



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:46 PM GMT

PDB ID : 4C7L
Title : Crystal structure of Mouse Hepatitis virus strain S Hemagglutinin- esterase
Authors : Zeng, Q.H.; Huizinga, E.G.
Deposited on : 2013-09-23
Resolution : 2.10 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>

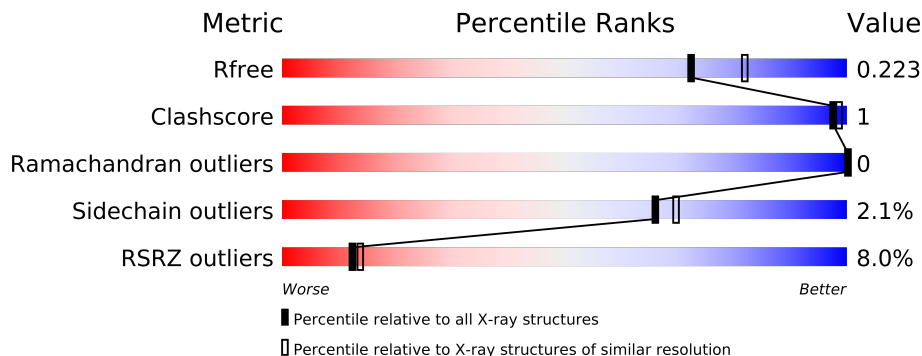
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	386	
1	B	386	

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	1403	-	X
3	NAG	A	1404	-	X
3	NAG	A	1405	-	X
3	NAG	B	1418	-	X
3	NAG	B	1422	-	X
7	GOL	B	1412	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6388 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	338	Total	C	N	O	S	0	4	0
			2714	1736	446	513	19			
1	B	368	Total	C	N	O	S	0	5	0
			2962	1885	488	569	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
A	404	SER	-	EXPRESSION TAG	UNP O55252
A	405	ASP	-	EXPRESSION TAG	UNP O55252
A	406	PRO	-	EXPRESSION TAG	UNP O55252
A	407	LEU	-	EXPRESSION TAG	UNP O55252
A	408	VAL	-	EXPRESSION TAG	UNP O55252
A	409	PRO	-	EXPRESSION TAG	UNP O55252
A	410	ARG	-	EXPRESSION TAG	UNP O55252
B	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
B	404	SER	-	EXPRESSION TAG	UNP O55252
B	405	ASP	-	EXPRESSION TAG	UNP O55252
B	406	PRO	-	EXPRESSION TAG	UNP O55252
B	407	LEU	-	EXPRESSION TAG	UNP O55252
B	408	VAL	-	EXPRESSION TAG	UNP O55252
B	409	PRO	-	EXPRESSION TAG	UNP O55252
B	410	ARG	-	EXPRESSION TAG	UNP O55252

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is SUGAR (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	B	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	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	SER	ENGINEERED MUTATION	UNP P28845

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Chain	Residue	Modelled	Actual	Comment	Reference
A	404	SER	-	EXPRESSION TAG	UNP O55252
A	405	ASP	-	EXPRESSION TAG	UNP O55252
A	406	PRO	-	EXPRESSION TAG	UNP O55252
A	407	LEU	-	EXPRESSION TAG	UNP O55252
A	408	VAL	-	EXPRESSION TAG	UNP O55252
A	409	PRO	-	EXPRESSION TAG	UNP O55252
A	410	ARG	-	EXPRESSION TAG	UNP O55252
B	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
B	404	SER	-	EXPRESSION TAG	UNP O55252
B	405	ASP	-	EXPRESSION TAG	UNP O55252
B	406	PRO	-	EXPRESSION TAG	UNP O55252
B	407	LEU	-	EXPRESSION TAG	UNP O55252
B	408	VAL	-	EXPRESSION TAG	UNP O55252
B	409	PRO	-	EXPRESSION TAG	UNP O55252
B	410	ARG	-	EXPRESSION TAG	UNP O55252

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

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

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
A	404	SER	-	EXPRESSION TAG	UNP O55252
A	405	ASP	-	EXPRESSION TAG	UNP O55252
A	406	PRO	-	EXPRESSION TAG	UNP O55252
A	407	LEU	-	EXPRESSION TAG	UNP O55252
A	408	VAL	-	EXPRESSION TAG	UNP O55252
A	409	PRO	-	EXPRESSION TAG	UNP O55252
A	410	ARG	-	EXPRESSION TAG	UNP O55252
B	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
B	404	SER	-	EXPRESSION TAG	UNP O55252
B	405	ASP	-	EXPRESSION TAG	UNP O55252

