



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 10:47 PM BST

PDB ID : 5GS0
Title : Crystal structure of the complex of TLR3 and bi-specific diabody
Authors : Kim, J.H.; Song, D.H.; Youn, S.J.; Kim, J.W.; Cho, G.; Lee, H.; Lee, J.O.
Deposited on : 2016-08-13
Resolution : 3.27 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

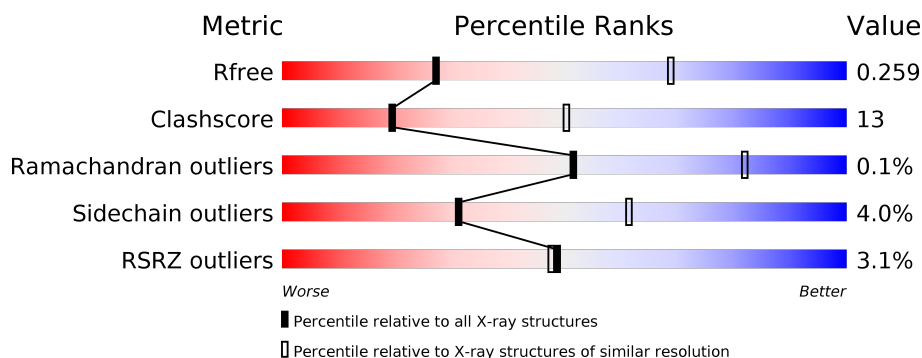
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 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	671	<div> <div>70%</div> <div>27%</div> <div>..</div> </div>
1	B	671	<div> <div>74%</div> <div>23%</div> <div>..</div> </div>
2	C	107	<div> <div>67%</div> <div>30%</div> <div>.</div> </div>
2	E	107	<div> <div>73%</div> <div>21%</div> <div>5%</div> <div>.</div> </div>
3	D	127	<div> <div>67%</div> <div>27%</div> <div>..</div> </div>
3	F	127	<div> <div>2%</div> <div>64%</div> <div>30%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	H	121	
4	X	121	
5	L	107	
5	Y	107	

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
6	NAG	A	804	-	-	-	X
6	NAG	A	805	-	-	-	X
6	NAG	A	813	-	-	-	X
6	NAG	B	705	-	-	-	X
6	NAG	B	706	-	-	-	X
6	NAG	B	719	-	-	-	X
7	BMA	A	819	-	-	-	X
7	BMA	B	720	-	-	-	X
8	MAN	A	820	-	-	-	X
8	MAN	B	701	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18219 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5323	3407	903	996	17			
1	B	663	Total	C	N	O	S	0	0	0
			5323	3407	903	996	17			

- Molecule 2 is a protein called light chain (anti-TLR3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	107	Total	C	N	O	S	0	0	0
			809	504	133	170	2			
2	E	107	Total	C	N	O	S	0	0	0
			809	504	133	170	2			

- Molecule 3 is a protein called heavy chain (anti-TLR3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	122	Total	C	N	O	S	0	0	0
			956	609	161	184	2			
3	F	122	Total	C	N	O	S	0	0	0
			956	609	161	184	2			

- Molecule 4 is a protein called heavy chain (anti-Lid).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	114	Total	C	N	O	S	0	0	0
			909	582	151	173	3			
4	H	116	Total	C	N	O	S	0	0	0
			921	588	153	177	3			

- Molecule 5 is a protein called light chain (anti-Lid).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Y	107	Total	C	N	O	S	0	0	0
			824	514	141	167	2			
5	L	105	Total	C	N	O	S	0	0	0
			807	502	138	165	2			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		

Continued on next page...

Continued from previous page...

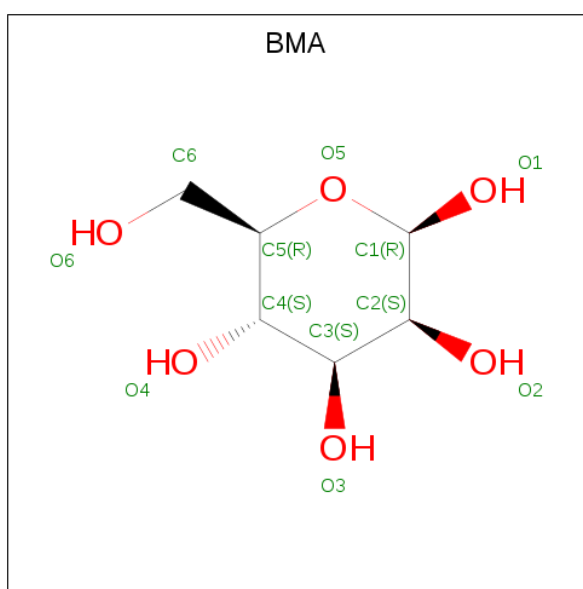
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	A	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 7 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	6	6		
7	A	1	Total	C	O	0	0
			12	6	6		
7	B	1	Total	C	O	0	0
			12	6	6		
7	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).

