



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:52 PM GMT

PDB ID : 4ARN
Title : Crystal structure of the N-terminal domain of Drosophila Toll receptor
Authors : Gangloff, M.; Gay, N.J.
Deposited on : 2012-04-25
Resolution : 2.41 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

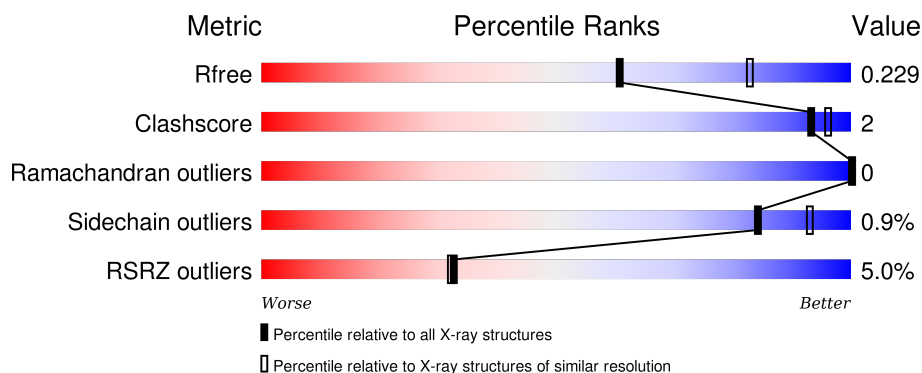
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	279	<div> <div>5%</div> <div>91%</div> <div>8%</div> </div>
1	B	279	<div> <div>5%</div> <div>91%</div> <div>7%</div> </div>
1	C	279	<div> <div>5%</div> <div>92%</div> <div>6%</div> </div>
1	D	279	<div> <div>4%</div> <div>92%</div> <div>6%</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	D	601	-	-	-	X
6	MAN	C	506	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9283 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 RECEPTOR, VARIABLE LYMPHOCYTE RECEPTOR B.61 CHIMERA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	2	0
			2217	1389	399	408	21			
1	B	273	Total	C	N	O	S	0	1	0
			2162	1354	388	399	21			
1	C	273	Total	C	N	O	S	0	1	0
			2172	1360	392	399	21			
1	D	272	Total	C	N	O	S	0	1	0
			2164	1355	391	397	21			

There are 36 discrepancies between the modelled and reference sequences:

