
1:A:603:LEU:O	1:A:606:THR:HG23	2.20	0.41
1:A:631:CYS:HA	1:A:632:PRO:HD3	1.92	0.41
1:A:716:LEU:O	1:A:744:ARG:HD3	2.21	0.41
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.82	0.41
2:J:9:LEU:HD11	2:K:9:LEU:HD22	2.03	0.41
1:A:230:SER:O	6:A:2019:EPE:H51	2.21	0.41
1:A:230:SER:HA	1:A:254:ASP:O	2.22	0.40
2:J:95:ILE:HA	2:J:96:PRO:HD3	1.91	0.40
1:A:575:LEU:HD21	1:A:585:SER:HB2	2.02	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	749/783 (96%)	701 (94%)	46 (6%)	2 (0%)	44	49
2	J	58/114 (51%)	55 (95%)	3 (5%)	0	100	100
2	K	60/114 (53%)	58 (97%)	2 (3%)	0	100	100
All	All	867/1011 (86%)	814 (94%)	51 (6%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	VAL
1	A	582	PRO

### 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	703/723 (97%)	679 (97%)	24 (3%)	42	53
2	J	57/101 (56%)	55 (96%)	2 (4%)	41	51
2	K	57/101 (56%)	55 (96%)	2 (4%)	41	51
All	All	817/925 (88%)	789 (97%)	28 (3%)	42	53

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	49	MET
1	A	59	ASN
1	A	84	THR
1	A	90	LEU
1	A	175	ASN
1	A	273	ASP
1	A	418	THR
1	A	427	ARG
1	A	481	ARG
1	A	497	LEU

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Mol	Chain	Res	Type
1	A	508	ASN
1	A	542	ASP
1	A	577	ARG
1	A	603	LEU
1	A	608	VAL
1	A	621	ASP
1	A	667	ASN
1	A	696	SER
1	A	714	THR
1	A	729	LEU
1	A	744	ARG
1	A	746	VAL
1	A	757	CYS
2	J	73	THR
2	J	107	LEU
2	K	1	VAL
2	K	107	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	70	GLN
1	A	150	HIS
1	A	232	GLN
1	A	239	HIS
1	A	583	GLN
1	A	610	GLN
1	A	677	ASN
2	J	52	GLN
2	J	109	HIS
2	K	43	GLN
2	K	65	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

19 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	0.40	0	15,19,21	0.53	0
3	NAG	A	2002	3,4	14,14,15	0.60	0	15,19,21	0.49	0
4	BMA	A	2003	3,4	11,11,12	1.62	3 (27%)	13,15,17	1.64	2 (15%)
4	BMA	A	2004	5,4	11,11,12	0.87	0	13,15,17	0.61	0
5	MAN	A	2005	4	11,11,12	0.84	0	13,15,17	1.12	1 (7%)
3	NAG	A	2006	1	14,14,15	0.32	0	15,19,21	0.59	0
3	NAG	A	2007	1,3	14,14,15	0.48	0	15,19,21	0.47	0
3	NAG	A	2008	3	14,14,15	0.40	0	15,19,21	0.47	0
3	NAG	A	2009	1,3	14,14,15	0.57	0	15,19,21	0.58	0
3	NAG	A	2010	3,4	14,14,15	0.21	0	15,19,21	0.66	0
4	BMA	A	2011	3	11,11,12	0.90	0	13,15,17	0.83	0
3	NAG	A	2012	1	14,14,15	0.39	0	15,19,21	0.49	0
3	NAG	A	2013	1	14,14,15	0.39	0	15,19,21	0.76	0
3	NAG	A	2014	1	14,14,15	0.25	0	15,19,21	0.61	0
3	NAG	A	2015	1,3	14,14,15	0.44	0	15,19,21	0.59	0
3	NAG	A	2016	3	14,14,15	0.20	0	15,19,21	0.43	0
3	NAG	A	2017	1	14,14,15	0.78	1 (7%)	15,19,21	0.88	1 (6%)
3	NAG	A	2018	1	14,14,15	0.76	1 (7%)	15,19,21	0.59	0
6	EPE	A	2019	-	15,15,15	0.94	1 (6%)	18,20,20	2.42	8 (44%)