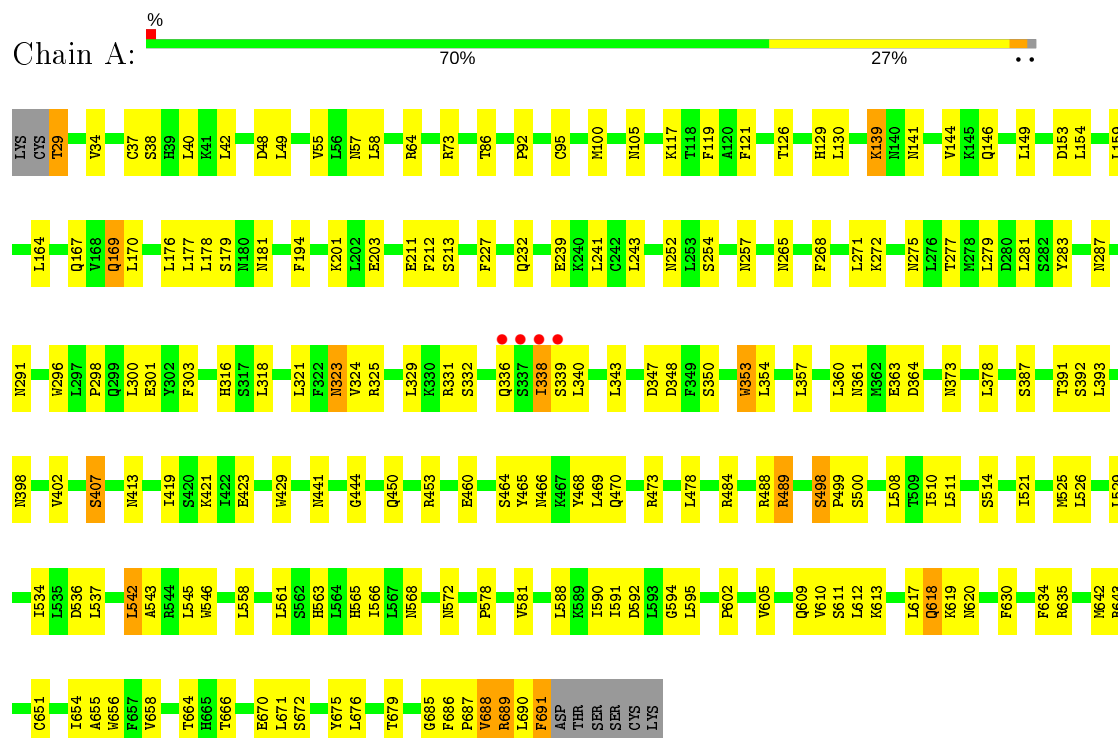


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	6	6		
8	B	1	Total	C	O	0	0
			12	6	6		