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Chain	Residue	Modelled	Actual	Comment	Reference
B	406	PRO	-	EXPRESSION TAG	UNP O55252
B	407	LEU	-	EXPRESSION TAG	UNP O55252
B	408	VAL	-	EXPRESSION TAG	UNP O55252
B	409	PRO	-	EXPRESSION TAG	UNP O55252
B	410	ARG	-	EXPRESSION TAG	UNP O55252
B	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
B	404	SER	-	EXPRESSION TAG	UNP O55252
B	405	ASP	-	EXPRESSION TAG	UNP O55252
B	406	PRO	-	EXPRESSION TAG	UNP O55252
B	407	LEU	-	EXPRESSION TAG	UNP O55252
B	408	VAL	-	EXPRESSION TAG	UNP O55252
B	409	PRO	-	EXPRESSION TAG	UNP O55252
B	410	ARG	-	EXPRESSION TAG	UNP O55252
B	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
B	404	SER	-	EXPRESSION TAG	UNP O55252
B	405	ASP	-	EXPRESSION TAG	UNP O55252
B	406	PRO	-	EXPRESSION TAG	UNP O55252
B	407	LEU	-	EXPRESSION TAG	UNP O55252
B	408	VAL	-	EXPRESSION TAG	UNP O55252
B	409	PRO	-	EXPRESSION TAG	UNP O55252
B	410	ARG	-	EXPRESSION TAG	UNP O55252

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			50	28	2	20		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
A	404	SER	-	EXPRESSION TAG	UNP O55252
A	405	ASP	-	EXPRESSION TAG	UNP O55252
A	406	PRO	-	EXPRESSION TAG	UNP O55252
A	407	LEU	-	EXPRESSION TAG	UNP O55252
A	408	VAL	-	EXPRESSION TAG	UNP O55252
A	409	PRO	-	EXPRESSION TAG	UNP O55252
A	410	ARG	-	EXPRESSION TAG	UNP O55252

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is a polymer of unknown type called SUGAR (7-MER).

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	ALA	SER	ENGINEERED MUTATION	UNP P28845
B	404	SER	-	EXPRESSION TAG	UNP O55252
B	405	ASP	-	EXPRESSION TAG	UNP O55252
B	406	PRO	-	EXPRESSION TAG	UNP O55252
B	407	LEU	-	EXPRESSION TAG	UNP O55252
B	408	VAL	-	EXPRESSION TAG	UNP O55252
B	409	PRO	-	EXPRESSION TAG	UNP O55252
B	410	ARG	-	EXPRESSION TAG	UNP O55252

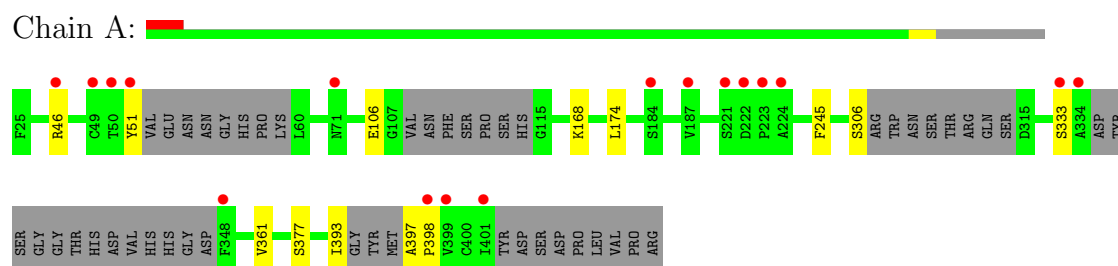
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	169	Total 169	O 169	0	0
9	B	122	Total 122	O 122	0	0

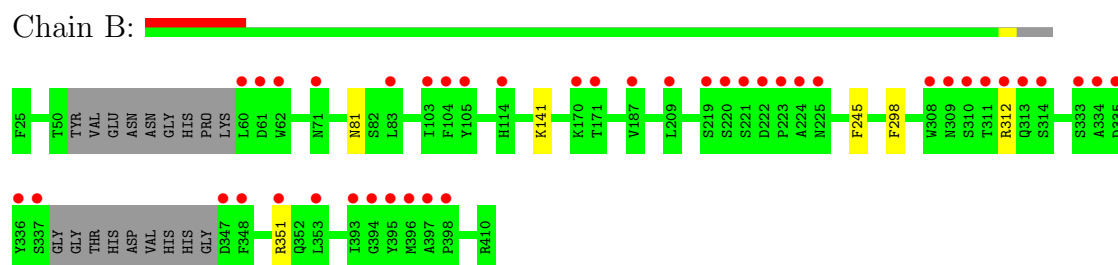
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