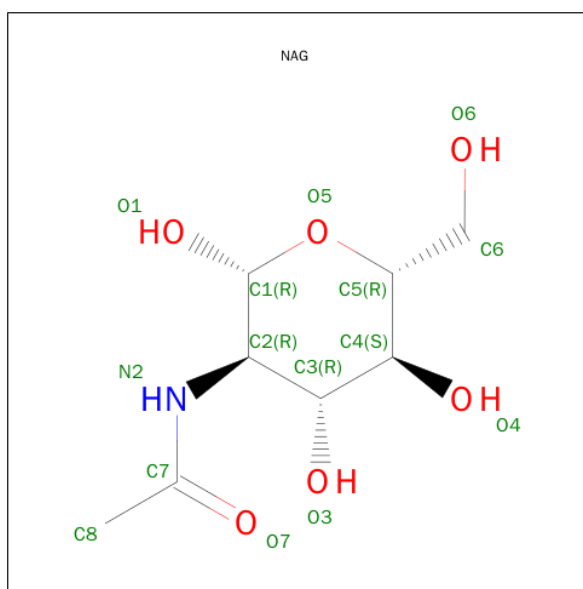
Chain	Residue	Modelled	Actual	Comment	Reference
A	229	ALA	ASP	CLONING ARTIFACT	UNP Q4G1L2
A	230	SER	THR	CLONING ARTIFACT	UNP Q4G1L2
A	300	GLY	-	EXPRESSION TAG	UNP Q4G1L2
A	301	GLU	-	EXPRESSION TAG	UNP Q4G1L2
A	302	ASN	-	EXPRESSION TAG	UNP Q4G1L2
A	303	LEU	-	EXPRESSION TAG	UNP Q4G1L2
A	304	TYR	-	EXPRESSION TAG	UNP Q4G1L2
A	305	PHE	-	EXPRESSION TAG	UNP Q4G1L2
A	306	GLN	-	EXPRESSION TAG	UNP Q4G1L2
B	229	ALA	ASP	CLONING ARTIFACT	UNP Q4G1L2
B	230	SER	THR	CLONING ARTIFACT	UNP Q4G1L2
B	300	GLY	-	EXPRESSION TAG	UNP Q4G1L2
B	301	GLU	-	EXPRESSION TAG	UNP Q4G1L2
B	302	ASN	-	EXPRESSION TAG	UNP Q4G1L2
B	303	LEU	-	EXPRESSION TAG	UNP Q4G1L2
B	304	TYR	-	EXPRESSION TAG	UNP Q4G1L2
B	305	PHE	-	EXPRESSION TAG	UNP Q4G1L2
B	306	GLN	-	EXPRESSION TAG	UNP Q4G1L2
C	229	ALA	ASP	CLONING ARTIFACT	UNP Q4G1L2
C	230	SER	THR	CLONING ARTIFACT	UNP Q4G1L2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	300	GLY	-	EXPRESSION TAG	UNP Q4G1L2
C	301	GLU	-	EXPRESSION TAG	UNP Q4G1L2
C	302	ASN	-	EXPRESSION TAG	UNP Q4G1L2
C	303	LEU	-	EXPRESSION TAG	UNP Q4G1L2
C	304	TYR	-	EXPRESSION TAG	UNP Q4G1L2
C	305	PHE	-	EXPRESSION TAG	UNP Q4G1L2
C	306	GLN	-	EXPRESSION TAG	UNP Q4G1L2
D	229	ALA	ASP	CLONING ARTIFACT	UNP Q4G1L2
D	230	SER	THR	CLONING ARTIFACT	UNP Q4G1L2
D	300	GLY	-	EXPRESSION TAG	UNP Q4G1L2
D	301	GLU	-	EXPRESSION TAG	UNP Q4G1L2
D	302	ASN	-	EXPRESSION TAG	UNP Q4G1L2
D	303	LEU	-	EXPRESSION TAG	UNP Q4G1L2
D	304	TYR	-	EXPRESSION TAG	UNP Q4G1L2
D	305	PHE	-	EXPRESSION TAG	UNP Q4G1L2
D	306	GLN	-	EXPRESSION TAG	UNP Q4G1L2

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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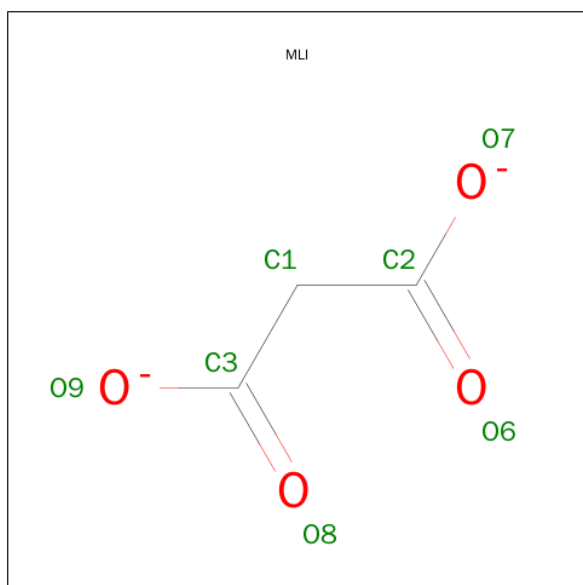
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	7	Total	C	N	O	0	0
			81	46	2	33		

