



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:15 PM GMT

PDB ID : 3I27
Title : Structure of bovine torovirus Hemagglutinin-Esterasein complex with receptor
Authors : Zeng, Q.H.; Huizinga, E.G.
Deposited on : 2009-06-29
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

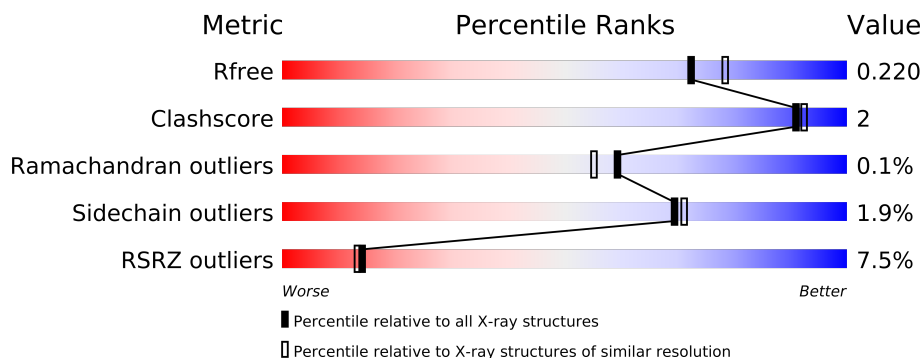
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	384	
1	B	384	
1	C	384	
1	D	384	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	5156	-	X
3	NAG	A	5157	-	X
3	NAG	B	5154	-	X
3	NAG	D	5157	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12866 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2862	1821	455	559	27			
1	B	364	Total	C	N	O	S	0	0	0
			2855	1819	454	555	27			
1	C	358	Total	C	N	O	S	0	0	0
			2813	1795	447	544	27			
1	D	369	Total	C	N	O	S	0	0	0
			2889	1837	460	565	27			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
A	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
A	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
A	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
A	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
A	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
B	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
B	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
B	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
B	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
B	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
B	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
C	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
C	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
C	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
C	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
C	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
C	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
D	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
D	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
D	395	LEU	-	EXPRESSION TAG	UNP P0C0V9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
D	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
D	398	ARG	-	EXPRESSION TAG	UNP P0C0V9

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		
2	C	3	Total	C	N	O	0	0
			39	22	2	15		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
A	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
A	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
A	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
A	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
A	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
B	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
B	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
B	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
B	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
B	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
B	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
C	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
C	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
C	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
C	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
C	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
C	398	ARG	-	EXPRESSION TAG	UNP P0C0V9

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

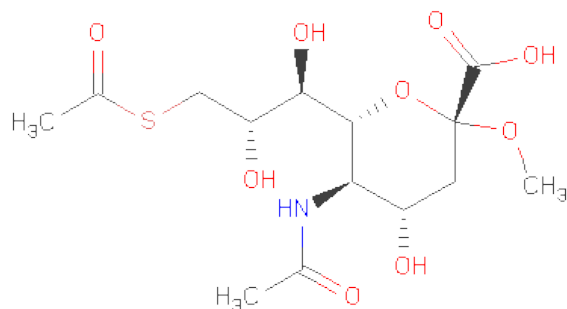
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
A	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
A	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
A	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
A	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
A	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
A	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
A	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
A	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
A	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
A	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
A	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
B	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
B	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
B	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
B	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
B	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
B	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
D	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
D	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
D	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
D	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
D	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
D	398	ARG	-	EXPRESSION TAG	UNP P0C0V9
D	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
D	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
D	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
D	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
D	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
D	398	ARG	-	EXPRESSION TAG	UNP P0C0V9

- Molecule 5 is SUGAR (METHYL 9-S-ACETYL-5-(ACETYLAMINO)-3,5-DIDEOXY-9-THIO-D-GLYCERO-ALPHA-D-GALACTO-NON-2-ULOPYRANOSIDONICACID) (three-letter code: SID) (formula: C₁₄H₂₃NO₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			25	14	1	9	1		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	7	Total	C	N	O	0	0
			83	46	2	35		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	393	ASP	-	EXPRESSION TAG	UNP P0C0V9
D	394	PRO	-	EXPRESSION TAG	UNP P0C0V9
D	395	LEU	-	EXPRESSION TAG	UNP P0C0V9
D	396	VAL	-	EXPRESSION TAG	UNP P0C0V9
D	397	PRO	-	EXPRESSION TAG	UNP P0C0V9
D	398	ARG	-	EXPRESSION TAG	UNP P0C0V9