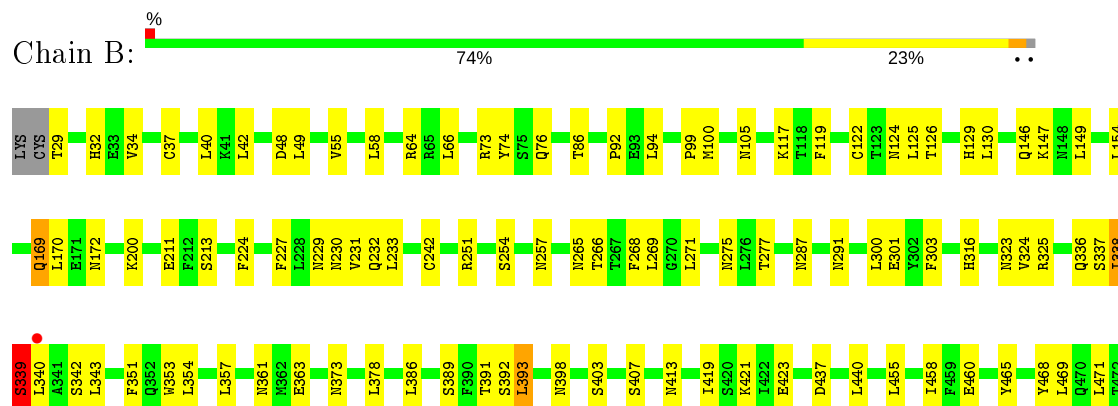
3 Residue-property plots

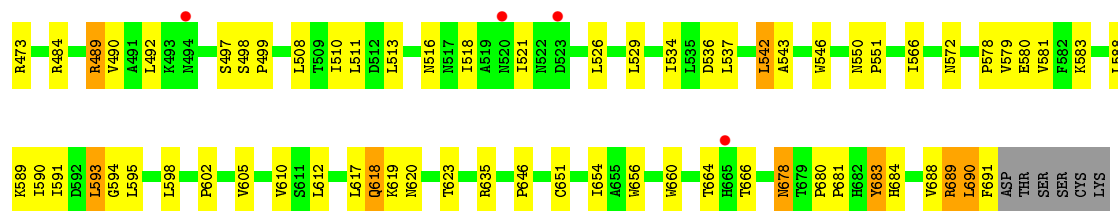
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 3



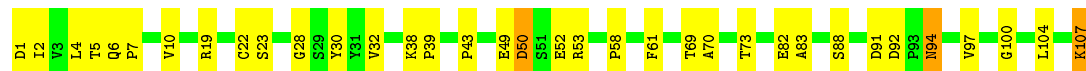
• Molecule 1: Toll-like receptor 3





• Molecule 2: light chain (anti-TLR3)

Chain C: 67% 30%



• Molecule 2: light chain (anti-TLR3)

Chain E: 73% 21% 5%



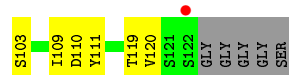
• Molecule 3: heavy chain (anti-TLR3)

Chain D: 67% 27%



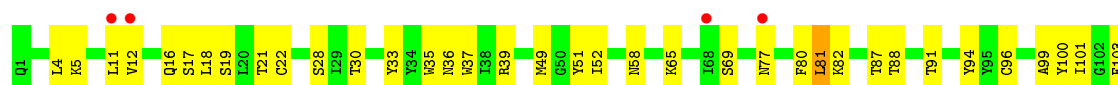
• Molecule 3: heavy chain (anti-TLR3)

Chain F: 2% 64% 30%



• Molecule 4: heavy chain (anti-Lid)

Chain X: 3% 61% 31% 6%

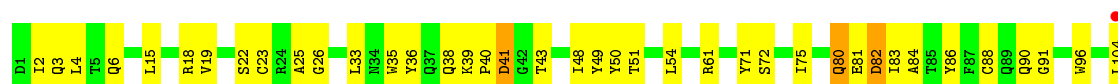




• Molecule 4: heavy chain (anti-Lid)



• Molecule 5: light chain (anti-Lid)



• Molecule 5: light chain (anti-Lid)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.52Å 141.33Å 150.83Å 90.00° 106.88° 90.00°	Depositor
Resolution (Å)	35.07 – 3.27 41.16 – 3.28	Depositor EDS
% Data completeness (in resolution range)	95.7 (35.07-3.27) 92.3 (41.16-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.192 , 0.248 0.208 , 0.259	Depositor DCC
R_{free} test set	2795 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18219	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.52	2/5436 (0.0%)	0.72	4/7380 (0.1%)
1	B	0.50	0/5436	0.73	4/7380 (0.1%)
2	C	0.56	0/829	0.76	2/1132 (0.2%)
2	E	0.67	2/829 (0.2%)	1.34	13/1132 (1.1%)
3	D	0.54	0/981	0.73	1/1337 (0.1%)
3	F	0.44	0/981	0.70	2/1337 (0.1%)
4	H	0.42	0/946	0.68	0/1287
4	X	0.47	0/934	0.67	0/1271
5	L	0.38	0/824	0.70	2/1119 (0.2%)
5	Y	0.48	0/841	0.70	1/1141 (0.1%)
All	All	0.51	4/18037 (0.0%)	0.76	29/24516 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	93	PRO	N-CD	9.73	1.61	1.47
1	A	407	SER	C-N	7.04	1.47	1.34
2	E	54	PRO	N-CD	6.39	1.56	1.47
1	A	353	TRP	CB-CG	-5.07	1.41	1.50