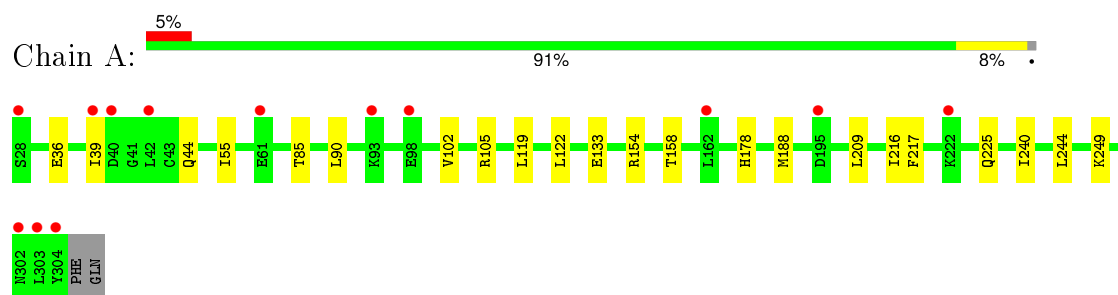
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	107	Total	O	0	0
			107	107		
7	B	90	Total	O	0	0
			90	90		
7	C	68	Total	O	0	0
			68	68		
7	D	58	Total	O	0	0
			58	58		

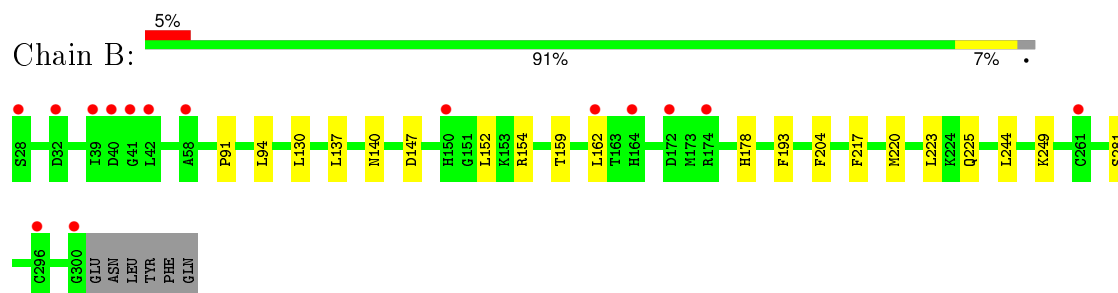
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

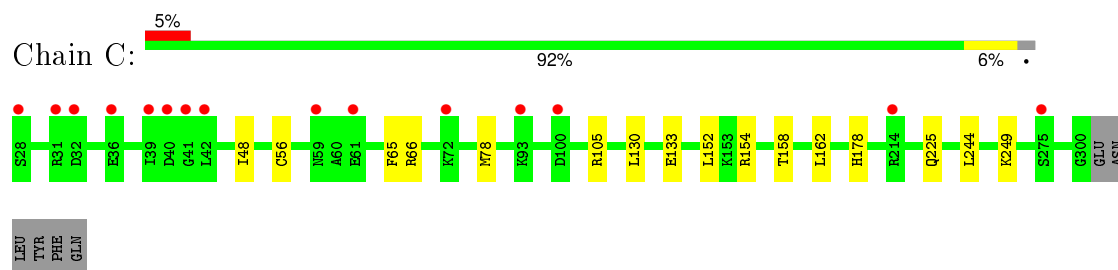
- Molecule 1: TOLL RECEPTOR, VARIABLE LYMPHOCYTE RECEPTOR B.61 CHIMERA



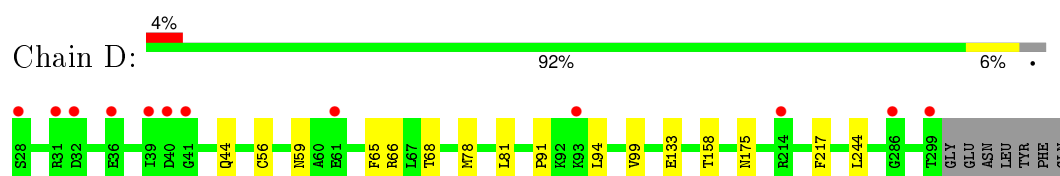
- Molecule 1: TOLL RECEPTOR, VARIABLE LYMPHOCYTE RECEPTOR B.61 CHIMERA