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	347	Total	O	0	0
			347	347		
7	B	338	Total	O	0	0
			338	338		

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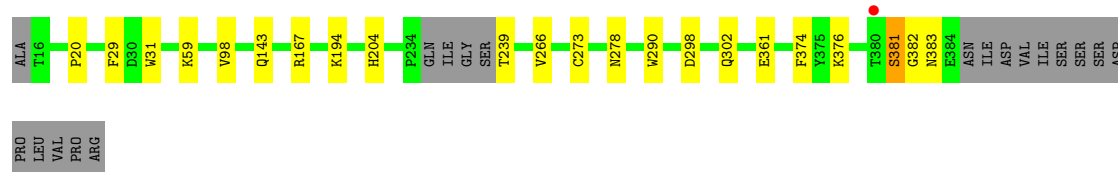
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	65	Total 65	O 65	0	0
7	D	262	Total 262	O 262	0	0

3 Residue-property plots

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.

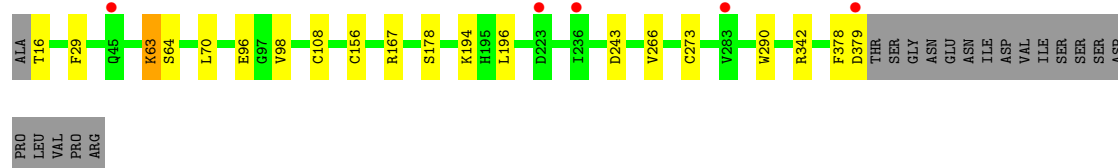
- Molecule 1: Hemagglutinin-esterase

Chain A: 



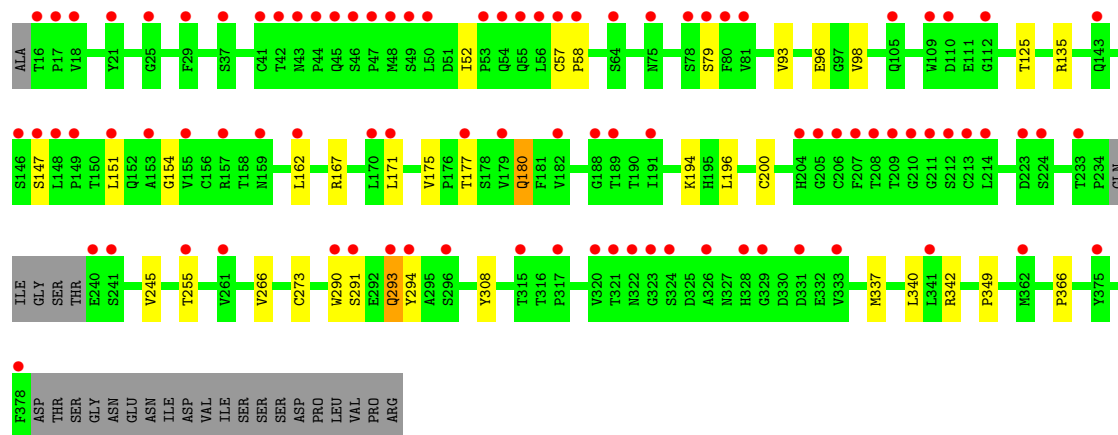
- Molecule 1: Hemagglutinin-esterase

Chain B: 



- Molecule 1: Hemagglutinin-esterase

Chain C: 