• Molecule 1: HEMAGGLUTININ-ESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.83Å 108.76Å 125.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.76 – 2.10 29.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.76-2.10) 99.7 (29.76-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.186 , 0.219 0.194 , 0.223	Depositor DCC
R_{free} test set	3707 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 73783 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: GOL, K, 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	0.53	0/2785	0.62	0/3773
1	B	0.49	0/3045	0.58	0/4134
All	All	0.51	0/5830	0.60	0/7907

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2714	0	0	2	0
1	B	2962	0	0	2	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	42	0	39	0	0
3	B	42	0	39	0	0
4	A	39	0	34	0	0
4	B	39	0	34	0	0
5	A	28	0	25	0	0
5	B	84	0	75	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	50	0	43	0	0
7	B	12	0	16	1	0
8	B	83	0	70	0	0
9	A	169	0	0	0	0
9	B	122	0	0	1	0
All	All	6388	0	375	5	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 1.

All (5) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:397:ALA:N	1:A:398:PRO:CD	2.57	0.66
1:B:298:PHE:N	7:B:1412:GOL:HO1	2.00	0.59
1:A:106:GLU:O	1:A:306:SER:N	2.50	0.45
1:B:141:LYS:NZ	9:B:2047:HOH:O	2.51	0.42
5:B:1424:NAG:HO3	5:B:1425:NAG:C1	2.34	0.41

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	330/386 (86%)	319 (97%)	11 (3%)	0	100	100
1	B	367/386 (95%)	355 (97%)	12 (3%)	0	100	100
All	All	697/772 (90%)	674 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	297/336 (88%)	288 (97%)	9 (3%)	53	55
1	B	327/336 (97%)	323 (99%)	4 (1%)	82	87
All	All	624/672 (93%)	611 (98%)	13 (2%)	66	70

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	51	TYR
1	A	168	LYS
1	A	174	LEU
1	A	245	PHE
1	A	333	SER
1	A	361	VAL
1	A	377	SER
1	A	393	ILE
1	B	81	ASN
1	B	245	PHE
1	B	312	ARG
1	B	351	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

25 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	$\# Z > 2$
4	NAG	A	1406	1,4	12,14,15	0.76	1 (8%)	15,19,21	1.15	1 (6%)
4	NAG	A	1407	4	12,14,15	0.73	1 (8%)	15,19,21	1.20	1 (6%)
4	BMA	A	1408	4	10,11,12	0.54	0	11,15,17	1.29	3 (27%)
5	NAG	A	1409	1,5	12,14,15	0.66	0	15,19,21	1.16	1 (6%)
5	NAG	A	1410	5	12,14,15	0.66	0	15,19,21	0.97	1 (6%)
6	NAG	A	1411	1,6	12,14,15	0.65	0	15,19,21	1.45	2 (13%)
6	NAG	A	1412	6	12,14,15	0.61	0	15,19,21	0.96	1 (6%)
6	BMA	A	1413	6	10,11,12	0.55	0	11,15,17	2.23	2 (18%)
6	MAN	A	1414	6	10,11,12	0.73	0	11,15,17	0.70	0
5	NAG	B	1414	1,5	12,14,15	0.61	0	15,19,21	0.84	0
5	NAG	B	1415	5	12,14,15	0.54	0	15,19,21	0.79	0
5	NAG	B	1416	1,5	12,14,15	0.57	0	15,19,21	0.96	1 (6%)
5	NAG	B	1417	5	12,14,15	0.58	0	15,19,21	1.17	1 (6%)
4	NAG	B	1419	1,4	12,14,15	0.67	0	15,19,21	1.49	1 (6%)
4	NAG	B	1420	4	12,14,15	0.64	0	15,19,21	1.21	1 (6%)
4	BMA	B	1421	4	10,11,12	0.53	0	11,15,17	0.95	1 (9%)
5	NAG	B	1424	1,5	12,14,15	0.96	1 (8%)	15,19,21	0.92	1 (6%)
5	NAG	B	1425	5	12,14,15	0.65	0	15,19,21	1.18	2 (13%)
8	NAG	B	1426	1,8	12,14,15	0.81	0	15,19,21	0.94	0
8	NAG	B	1427	8	12,14,15	0.64	0	15,19,21	1.01	2 (13%)
8	BMA	B	1428	8	10,11,12	0.63	0	11,15,17	0.85	0
8	MAN	B	1429	8	10,11,12	0.86	0	11,15,17	1.04	1 (9%)
8	MAN	B	1430	8	10,11,12	0.69	0	11,15,17	0.79	0
8	MAN	B	1431	8	10,11,12	0.74	0	11,15,17	1.35	1 (9%)
8	MAN	B	1432	8	10,11,12	0.81	0	11,15,17	1.64	1 (9%)