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	91	ASP	CB-CA-C	20.47	151.35	110.40
2	E	54	PRO	N-CA-CB	-14.08	86.40	103.30
2	E	91	ASP	N-CA-C	-10.81	81.82	111.00
2	E	53	ARG	C-N-CD	-10.30	97.93	120.60
2	E	54	PRO	N-CD-CG	-10.22	87.86	103.20

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	5323	0	5345	129	0
1	B	5323	0	5345	111	0
2	C	809	0	755	20	0
2	E	809	0	755	17	0
3	D	956	0	938	25	0
3	F	956	0	938	30	0
4	H	921	0	885	22	0
4	X	909	0	875	30	0
5	L	807	0	772	32	0
5	Y	824	0	796	37	0
6	A	255	0	255	18	0
6	B	255	0	255	13	0
7	A	24	0	24	2	0
7	B	24	0	24	2	0
8	A	12	0	12	0	0
8	B	12	0	12	0	0
All	All	18219	0	17986	462	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 13.

The worst 5 of 462 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:B:338:ILE:HG12	1:B:338:ILE:O	1.50	1.06
4:X:12:VAL:O	4:X:114:VAL:HG22	1.60	1.01
2:E:53:ARG:NH1	2:E:61:PHE:O	2.03	0.92
4:X:69:SER:HB3	4:X:82:LYS:HB3	1.52	0.91
4:X:28:SER:HA	4:X:77:ASN:HD21	1.36	0.90

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	661/671 (98%)	611 (92%)	50 (8%)	0	100	100
1	B	661/671 (98%)	613 (93%)	48 (7%)	0	100	100
2	C	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	E	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	D	120/127 (94%)	110 (92%)	10 (8%)	0	100	100
3	F	120/127 (94%)	109 (91%)	11 (9%)	0	100	100
4	H	114/121 (94%)	103 (90%)	11 (10%)	0	100	100
4	X	112/121 (93%)	102 (91%)	10 (9%)	0	100	100
5	L	103/107 (96%)	88 (85%)	15 (15%)	0	100	100
5	Y	105/107 (98%)	93 (89%)	10 (10%)	2 (2%)	8	35
All	All	2206/2266 (97%)	2026 (92%)	178 (8%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Y	82	ASP
5	Y	106	ILE

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	618/626 (99%)	598 (97%)	20 (3%)	39	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	618/626 (99%)	596 (96%)	22 (4%)	35	63
2	C	90/90 (100%)	83 (92%)	7 (8%)	12	38
2	E	90/90 (100%)	83 (92%)	7 (8%)	12	38
3	D	107/108 (99%)	103 (96%)	4 (4%)	34	62
3	F	107/108 (99%)	103 (96%)	4 (4%)	34	62
4	H	101/102 (99%)	96 (95%)	5 (5%)	24	55
4	X	99/102 (97%)	95 (96%)	4 (4%)	31	61
5	L	91/93 (98%)	87 (96%)	4 (4%)	28	59
5	Y	93/93 (100%)	89 (96%)	4 (4%)	29	59
All	All	2014/2038 (99%)	1933 (96%)	81 (4%)	31	61

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	303	PHE
1	B	536	ASP
4	H	65	LYS
1	B	323	ASN
1	B	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	291	ASN
1	B	413	ASN
1	B	684	HIS
1	B	230	ASN
1	B	678	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