- Molecule 1: TOLL RECEPTOR, VARIABLE LYMPHOCYTE RECEPTOR B.61 CHIMERA



- Molecule 1: TOLL RECEPTOR, VARIABLE LYMPHOCYTE RECEPTOR B.61 CHIMERA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.79Å 93.28Å 225.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 2.41 29.34 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.95-2.41) 99.6 (29.34-2.41)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.201 , 0.216 0.211 , 0.229	Depositor DCC
R_{free} test set	3668 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.3	EDS
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 72763 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9283	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, BMA, NAG, MLI, FUC

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	0.39	0/2268	0.58	0/3065
1	B	0.41	1/2208 (0.0%)	0.59	0/2986
1	C	0.40	0/2218	0.58	0/2997
1	D	0.39	0/2210	0.58	0/2987
All	All	0.40	1/8904 (0.0%)	0.58	0/12035

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	ASN	CG-ND2	-5.52	1.19	1.32

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	2217	0	2217	11	0
1	B	2162	0	2152	8	0
1	C	2172	0	2175	8	0
1	D	2164	0	2160	7	0
2	A	14	0	13	0	0
2	B	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	14	0	13	1	0
3	A	24	0	22	0	0
4	A	7	0	2	0	0
4	B	7	0	2	0	0
5	C	28	0	25	0	0
5	D	28	0	25	0	0
6	C	81	0	70	0	0
7	A	107	0	0	0	0
7	B	90	0	0	0	0
7	C	68	0	0	0	0
7	D	58	0	0	0	0
All	All	9283	0	8915	33	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 2.

All (33) 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:44:GLN:HG2	1:A:55:ILE:HB	1.84	0.60
1:C:225:GLN:HG2	1:C:249:LYS:HB2	1.86	0.57
1:D:44:GLN:HE21	1:D:59:ASN:H	1.53	0.56
1:A:217:PHE:HB3	1:A:244:LEU:HD21	1.87	0.56
1:C:66:ARG:HB3	1:C:78:MET:HB3	1.88	0.56
1:B:130:LEU:HB3	1:B:152:LEU:HD21	1.88	0.55
1:D:217:PHE:HB3	1:D:244:LEU:HD21	1.90	0.54
1:A:154:ARG:HG3	1:A:178:HIS:HB2	1.92	0.51
1:A:225:GLN:HG2	1:A:249:LYS:HB2	1.93	0.51
1:B:91:PRO:HB2	1:B:94:LEU:HG	1.92	0.50
1:B:154:ARG:HG3	1:B:178:HIS:HB2	1.94	0.49
1:C:105:ARG:HD2	1:C:133:GLU:HB3	1.95	0.49
1:A:90:LEU:HD22	1:A:122:LEU:HD21	1.96	0.48
1:C:130:LEU:HB3	1:C:152:LEU:HD21	1.95	0.48
1:D:133:GLU:HG3	1:D:158:THR:HB	1.96	0.47
1:D:66:ARG:HB3	1:D:78:MET:HB3	1.97	0.47
1:C:56:CYS:HB2	1:C:65:PHE:HB2	1.97	0.47
1:B:217:PHE:HB3	1:B:244:LEU:HD21	1.97	0.46
1:B:193:PHE:HZ	1:B:204:PHE:CE2	2.33	0.46
1:B:220:MET:HE3	1:B:223:LEU:HD13	1.99	0.45
1:A:85:THR:HA	1:C:48:ILE:HD12	1.98	0.45
1:D:175:ASN:OD1	2:D:601:NAG:N2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:CYS:HB2	1:D:65:PHE:HB2	2.00	0.44
1:A:133:GLU:HG3	1:A:158:THR:HB	1.99	0.44
1:A:188[A]:MET:HG2	1:A:209:LEU:HD21	2.00	0.43
1:A:216:ILE:HG22	1:A:240:ILE:HD11	2.01	0.43
1:D:91:PRO:HG2	1:D:94:LEU:HD22	2.01	0.42
1:C:154:ARG:HG3	1:C:178:HIS:HB2	2.01	0.42
1:C:133:GLU:HG3	1:C:158:THR:HB	2.02	0.42
1:A:36:GLU:HA	1:A:39:ILE:HD12	2.02	0.42
1:B:225:GLN:HG2	1:B:249:LYS:HB2	2.02	0.41
1:B:137:LEU:HD11	1:B:159:THR:HG21	2.02	0.41
1:A:102:VAL:HG11	1:A:119:LEU:HD11	2.03	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	277/279 (99%)	264 (95%)	13 (5%)	0	100	100
1	B	272/279 (98%)	254 (93%)	18 (7%)	0	100	100
1	C	272/279 (98%)	257 (94%)	15 (6%)	0	100	100
1	D	271/279 (97%)	257 (95%)	14 (5%)	0	100	100
All	All	1092/1116 (98%)	1032 (94%)	60 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	253/255 (99%)	252 (100%)	1 (0%)	93	98
1	B	245/255 (96%)	242 (99%)	3 (1%)	78	90
1	C	247/255 (97%)	245 (99%)	2 (1%)	86	94
1	D	245/255 (96%)	242 (99%)	3 (1%)	78	90
All	All	990/1020 (97%)	981 (99%)	9 (1%)	84	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	B	147	ASP
1	B	162	LEU
1	B	281	SER
1	C	162	LEU
1	C	244	LEU
1	D	68	THR
1	D	81	LEU
1	D	99	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	144	GLN
1	C	232	GLN
1	D	44	GLN
1	D	76	GLN
1	D	232	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 ⓘ