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
4	NAG	A	1406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1408	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1409	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1410	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1411	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1412	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1413	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1414	6	-	0/2/19/22	0/1/1/1
5	NAG	B	1414	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1415	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1416	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1417	5	-	0/6/23/26	0/1/1/1
4	NAG	B	1419	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1420	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1421	4	-	0/2/19/22	0/1/1/1
5	NAG	B	1424	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1425	5	-	0/6/23/26	0/1/1/1
8	NAG	B	1426	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1427	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1428	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1429	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1430	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1431	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1432	8	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1424	NAG	O5-C5	-3.05	1.39	1.45
4	A	1406	NAG	O5-C5	-2.21	1.41	1.45
4	A	1407	NAG	O5-C5	-2.05	1.41	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1413	BMA	O5-C5-C6	5.87	113.14	106.98
4	B	1419	NAG	C3-C2-N2	-5.31	103.68	111.76
6	A	1413	BMA	O5-C5-C4	-4.19	105.34	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1411	NAG	O5-C5-C6	4.16	111.35	106.98
8	B	1432	MAN	O5-C5-C6	3.87	111.04	106.98
4	A	1406	NAG	C3-C2-N2	-3.82	105.94	111.76
4	B	1420	NAG	C3-C2-N2	-3.79	106.00	111.76
4	A	1407	NAG	C3-C2-N2	-3.71	106.11	111.76
8	B	1431	MAN	O5-C5-C6	3.64	110.80	106.98
5	A	1409	NAG	C3-C2-N2	-3.48	106.45	111.76
8	B	1429	MAN	O5-C5-C6	2.89	110.01	106.98
5	B	1425	NAG	O5-C5-C4	-2.79	107.11	110.65
5	B	1417	NAG	C3-C2-N2	-2.75	107.57	111.76
8	B	1427	NAG	O5-C5-C6	2.55	109.66	106.98
5	B	1425	NAG	O5-C5-C6	2.53	109.63	106.98
4	B	1421	BMA	O5-C5-C6	2.50	109.60	106.98
6	A	1411	NAG	C3-C2-N2	-2.49	107.97	111.76
5	A	1410	NAG	C3-C2-N2	-2.40	108.11	111.76
5	B	1424	NAG	O5-C5-C4	-2.35	107.67	110.65
4	A	1408	BMA	C3-C4-C5	2.34	114.38	110.20
4	A	1408	BMA	C4-C3-C2	2.27	113.56	110.50
5	B	1416	NAG	O5-C5-C6	2.15	109.24	106.98
8	B	1427	NAG	O5-C5-C4	-2.12	107.96	110.65
4	A	1408	BMA	O5-C5-C6	2.11	109.19	106.98
6	A	1412	NAG	O5-C5-C6	2.07	109.16	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	1403	1	12,14,15	0.64	0	15,19,21	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1404	1	12,14,15	0.55	0	15,19,21	0.84	0
3	NAG	A	1405	1	12,14,15	0.66	0	15,19,21	1.20	2 (13%)
7	GOL	B	1412	-	5,5,5	0.30	0	5,5,5	0.59	0
7	GOL	B	1413	-	5,5,5	0.36	0	5,5,5	0.21	0
3	NAG	B	1418	1	12,14,15	0.58	0	15,19,21	1.26	1 (6%)
3	NAG	B	1422	1	12,14,15	0.48	0	15,19,21	0.78	0
3	NAG	B	1423	1	12,14,15	0.47	0	15,19,21	1.00	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	1403	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
7	GOL	B	1412	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1413	-	-	0/4/4/4	0/0/0/0
3	NAG	B	1418	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1422	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1423	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1418	NAG	C3-C2-N2	-3.59	106.30	111.76
3	A	1405	NAG	O5-C5-C4	-2.69	107.23	110.65
3	A	1403	NAG	O5-C5-C6	2.31	109.41	106.98
3	A	1403	NAG	O5-C5-C4	-2.30	107.74	110.65
3	A	1405	NAG	O5-C5-C6	2.17	109.26	106.98

There are no chirality outliers.