- Molecule 1: Hemagglutinin-esterase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.63Å 112.89Å 273.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.00 48.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.92-2.00) 99.4 (48.92-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.179 , 0.210 0.190 , 0.220	Depositor DCC
R_{free} test set	7106 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 141522 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12866	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SID, 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	0.68	0/2949	0.70	0/4021
1	B	0.68	0/2943	0.69	1/4014 (0.0%)
1	C	0.48	0/2900	0.57	0/3954
1	D	0.63	0/2977	0.69	0/4060
All	All	0.62	0/11769	0.66	1/16049 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ASP	CB-CG-OD1	5.15	122.93	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2862	0	2669	11	0
1	B	2855	0	2672	9	0
1	C	2813	0	2635	14	0
1	D	2889	0	2697	11	0
2	A	39	0	34	0	0
2	B	39	0	34	0	0
2	C	39	0	34	0	0
3	A	28	0	26	0	0
3	B	14	0	13	1	0
3	D	28	0	26	0	0
4	A	56	0	50	0	0
4	B	28	0	25	0	0
4	D	56	0	50	0	0
5	D	25	0	22	2	0
6	D	83	0	70	0	0
7	A	347	0	0	3	0
7	B	338	0	0	0	0
7	C	65	0	0	0	0
7	D	262	0	0	0	0
All	All	12866	0	11057	45	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:211:GLY:HA3	1:D:212:SER:CB	2.15	0.76
1:D:211:GLY:HA3	1:D:212:SER:HB2	1.78	0.64
1:C:98:VAL:HG22	1:C:290:TRP:CE2	2.33	0.64
1:A:381:SER:HB2	1:A:383:ASN:H	1.64	0.62
1:B:63:LYS:HD3	1:B:64:SER:N	2.20	0.56
1:D:211:GLY:HA3	1:D:212:SER:HB3	1.86	0.55
1:D:167:ARG:O	1:D:266:VAL:HA	2.07	0.55
1:B:29:PHE:HB3	3:B:5154:NAG:H5	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:HIS:ND1	7:A:671:HOH:O	2.32	0.54
1:D:78:SER:O	1:D:79:SER:CB	2.56	0.53
1:B:378:PHE:O	1:B:379:ASP:HB2	2.10	0.52
1:D:207:PHE:CE2	5:D:1001:SID:HM9B	2.48	0.48
1:D:207:PHE:CZ	5:D:1001:SID:HM9B	2.49	0.48
1:C:154:GLY:O	1:C:162:LEU:HD22	2.13	0.48
1:D:78:SER:O	1:D:79:SER:HB3	2.14	0.48
1:A:98:VAL:HG22	1:A:290:TRP:CE2	2.48	0.47
1:D:98:VAL:HG22	1:D:290:TRP:CE2	2.49	0.47
1:C:93:VAL:HG21	1:C:340:LEU:HD21	1.95	0.47
1:C:349:PRO:HD3	1:C:366:PRO:O	2.16	0.46
1:B:63:LYS:HD3	1:B:63:LYS:C	2.36	0.46
1:B:70:LEU:HD23	1:B:70:LEU:C	2.37	0.45
1:B:108:CYS:O	1:B:156:CYS:HB3	2.17	0.45
1:A:381:SER:CB	1:A:383:ASN:H	2.29	0.45
1:C:167:ARG:O	1:C:266:VAL:HA	2.16	0.45
1:A:167:ARG:O	1:A:266:VAL:HA	2.18	0.44
1:D:211:GLY:CA	1:D:212:SER:CB	2.93	0.44
1:B:167:ARG:O	1:B:266:VAL:HA	2.19	0.43
1:C:180:GLN:HG2	1:C:255:THR:CG2	2.48	0.43
1:A:278:ASN:ND2	7:A:1019:HOH:O	2.52	0.43
1:A:382:GLY:HA2	7:A:959:HOH:O	2.18	0.43
1:C:196:LEU:C	1:C:196:LEU:HD23	2.38	0.43
1:B:98:VAL:HG22	1:B:290:TRP:CE2	2.54	0.42
1:C:52:ILE:HG22	1:C:337:MET:HG3	2.01	0.42
1:C:291:SER:OG	1:C:293:GLN:NE2	2.47	0.42
1:C:125:THR:HG23	1:C:308:TYR:OH	2.19	0.42
1:D:169:ALA:C	1:D:170:LEU:HD12	2.41	0.41
1:C:293:GLN:HG2	1:C:294:TYR:CD1	2.55	0.41
1:A:298:ASP:O	1:A:302:GLN:HG2	2.19	0.41
1:A:374:PHE:CZ	1:A:376:LYS:HD2	2.54	0.41
1:B:196:LEU:C	1:B:196:LEU:HD23	2.40	0.41
1:C:57:CYS:N	1:C:58:PRO:CD	2.84	0.41
1:A:20:PRO:HD2	1:A:361:GLU:HG2	2.04	0.40
1:C:151:LEU:HD23	1:C:171:LEU:HD23	2.02	0.40
1:C:200:CYS:HA	1:C:245:VAL:O	2.22	0.40
1:A:31:TRP:CZ2	1:A:59:LYS:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	361/384 (94%)	345 (96%)	16 (4%)	0	100	100
1	B	362/384 (94%)	347 (96%)	15 (4%)	0	100	100
1	C	354/384 (92%)	341 (96%)	13 (4%)	0	100	100
1	D	367/384 (96%)	349 (95%)	17 (5%)	1 (0%)	50	44
All	All	1444/1536 (94%)	1382 (96%)	61 (4%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	212	SER