40 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	$\# Z > 2$
6	NAG	B	711	-	15,15,15	0.23	0	21,21,21	0.68	0
6	NAG	B	702	-	15,15,15	0.73	1 (6%)	21,21,21	0.39	0
6	NAG	B	705	-	15,15,15	0.57	0	21,21,21	0.92	1 (4%)
6	NAG	A	807	-	15,15,15	0.90	1 (6%)	21,21,21	0.71	0
6	NAG	A	808	-	15,15,15	0.84	1 (6%)	21,21,21	0.89	2 (9%)
7	BMA	A	816	-	12,12,12	1.21	0	17,17,17	0.72	0
6	NAG	A	817	-	15,15,15	0.54	0	21,21,21	0.66	0
8	MAN	B	701	-	12,12,12	1.11	0	17,17,17	1.17	1 (5%)
6	NAG	B	709	-	15,15,15	1.00	1 (6%)	21,21,21	0.97	1 (4%)
6	NAG	A	812	-	15,15,15	0.93	1 (6%)	21,21,21	1.16	2 (9%)
6	NAG	B	715	-	15,15,15	0.47	0	21,21,21	0.85	1 (4%)
6	NAG	A	813	-	15,15,15	0.88	1 (6%)	21,21,21	0.56	0
6	NAG	A	803	-	15,15,15	0.41	0	21,21,21	0.52	0
6	NAG	B	710	-	15,15,15	0.29	0	21,21,21	0.34	0
6	NAG	A	815	-	15,15,15	0.47	0	21,21,21	0.74	0
6	NAG	A	818	-	15,15,15	0.70	1 (6%)	21,21,21	1.11	2 (9%)
6	NAG	B	713	-	15,15,15	1.12	2 (13%)	21,21,21	1.22	2 (9%)
6	NAG	A	811	-	15,15,15	0.38	0	21,21,21	0.88	1 (4%)
6	NAG	A	805	-	15,15,15	0.28	0	21,21,21	0.40	0
7	BMA	B	717	-	12,12,12	1.14	2 (16%)	17,17,17	0.78	0
6	NAG	B	712	-	15,15,15	0.48	0	21,21,21	1.19	3 (14%)
6	NAG	A	809	-	15,15,15	0.25	0	21,21,21	0.37	0
6	NAG	B	716	-	15,15,15	0.50	0	21,21,21	0.85	0
6	NAG	A	814	-	15,15,15	0.39	0	21,21,21	0.84	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	804	-	15,15,15	0.58	0	21,21,21	0.93	1 (4%)
6	NAG	B	718	-	15,15,15	0.52	0	21,21,21	0.58	0
6	NAG	B	719	-	15,15,15	0.70	1 (6%)	21,21,21	1.12	3 (14%)
6	NAG	B	704	-	15,15,15	0.37	0	21,21,21	0.53	0
6	NAG	B	714	-	15,15,15	0.70	1 (6%)	21,21,21	0.70	0
6	NAG	A	801	-	15,15,15	0.78	1 (6%)	21,21,21	0.36	0
6	NAG	B	706	-	15,15,15	0.43	0	21,21,21	0.47	0
7	BMA	A	819	-	12,12,12	1.18	1 (8%)	17,17,17	0.70	0
6	NAG	A	810	-	15,15,15	0.51	0	21,21,21	0.45	0
6	NAG	B	708	-	15,15,15	0.73	1 (6%)	21,21,21	0.58	0
6	NAG	B	703	-	15,15,15	0.53	0	21,21,21	0.65	0
6	NAG	A	806	-	15,15,15	1.43	2 (13%)	21,21,21	1.31	3 (14%)
6	NAG	B	707	-	15,15,15	1.24	2 (13%)	21,21,21	1.18	2 (9%)
7	BMA	B	720	-	12,12,12	0.96	0	17,17,17	0.77	0
6	NAG	A	802	-	15,15,15	0.31	0	21,21,21	0.61	0
8	MAN	A	820	-	12,12,12	1.12	1 (8%)	17,17,17	1.17	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
6	NAG	B	711	-	-	1/6/26/26	0/1/1/1
6	NAG	B	702	-	-	1/6/26/26	0/1/1/1
6	NAG	B	705	-	-	2/6/26/26	0/1/1/1
6	NAG	A	807	-	-	1/6/26/26	0/1/1/1
6	NAG	A	808	-	-	4/6/26/26	0/1/1/1
7	BMA	A	816	-	-	2/2/22/22	0/1/1/1
6	NAG	A	817	-	-	1/6/26/26	0/1/1/1
8	MAN	B	701	-	-	2/2/22/22	0/1/1/1
6	NAG	B	709	-	-	4/6/26/26	0/1/1/1
6	NAG	A	812	-	-	4/6/26/26	0/1/1/1
6	NAG	B	715	-	-	0/6/26/26	0/1/1/1
6	NAG	A	813	-	-	2/6/26/26	0/1/1/1
6	NAG	A	803	-	-	2/6/26/26	0/1/1/1
6	NAG	B	710	-	-	2/6/26/26	0/1/1/1
6	NAG	A	815	-	-	2/6/26/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	818	-	-	4/6/26/26	0/1/1/1
6	NAG	B	713	-	-	4/6/26/26	0/1/1/1
6	NAG	A	811	-	-	3/6/26/26	0/1/1/1
6	NAG	A	805	-	-	2/6/26/26	0/1/1/1
7	BMA	B	717	-	-	2/2/22/22	0/1/1/1
6	NAG	B	712	-	-	3/6/26/26	0/1/1/1
6	NAG	A	809	-	-	2/6/26/26	0/1/1/1
6	NAG	B	716	-	-	2/6/26/26	0/1/1/1
6	NAG	A	814	-	-	0/6/26/26	0/1/1/1
6	NAG	A	804	-	-	2/6/26/26	0/1/1/1
6	NAG	B	718	-	-	2/6/26/26	0/1/1/1
6	NAG	B	719	-	-	4/6/26/26	0/1/1/1
6	NAG	B	704	-	-	3/6/26/26	0/1/1/1
6	NAG	B	714	-	-	2/6/26/26	0/1/1/1
6	NAG	A	801	-	-	1/6/26/26	0/1/1/1
6	NAG	B	706	-	-	2/6/26/26	0/1/1/1
7	BMA	A	819	-	-	1/2/22/22	0/1/1/1
6	NAG	A	810	-	-	1/6/26/26	0/1/1/1
6	NAG	B	708	-	-	1/6/26/26	0/1/1/1
6	NAG	B	703	-	-	2/6/26/26	0/1/1/1
6	NAG	A	806	-	-	3/6/26/26	0/1/1/1
6	NAG	B	707	-	-	2/6/26/26	0/1/1/1
7	BMA	B	720	-	-	1/2/22/22	0/1/1/1
6	NAG	A	802	-	-	4/6/26/26	0/1/1/1
8	MAN	A	820	-	-	2/2/22/22	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	806	NAG	C1-C2	4.69	1.58	1.52
6	B	707	NAG	C1-C2	3.86	1.57	1.52
6	B	709	NAG	C1-C2	3.44	1.57	1.52
6	B	713	NAG	C1-C2	3.29	1.56	1.52
6	A	807	NAG	C1-C2	3.07	1.56	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	713	NAG	C1-C2-N2	4.32	115.73	110.73
6	B	712	NAG	C1-C2-N2	3.78	115.11	110.73
6	B	707	NAG	C4-C3-C2	3.41	115.33	110.34
6	A	806	NAG	C4-C3-C2	3.24	115.09	110.34
6	A	814	NAG	O1-C1-O5	-3.03	101.29	110.38