13 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	501	1,3	14,14,15	0.27	0	15,19,21	0.78	1 (6%)
3	FUC	A	502	3	10,10,11	2.15	4 (40%)	14,14,16	1.91	3 (21%)
5	NAG	C	401	1,5	14,14,15	0.30	0	15,19,21	0.63	0
5	NAG	C	402	5	14,14,15	0.26	0	15,19,21	0.38	0
6	NAG	C	501	1,6	14,14,15	0.25	0	15,19,21	0.71	1 (6%)
6	NAG	C	502	6	14,14,15	0.26	0	15,19,21	0.47	0
6	BMA	C	503	6	11,11,12	2.17	3 (27%)	14,15,17	2.39	2 (14%)
6	FUC	C	504	6	10,10,11	2.12	4 (40%)	14,14,16	1.68	3 (21%)
6	FUC	C	505	6	10,10,11	2.09	4 (40%)	14,14,16	1.74	4 (28%)
6	MAN	C	506	6	11,11,12	1.69	3 (27%)	14,15,17	3.14	3 (21%)
6	BMA	C	507	6	11,11,12	1.96	4 (36%)	14,15,17	1.45	1 (7%)
5	NAG	D	401	1,5	14,14,15	0.27	0	15,19,21	0.46	0
5	NAG	D	402	5	14,14,15	0.26	0	15,19,21	0.42	0