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	327/344 (95%)	322 (98%)	5 (2%)	76	79
1	B	326/344 (95%)	319 (98%)	7 (2%)	66	67
1	C	321/344 (93%)	310 (97%)	11 (3%)	49	45
1	D	330/344 (96%)	328 (99%)	2 (1%)	92	94
All	All	1304/1376 (95%)	1279 (98%)	25 (2%)	69	71

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	143	GLN

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Mol	Chain	Res	Type
1	A	194	LYS
1	A	239	THR
1	A	273	CYS
1	B	16	THR
1	B	63	LYS
1	B	96	GLU
1	B	178	SER
1	B	194	LYS
1	B	273	CYS
1	B	342	ARG
1	C	79	SER
1	C	96	GLU
1	C	135	ARG
1	C	147	SER
1	C	175	VAL
1	C	177	THR
1	C	180	GLN
1	C	194	LYS
1	C	273	CYS
1	C	293	GLN
1	C	342	ARG
1	D	236	ILE
1	D	238	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	278	ASN
1	C	180	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

26 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$
2	NAG	A	5151	1,2	12,14,15	0.73	1 (8%)	15,19,21	0.86	0
2	NAG	A	5152	2	12,14,15	0.65	0	15,19,21	1.65	2 (13%)
2	BMA	A	5153	2	10,11,12	0.57	0	11,15,17	1.60	3 (27%)
4	NAG	A	5154	1,4	12,14,15	0.69	0	15,19,21	1.22	1 (6%)
4	NAG	A	5155	4	12,14,15	0.61	0	15,19,21	1.47	3 (20%)
4	NAG	A	5158	1,4	12,14,15	0.73	0	15,19,21	0.99	1 (6%)
4	NAG	A	5159	4	12,14,15	0.58	0	15,19,21	1.44	1 (6%)
2	NAG	B	5151	1,2	12,14,15	0.83	0	15,19,21	1.18	3 (20%)
2	NAG	B	5152	2	12,14,15	0.60	0	15,19,21	1.00	0
2	BMA	B	5153	2	10,11,12	0.49	0	11,15,17	2.04	3 (27%)
4	NAG	B	5158	1,4	12,14,15	0.71	0	15,19,21	1.36	2 (13%)
4	NAG	B	5159	4	12,14,15	0.79	1 (8%)	15,19,21	0.94	1 (6%)
2	NAG	C	5158	1,2	12,14,15	0.69	1 (8%)	15,19,21	0.77	0
2	NAG	C	5159	2	12,14,15	0.64	0	15,19,21	1.61	2 (13%)
2	BMA	C	5160	2	10,11,12	0.46	0	11,15,17	0.92	1 (9%)
4	NAG	D	5151	1,4	12,14,15	1.34	2 (16%)	15,19,21	0.91	1 (6%)
4	NAG	D	5152	4	12,14,15	0.62	0	15,19,21	0.93	0
4	NAG	D	5154	1,4	12,14,15	1.06	1 (8%)	15,19,21	1.29	3 (20%)
4	NAG	D	5155	4	12,14,15	0.53	0	15,19,21	0.92	0
6	NAG	D	5158	1,6	12,14,15	1.03	1 (8%)	15,19,21	1.23	1 (6%)
6	NAG	D	5159	6	12,14,15	0.85	0	15,19,21	1.15	1 (6%)
6	BMA	D	5160	6	10,11,12	0.45	0	11,15,17	1.10	0
6	MAN	D	5161	6	10,11,12	0.76	0	11,15,17	1.39	0
6	MAN	D	5162	6	10,11,12	0.70	0	11,15,17	0.95	0
6	MAN	D	5163	6	10,11,12	0.72	0	11,15,17	1.25	1 (9%)
6	MAN	D	5164	6	10,11,12	0.63	0	11,15,17	0.96	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
2	NAG	A	5151	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	5152	2	-	0/6/23/26	0/1/1/1
2	BMA	A	5153	2	-	0/2/19/22	0/1/1/1
4	NAG	A	5154	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	5155	4	-	0/6/23/26	0/1/1/1
4	NAG	A	5158	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	5159	4	-	0/6/23/26	0/1/1/1