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	811	NAG	C1-C2-N2-C7
6	B	712	NAG	C1-C2-N2-C7
6	A	806	NAG	C1-C2-N2-C7
6	B	707	NAG	C1-C2-N2-C7
6	A	818	NAG	C4-C5-C6-O6

There are no ring outliers.

28 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	711	NAG	1	0
6	A	807	NAG	3	0
6	A	808	NAG	2	0
7	A	816	BMA	1	0
6	A	817	NAG	1	0
6	A	812	NAG	3	0
6	B	715	NAG	2	0
6	A	803	NAG	1	0
6	B	710	NAG	1	0
6	A	815	NAG	2	0
6	A	818	NAG	2	0
6	B	713	NAG	2	0
6	A	811	NAG	2	0
7	B	717	BMA	1	0
6	B	712	NAG	1	0
6	A	809	NAG	1	0
6	B	716	NAG	3	0
6	A	814	NAG	2	0
6	B	719	NAG	1	0
6	B	704	NAG	1	0
6	B	714	NAG	1	0
7	A	819	BMA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	810	NAG	1	0
6	B	708	NAG	1	0
6	B	703	NAG	1	0
6	A	806	NAG	1	0
7	B	720	BMA	1	0
6	A	802	NAG	2	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	663/671 (98%)	-0.20	4 (0%) 89 90	58, 85, 118, 174	0
1	B	663/671 (98%)	-0.17	5 (0%) 86 86	53, 88, 119, 184	0
2	C	107/107 (100%)	-0.27	0 100 100	61, 83, 109, 136	0
2	E	107/107 (100%)	-0.14	0 100 100	70, 88, 113, 145	0
3	D	122/127 (96%)	-0.09	0 100 100	58, 90, 124, 145	0
3	F	122/127 (96%)	-0.06	2 (1%) 72 69	81, 116, 135, 157	0
4	H	116/121 (95%)	0.98	20 (17%) 1 1	106, 152, 186, 196	0
4	X	114/121 (94%)	0.42	4 (3%) 44 42	90, 141, 186, 204	0
5	L	105/107 (98%)	1.72	34 (32%) 0 0	96, 176, 209, 243	0
5	Y	107/107 (100%)	-0.15	1 (0%) 84 84	65, 109, 136, 157	0
All	All	2226/2266 (98%)	0.01	70 (3%) 49 48	53, 94, 168, 243	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	10	SER	13.4
5	L	48	ILE	5.8
5	L	46	LEU	5.2
5	L	11	LEU	5.2
5	L	9	SER	5.1