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	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	502	3	-	0/0/17/20	0/1/1/1
5	NAG	C	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	402	5	-	0/6/23/26	0/1/1/1
6	NAG	C	501	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	502	6	-	0/6/23/26	0/1/1/1
6	BMA	C	503	6	-	0/2/19/22	0/1/1/1
6	FUC	C	504	6	-	0/0/17/20	0/1/1/1
6	FUC	C	505	6	-	0/0/17/20	0/1/1/1
6	MAN	C	506	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	C	507	6	-	0/2/19/22	0/1/1/1
5	NAG	D	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	402	5	-	0/6/23/26	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	507	BMA	C4-C3	2.39	1.58	1.52
6	C	507	BMA	C1-C2	2.40	1.57	1.52
6	C	506	MAN	C4-C5	2.41	1.58	1.53
6	C	503	BMA	C4-C3	2.42	1.58	1.52
3	A	502	FUC	C4-C3	2.44	1.58	1.52
6	C	505	FUC	C4-C3	2.45	1.58	1.52
6	C	504	FUC	C4-C3	2.46	1.58	1.52
6	C	506	MAN	C1-C2	2.60	1.58	1.52
6	C	507	BMA	C4-C5	2.69	1.58	1.53
6	C	504	FUC	C4-C5	2.70	1.58	1.52
6	C	505	FUC	C4-C5	2.70	1.58	1.52
6	C	505	FUC	C1-C2	2.82	1.58	1.52
3	A	502	FUC	C4-C5	2.83	1.58	1.52
6	C	504	FUC	C1-C2	2.86	1.59	1.52
6	C	506	MAN	C2-C3	2.86	1.56	1.52
6	C	503	BMA	C4-C5	2.90	1.59	1.53
3	A	502	FUC	C1-C2	2.90	1.59	1.52
6	C	507	BMA	C2-C3	3.87	1.57	1.52
6	C	505	FUC	C2-C3	4.10	1.58	1.52
6	C	504	FUC	C2-C3	4.22	1.58	1.52
3	A	502	FUC	C2-C3	4.35	1.58	1.52
6	C	503	BMA	C2-C3	5.02	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	503	BMA	C1-C2-C3	-3.67	105.20	109.54
6	C	507	BMA	C1-C2-C3	-2.54	106.54	109.54
6	C	505	FUC	O2-C2-C3	-2.37	105.36	110.12
3	A	502	FUC	O2-C2-C3	-2.29	105.52	110.12
6	C	504	FUC	O2-C2-C3	-2.22	105.66	110.12
6	C	506	MAN	C1-C2-C3	2.01	111.92	109.54
6	C	501	NAG	C1-O5-C5	2.03	114.82	112.25
6	C	504	FUC	O2-C2-C1	2.10	113.42	109.21
6	C	505	FUC	O2-C2-C1	2.17	113.55	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	505	FUC	O5-C1-C2	2.21	114.45	110.86
3	A	502	FUC	O5-C1-C2	2.58	115.05	110.86
3	A	501	NAG	C1-O5-C5	2.77	115.76	112.25
6	C	505	FUC	C1-O5-C5	4.25	118.94	112.38
6	C	504	FUC	C1-O5-C5	4.32	119.05	112.38
3	A	502	FUC	C1-O5-C5	4.88	119.91	112.38
6	C	506	MAN	O5-C1-C2	5.84	120.34	110.86
6	C	503	BMA	O3-C3-C2	7.81	124.11	110.00
6	C	506	MAN	C1-O5-C5	9.29	124.04	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

7 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	401	1	14,14,15	0.27	0	15,19,21	0.48	0
4	MLI	A	601	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAG	B	401	1	14,14,15	0.25	0	15,19,21	0.45	0
2	NAG	B	501	1	14,14,15	0.27	0	15,19,21	0.49	0
2	NAG	B	601	1	14,14,15	0.27	0	15,19,21	0.63	1 (6%)
4	MLI	B	602	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAG	D	601	1	14,14,15	0.35	0	15,19,21	0.90	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	401	1	-	0/6/23/26	0/1/1/1
4	MLI	A	601	-	-	0/0/4/4	0/0/0/0
2	NAG	B	401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	MLI	B	602	-	-	0/0/4/4	0/0/0/0
2	NAG	D	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAG	C1-O5-C5	2.19	115.03	112.25
2	D	601	NAG	C1-O5-C5	3.12	116.21	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	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