2	NAG	B	5151	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	5152	2	-	0/6/23/26	0/1/1/1
2	BMA	B	5153	2	-	0/2/19/22	0/1/1/1
4	NAG	B	5158	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	5159	4	-	0/6/23/26	0/1/1/1
2	NAG	C	5158	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	5159	2	-	0/6/23/26	0/1/1/1
2	BMA	C	5160	2	-	0/2/19/22	0/1/1/1
4	NAG	D	5151	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	5152	4	-	0/6/23/26	0/1/1/1
4	NAG	D	5154	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	5155	4	-	0/6/23/26	0/1/1/1
6	NAG	D	5158	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	5159	6	-	0/6/23/26	0/1/1/1
6	BMA	D	5160	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5161	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5162	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5163	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5164	6	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5151	NAG	O5-C5	-3.10	1.39	1.45
4	D	5154	NAG	O5-C5	-3.10	1.39	1.45
6	D	5158	NAG	O5-C5	-2.95	1.39	1.45
4	D	5151	NAG	C2-N2	-2.84	1.43	1.46
4	B	5159	NAG	O5-C5	-2.37	1.41	1.45
2	C	5158	NAG	O5-C5	-2.07	1.41	1.45
2	A	5151	NAG	O5-C5	-2.03	1.41	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5152	NAG	O5-C5-C6	5.09	112.32	106.98
2	B	5153	BMA	O5-C5-C6	4.83	112.05	106.98
2	C	5159	NAG	O5-C5-C6	4.41	111.61	106.98
4	A	5154	NAG	C3-C2-N2	-3.75	106.06	111.76
4	A	5155	NAG	C3-C2-N2	-3.31	106.73	111.76
4	A	5159	NAG	C3-C2-N2	-3.26	106.79	111.76
2	B	5153	BMA	O5-C5-C4	-3.16	106.64	110.65
2	C	5159	NAG	O5-C5-C4	-3.10	106.72	110.65
2	A	5152	NAG	C3-C2-N2	-2.83	107.45	111.76
4	A	5158	NAG	O5-C5-C6	2.76	109.88	106.98
4	B	5158	NAG	C3-C2-N2	-2.67	107.69	111.76
4	D	5154	NAG	O5-C5-C6	-2.65	104.20	106.98
2	C	5160	BMA	O5-C5-C6	2.54	109.64	106.98
4	B	5159	NAG	O5-C5-C4	-2.54	107.44	110.65
2	A	5153	BMA	C4-C3-C2	-2.52	107.12	110.50
6	D	5163	MAN	O5-C5-C6	2.52	109.62	106.98
4	A	5155	NAG	O6-C6-C5	-2.44	102.95	111.36
4	B	5158	NAG	O5-C5-C6	2.44	109.54	106.98
6	D	5159	NAG	O5-C5-C6	2.39	109.49	106.98
2	A	5153	BMA	O5-C5-C6	2.38	109.48	106.98
6	D	5158	NAG	C3-C4-C5	-2.35	106.00	110.20
2	A	5153	BMA	O3-C3-C2	2.25	114.04	109.94
2	B	5151	NAG	C3-C2-N2	-2.21	108.39	111.76
2	B	5151	NAG	O3-C3-C4	2.11	115.09	110.35
4	D	5154	NAG	C3-C2-N2	-2.10	108.56	111.76
4	D	5151	NAG	O4-C4-C5	-2.10	103.75	109.28
2	B	5151	NAG	O5-C5-C4	2.09	113.30	110.65
4	D	5154	NAG	O3-C3-C2	-2.08	104.72	109.09
4	A	5155	NAG	C3-C4-C5	-2.05	106.55	110.20
2	B	5153	BMA	C3-C4-C5	-2.03	106.58	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