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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2008	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2009	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2010	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	2011	3	-	0/2/19/22	0/1/1/1
3	NAG	A	2012	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2013	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2014	1	-	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	-	0/6/23/26	0/1/1/1
3	NAG	A	2018	1	-	0/6/23/26	0/1/1/1
6	EPE	A	2019	-	-	0/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2018	NAG	O5-C1	-2.01	1.40	1.43
4	A	2003	BMA	C4-C5	2.02	1.57	1.53
3	A	2017	NAG	C1-C2	2.60	1.56	1.52
4	A	2003	BMA	C2-C3	2.89	1.56	1.52
4	A	2003	BMA	O3-C3	3.18	1.50	1.43
6	A	2019	EPE	C10-S	3.21	1.82	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2019	EPE	C9-N1-C6	-2.28	105.42	111.26
6	A	2019	EPE	C5-C6-N1	2.44	115.57	110.63
6	A	2019	EPE	O3S-S-C10	2.53	109.16	106.06
3	A	2017	NAG	C1-O5-C5	2.58	115.72	112.17
6	A	2019	EPE	O2S-S-C10	2.70	109.11	106.79
5	A	2005	MAN	C1-O5-C5	2.71	115.90	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2019	EPE	C7-N4-C3	2.73	118.25	111.26
4	A	2003	BMA	C1-O5-C5	2.91	116.18	112.17
6	A	2019	EPE	C6-C5-N4	3.16	117.02	110.63
6	A	2019	EPE	O1S-S-C10	4.65	110.78	106.79
4	A	2003	BMA	O3-C3-C2	4.67	118.53	110.02
6	A	2019	EPE	C5-N4-C3	5.47	121.27	108.87

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	2009	NAG	2	0
6	A	2019	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	755/783 (96%)	-0.22	20 (2%) 56 54	16, 40, 84, 125	0
2	J	64/114 (56%)	0.74	9 (14%) 3 3	19, 50, 96, 107	0
2	K	66/114 (57%)	0.33	6 (9%) 10 9	18, 50, 83, 101	0
All	All	885/1011 (87%)	-0.11	35 (3%) 39 37	16, 42, 86, 125	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	17	VAL	5.6
1	A	622	PHE	5.4
2	J	41	ALA	5.0
1	A	609	ARG	4.9
2	J	16	LEU	4.8
2	K	41	ALA	4.7
2	K	95	ILE	4.0
2	J	42	ILE	3.7
2	J	15	LYS	3.5
1	A	783	ASN	3.5
2	J	110	HIS	3.4
2	K	74	GLN	3.3
2	K	42	ILE	3.0
1	A	608	VAL	3.0
1	A	652	SER	2.9
1	A	660	ARG	2.8
2	J	14	ARG	2.8
1	A	754	MET	2.5
1	A	666	LYS	2.5
1	A	782	VAL	2.4
2	J	43	GLN	2.4
1	A	48	ILE	2.3
2	K	17	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	579	VAL	2.3
1	A	586	ARG	2.3
1	A	543	VAL	2.2
1	A	621	ASP	2.2
1	A	50	SER	2.2
1	A	784	ALA	2.1
1	A	59	ASN	2.0
1	A	605	GLY	2.0
1	A	758	THR	2.0
2	K	40	GLN	2.0
2	J	74	GLN	2.0
1	A	542	ASP	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	2013	14/15	0.88	0.15	3.54	53,69,83,86	0
3	NAG	A	2015	14/15	0.96	0.14	0.41	43,64,73,81	0
3	NAG	A	2001	14/15	0.96	0.10	-0.37	21,27,35,37	0
3	NAG	A	2009	14/15	0.95	0.10	-0.81	35,46,58,64	0
6	EPE	A	2019	15/15	0.98	0.09	-1.66	30,40,47,50	0
4	BMA	A	2003	11/12	0.93	0.08	-	56,59,78,79	0
3	NAG	A	2002	14/15	0.97	0.08	-	31,40,51,51	0
5	MAN	A	2005	11/12	0.93	0.08	-	55,60,69,70	0
3	NAG	A	2018	14/15	0.82	0.26	-	62,84,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	2014	14/15	0.91	0.15	-	53,66,77,79	0
3	NAG	A	2010	14/15	0.89	0.14	-	55,64,76,91	0
3	NAG	A	2016	14/15	0.86	0.21	-	76,80,85,87	0
3	NAG	A	2017	14/15	0.89	0.18	-	47,60,67,75	0
4	BMA	A	2011	11/12	0.77	0.30	-	96,102,111,112	0
4	BMA	A	2004	11/12	0.87	0.11	-	73,80,86,96	0
3	NAG	A	2007	14/15	0.93	0.12	-	39,53,59,62	0
3	NAG	A	2012	14/15	0.88	0.11	-	52,60,64,67	0
3	NAG	A	2008	14/15	0.89	0.12	-	61,71,77,81	0
3	NAG	A	2006	14/15	0.93	0.14	-	50,62,71,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.