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 monosaccharides 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. 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(Å ²)	Q<0.9
6	NAG	B	705	15/15	0.34	0.60	180,202,208,209	0
6	NAG	A	813	15/15	0.45	0.41	161,184,192,194	0
6	NAG	A	804	15/15	0.52	0.64	178,194,206,206	0
8	MAN	B	701	12/12	0.54	0.54	192,213,216,217	0
6	NAG	B	706	15/15	0.64	0.51	150,171,187,187	0
8	MAN	A	820	12/12	0.66	0.50	194,200,204,204	0
7	BMA	A	816	12/12	0.67	0.37	165,176,181,184	0
6	NAG	B	719	15/15	0.68	0.46	151,158,173,176	0
6	NAG	B	707	15/15	0.71	0.28	109,133,145,156	0
6	NAG	A	808	15/15	0.72	0.40	135,159,166,174	0
6	NAG	B	712	15/15	0.73	0.29	152,173,179,179	0
7	BMA	B	717	12/12	0.75	0.40	174,186,193,193	0
6	NAG	B	708	15/15	0.75	0.20	116,145,157,162	0
6	NAG	A	805	15/15	0.76	0.55	140,164,172,174	0
6	NAG	B	714	15/15	0.76	0.34	133,159,168,176	0
7	BMA	B	720	12/12	0.77	0.40	157,176,180,180	0
6	NAG	B	710	15/15	0.78	0.19	93,126,154,156	0
7	BMA	A	819	12/12	0.78	0.54	169,179,186,188	0
6	NAG	A	812	15/15	0.78	0.28	117,140,153,154	0
6	NAG	A	811	15/15	0.79	0.23	148,169,183,183	0
6	NAG	A	807	15/15	0.80	0.16	111,128,145,145	0
6	NAG	A	818	15/15	0.80	0.28	143,158,163,165	0
6	NAG	A	803	15/15	0.81	0.21	104,135,142,142	0
6	NAG	A	806	15/15	0.82	0.29	106,129,147,147	0
6	NAG	B	704	15/15	0.83	0.34	129,144,159,162	0
6	NAG	A	802	15/15	0.83	0.21	97,118,126,129	0
6	NAG	B	703	15/15	0.83	0.23	117,133,145,147	0
6	NAG	A	815	15/15	0.84	0.27	117,131,140,143	0
6	NAG	A	809	15/15	0.85	0.17	96,124,135,138	0
6	NAG	B	709	15/15	0.86	0.18	140,160,166,167	0
6	NAG	B	702	15/15	0.86	0.20	104,136,158,159	0
6	NAG	A	801	15/15	0.87	0.14	104,132,144,145	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	B	711	15/15	0.87	0.20	97,107,148,154	0
6	NAG	B	716	15/15	0.88	0.25	110,121,139,154	0
6	NAG	A	810	15/15	0.91	0.16	94,109,143,145	0
6	NAG	A	814	15/15	0.92	0.15	49,66,82,82	0
6	NAG	B	713	15/15	0.92	0.12	91,108,123,131	0
6	NAG	B	718	15/15	0.93	0.24	90,96,99,100	0
6	NAG	A	817	15/15	0.94	0.11	80,92,102,104	0
6	NAG	B	715	15/15	0.96	0.20	58,64,84,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.