6 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	5156	1	12,14,15	0.65	0	15,19,21	1.66	4 (26%)
3	NAG	A	5157	1	12,14,15	0.49	0	15,19,21	1.44	1 (6%)
3	NAG	B	5154	1	12,14,15	0.83	1 (8%)	15,19,21	1.44	2 (13%)
5	SID	D	1001	-	25,25,25	1.14	2 (8%)	36,36,36	1.25	4 (11%)
3	NAG	D	5156	1	12,14,15	0.59	0	15,19,21	1.22	1 (6%)
3	NAG	D	5157	1	12,14,15	0.56	0	15,19,21	0.95	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
3	NAG	A	5156	1	-	0/6/23/26	0/1/1/1
3	NAG	A	5157	1	-	0/6/23/26	0/1/1/1
3	NAG	B	5154	1	-	0/6/23/26	0/1/1/1
5	SID	D	1001	-	-	1/26/44/44	0/1/1/1
3	NAG	D	5156	1	-	0/6/23/26	0/1/1/1
3	NAG	D	5157	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1001	SID	O6-C2	2.74	1.46	1.42
5	D	1001	SID	C3-C2	2.57	1.56	1.52
3	B	5154	NAG	O5-C5	-2.37	1.41	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5157	NAG	O5-C5-C6	4.95	112.17	106.98
3	B	5154	NAG	O5-C5-C6	4.13	111.31	106.98
3	A	5156	NAG	O5-C5-C6	3.66	110.82	106.98
5	D	1001	SID	C8-C7-C6	-3.18	106.83	112.99
3	B	5154	NAG	O5-C5-C4	-2.86	107.02	110.65
3	D	5157	NAG	O5-C5-C6	2.63	109.74	106.98
3	A	5156	NAG	C3-C4-C5	-2.62	105.52	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1001	SID	C9-C8-C7	-2.33	107.74	113.07
5	D	1001	SID	C7-C6-C5	-2.28	110.88	114.24
3	A	5156	NAG	C3-C2-N2	-2.27	108.31	111.76
3	A	5156	NAG	O7-C7-C8	-2.20	117.75	122.04
3	D	5156	NAG	C3-C4-C5	2.19	114.12	110.20
5	D	1001	SID	O6-C6-C5	2.09	111.52	109.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1001	SID	CM9-CA9-S9-C9