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	277/279 (99%)	0.06	13 (4%) 35 35	38, 59, 93, 110	3 (1%)
1	B	273/279 (97%)	0.08	15 (5%) 29 28	37, 59, 90, 103	5 (1%)
1	C	273/279 (97%)	0.16	15 (5%) 29 28	45, 68, 98, 116	5 (1%)
1	D	272/279 (97%)	0.05	12 (4%) 38 38	47, 67, 96, 131	3 (1%)
All	All	1095/1116 (98%)	0.09	55 (5%) 32 32	37, 64, 95, 131	16 (1%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	ASP	5.7
1	C	41	GLY	5.6
1	A	42	LEU	5.5
1	D	299	THR	5.4
1	D	28	SER	5.2
1	C	42	LEU	5.0
1	C	59	ASN	4.1
1	D	214	ARG	4.1
1	C	28	SER	4.0
1	A	39	ILE	4.0
1	C	39	ILE	3.8
1	C	61	GLU	3.7
1	D	41	GLY	3.6
1	B	39	ILE	3.5
1	D	39	ILE	3.4
1	C	275	SER	3.4
1	B	42	LEU	3.3
1	B	296	CYS	3.2
1	A	28	SER	3.2
1	C	31	ARG	3.1
1	A	302	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	41	GLY	3.1
1	A	304	TYR	3.0
1	B	32	ASP	2.9
1	B	28	SER	2.9
1	A	40	ASP	2.9
1	A	93	LYS	2.9
1	B	40	ASP	2.8
1	B	172	ASP	2.8
1	D	40	ASP	2.8
1	A	61	GLU	2.7
1	B	150	HIS	2.7
1	D	61	GLU	2.7
1	C	93	LYS	2.7
1	A	162	LEU	2.7
1	A	303	LEU	2.7
1	B	261	CYS	2.6
1	C	36	GLU	2.6
1	D	93	LYS	2.6
1	C	32	ASP	2.6
1	B	162	LEU	2.5
1	D	32	ASP	2.4
1	D	31	ARG	2.4
1	D	286	GLY	2.3
1	C	100	ASP	2.3
1	C	72	LYS	2.2
1	B	58	ALA	2.2
1	A	195	ASP	2.2
1	A	98	GLU	2.2
1	B	300	GLY	2.1
1	B	164	HIS	2.1
1	C	214	ARG	2.0
1	A	222	LYS	2.0
1	D	36	GLU	2.0
1	B	174	ARG	2.0

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 ⓘ

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
6	MAN	C	506	11/12	0.67	0.36	7.85	114,118,126,127	0
6	NAG	C	501	14/15	0.92	0.13	-0.35	76,81,87,92	0
5	NAG	C	401	14/15	0.93	0.23	-	80,88,94,96	0
5	NAG	C	402	14/15	0.89	0.50	-	100,103,109,110	0
6	FUC	C	504	10/11	0.73	0.33	-	97,102,107,108	10
6	BMA	C	507	11/12	0.61	0.77	-	92,96,101,103	11
6	NAG	C	502	14/15	0.90	0.21	-	83,89,94,98	0
6	BMA	C	503	11/12	0.68	0.43	-	101,105,110,114	11
5	NAG	D	402	14/15	0.80	0.46	-	98,102,109,111	14
3	NAG	A	501	14/15	0.87	0.32	-	103,108,110,111	0
5	NAG	D	401	14/15	0.80	0.31	-	81,91,97,97	0
6	FUC	C	505	10/11	0.95	0.24	-	78,80,82,84	10
3	FUC	A	502	10/11	0.77	0.46	-	113,116,118,119	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(Å ²)	Q<0.9
2	NAG	D	601	14/15	0.65	0.39	8.39	108,111,113,115	14
2	NAG	B	501	14/15	0.69	0.34	1.62	88,90,93,94	14
4	MLI	B	602	7/7	0.89	0.18	1.24	80,80,82,83	0
4	MLI	A	601	7/7	0.97	0.15	-2.27	40,41,43,44	0
2	NAG	B	401	14/15	0.94	0.22	-	81,85,88,88	0
2	NAG	B	601	14/15	0.83	0.42	-	102,104,109,112	0
2	NAG	A	401	14/15	0.93	0.23	-	87,91,94,96	0

6.5 Other polymers

There are no such residues in this entry.