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	365/384 (95%)	0.02	1 (0%) 91 93	9, 13, 21, 35	0
1	B	364/384 (94%)	0.04	5 (1%) 72 72	8, 13, 21, 30	0
1	C	358/384 (93%)	1.19	91 (25%) 1 1	15, 25, 32, 37	0
1	D	369/384 (96%)	0.26	13 (3%) 42 41	10, 17, 28, 45	0
All	All	1456/1536 (94%)	0.37	110 (7%) 14 13	8, 17, 29, 45	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	GLY	9.0
1	D	236	ILE	8.4
1	D	239	THR	8.2
1	D	238	SER	7.4
1	C	47	PRO	6.9
1	C	146	SER	6.1
1	C	78	SER	6.1
1	C	320	VAL	5.9
1	C	48	MET	4.9
1	C	147	SER	4.5
1	C	41	CYS	4.1
1	D	235	GLN	4.0
1	C	188	GLY	3.9
1	C	378	PHE	3.9
1	C	42	THR	3.9
1	C	204	HIS	3.8
1	C	211	GLY	3.7
1	C	148	LEU	3.6
1	C	179	VAL	3.6
1	D	210	GLY	3.6
1	C	223	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	57	CYS	3.6
1	C	189	THR	3.6
1	C	209	THR	3.6
1	C	208	THR	3.5
1	C	17	PRO	3.4
1	C	54	GLN	3.4
1	C	214	LEU	3.4
1	C	333	VAL	3.4
1	C	159	ASN	3.4
1	C	210	GLY	3.2
1	C	241	SER	3.2
1	C	109	TRP	3.2
1	C	44	PRO	3.2
1	C	323	GLY	3.1
1	C	157	ARG	3.0
1	C	56	LEU	3.0
1	C	155	VAL	3.0
1	C	321	THR	3.0
1	C	81	VAL	3.0
1	C	162	LEU	3.0
1	C	105	GLN	3.0
1	C	170	LEU	3.0
1	C	46	SER	2.9
1	C	143	GLN	2.9
1	C	224	SER	2.9
1	C	53	PRO	2.9
1	B	223	ASP	2.9
1	C	45	GLN	2.9
1	C	79	SER	2.9
1	C	50	LEU	2.8
1	C	341	LEU	2.8
1	B	379	ASP	2.8
1	C	149	PRO	2.8
1	D	211	GLY	2.8
1	C	205	GLY	2.8
1	C	191	ILE	2.7
1	C	58	PRO	2.7
1	C	296	SER	2.7
1	C	182	VAL	2.7
1	C	293	GLN	2.7
1	C	29	PHE	2.6
1	C	80	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	123	PHE	2.6
1	C	16	THR	2.6
1	C	207	PHE	2.6
1	C	326	ALA	2.6
1	C	240	GLU	2.6
1	B	236	ILE	2.5
1	C	37	SER	2.5
1	C	110	ASP	2.5
1	C	375	TYR	2.4
1	C	328	HIS	2.4
1	C	18	VAL	2.4
1	C	291	SER	2.3
1	C	322	ASN	2.3
1	C	49	SER	2.3
1	C	75	ASN	2.3
1	C	25	GLY	2.3
1	C	206	CYS	2.3
1	C	64	SER	2.3
1	A	380	THR	2.3
1	C	177	THR	2.3
1	C	362	MET	2.3
1	D	249	LEU	2.3
1	C	255	THR	2.2
1	C	153	ALA	2.2
1	C	261	VAL	2.2
1	C	329	GLY	2.2
1	C	294	TYR	2.2
1	C	212	SER	2.2
1	C	171	LEU	2.2
1	D	248	TYR	2.2
1	C	331	ASP	2.1
1	C	233	THR	2.1
1	C	324	SER	2.1
1	C	151	LEU	2.1
1	C	43	ASN	2.1
1	C	55	GLN	2.1
1	C	21	TYR	2.1
1	D	124	TYR	2.1
1	C	213	CYS	2.1
1	D	127	LEU	2.1
1	C	315	THR	2.1
1	B	45	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	112	GLY	2.1
1	C	317	PRO	2.1
1	B	283	VAL	2.0
1	D	240	GLU	2.0
1	C	290	TRP	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MAN	D	5162	11/12	0.29	13.45	36,43,45,48	0
2	NAG	B	5152	14/15	0.16	1.90	31,34,41,42	0
2	BMA	B	5153	11/12	0.17	1.84	44,48,49,52	0
2	NAG	C	5158	14/15	0.17	0.81	38,42,46,50	0
2	NAG	B	5151	14/15	0.13	0.70	22,24,26,29	0
4	NAG	A	5155	14/15	0.14	0.69	30,35,39,41	0
4	NAG	A	5154	14/15	0.13	-0.01	19,22,25,27	0
4	NAG	A	5158	14/15	0.11	-0.16	20,24,27,31	0
4	NAG	D	5154	14/15	0.17	-0.23	33,36,37,37	0
2	NAG	A	5151	14/15	0.11	-0.24	17,20,26,28	0
4	NAG	D	5151	14/15	0.14	-0.56	15,18,25,27	0
4	NAG	D	5155	14/15	0.15	-0.59	40,42,47,49	0
6	NAG	D	5158	14/15	0.11	-0.70	22,25,29,32	0
4	NAG	D	5152	14/15	0.12	-0.73	29,31,34,35	0
4	NAG	B	5158	14/15	0.11	-1.69	19,22,27,30	0
2	NAG	A	5152	14/15	0.11	-2.02	27,32,35,40	0
2	BMA	A	5153	11/12	0.21	-	41,47,50,50	0
6	MAN	D	5161	11/12	0.22	-	46,47,51,53	0
6	MAN	D	5164	11/12	0.56	-	63,66,66,67	0
4	NAG	B	5159	14/15	0.13	-	34,36,42,42	0
4	NAG	A	5159	14/15	0.24	-	38,45,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BMA	D	5160	11/12	0.27	-	49,51,54,59	0
2	BMA	C	5160	11/12	0.31	-	64,66,67,67	0
6	MAN	D	5163	11/12	0.27	-	53,55,56,57	0
2	NAG	C	5159	14/15	0.23	-	55,57,60,63	0
6	NAG	D	5159	14/15	0.17	-	31,36,40,46	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	D	5157	14/15	0.21	86.00	41,47,50,52	0
3	NAG	B	5154	14/15	0.38	6.89	50,55,57,57	0
3	NAG	A	5157	14/15	0.29	3.35	47,54,56,57	0
3	NAG	A	5156	14/15	0.23	2.41	32,36,40,40	0
3	NAG	D	5156	14/15	0.24	1.99	36,42,45,46	0
5	SID	D	1001	25/25	0.24	1.05	49,55,62,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.