There are no torsion outliers.

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	338/386 (87%)	0.12	17 (5%)	28 30	28, 43, 93, 158	6 (1%)
1	B	368/386 (95%)	0.43	42 (11%)	6 6	34, 52, 104, 169	0
All	All	706/772 (91%)	0.28	59 (8%)	12 12	28, 48, 100, 169	6 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	8.2
1	B	62	TRP	8.1
1	B	336	TYR	8.0
1	B	60	LEU	7.8
1	B	337	SER	7.3
1	B	395	TYR	6.5
1	B	220	SER	6.1
1	B	61	ASP	6.1
1	B	310	SER	6.0
1	B	311	THR	5.6
1	B	334	ALA	5.5
1	B	335	ASP	5.4
1	B	348	PHE	5.2
1	A	51	TYR	4.9
1	A	221	SER	4.7
1	A	401	ILE	4.5
1	A	187	VAL	4.4
1	B	219	SER	4.4
1	B	313	GLN	4.4
1	B	314	SER	4.3
1	B	221	SER	4.3
1	B	312	ARG	4.1
1	B	397	ALA	3.9
1	B	170	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	393	ILE	3.9
1	A	71	ASN	3.9
1	A	50	THR	3.9
1	A	49	CYS	3.8
1	B	333	SER	3.8
1	A	333	SER	3.7
1	B	71	ASN	3.7
1	B	396	MET	3.6
1	B	225	ASN	3.5
1	A	348	PHE	3.4
1	B	114	HIS	3.4
1	B	398	PRO	3.3
1	B	224	ALA	3.3
1	B	171	THR	3.2
1	B	187	VAL	2.7
1	B	394	GLY	2.7
1	B	222	ASP	2.7
1	B	347	ASP	2.6
1	B	105	TYR	2.5
1	A	223	PRO	2.4
1	B	309	ASN	2.3
1	B	351	ARG	2.3
1	B	353	LEU	2.3
1	B	223	PRO	2.3
1	A	184	SER	2.2
1	A	222	ASP	2.2
1	A	46	ARG	2.2
1	B	103	ILE	2.2
1	B	104	PHE	2.1
1	B	83	LEU	2.1
1	A	399	VAL	2.1
1	B	308	TRP	2.1
1	B	209	LEU	2.0
1	A	224	ALA	2.0
1	A	398	PRO	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
5	NAG	B	1417	14/15	0.38	54.51	83,84,85,86	0
5	NAG	B	1415	14/15	0.45	44.60	84,88,89,90	0
5	NAG	B	1416	14/15	0.32	32.14	63,72,74,79	0
5	NAG	B	1414	14/15	0.29	23.69	62,70,73,79	0
8	MAN	B	1432	11/12	0.15	10.54	56,60,63,66	0
6	MAN	A	1414	11/12	0.27	5.44	83,84,85,85	0
4	NAG	A	1407	14/15	0.21	3.15	60,66,72,77	0
8	MAN	B	1429	11/12	0.15	2.73	47,50,52,54	0
4	NAG	B	1420	14/15	0.21	2.72	62,66,72,77	0
6	NAG	A	1412	14/15	0.18	1.99	68,70,74,77	0
8	MAN	B	1431	11/12	0.11	1.57	46,51,53,55	0
5	NAG	B	1424	14/15	0.14	1.03	56,65,69,76	0
8	MAN	B	1430	11/12	0.08	0.15	39,43,47,53	0
6	NAG	A	1411	14/15	0.11	-0.49	47,53,58,63	0
4	NAG	A	1406	14/15	0.10	-0.58	45,51,54,60	0
8	NAG	B	1427	14/15	0.08	-0.75	46,47,48,48	0
8	NAG	B	1426	14/15	0.09	-0.81	41,46,49,50	0
8	BMA	B	1428	11/12	0.05	-0.97	40,41,44,45	0
4	NAG	B	1419	14/15	0.06	-1.38	44,51,53,59	0
5	NAG	A	1409	14/15	0.08	-1.74	44,50,59,66	0
5	NAG	B	1425	14/15	0.46	-	82,87,88,89	0
4	BMA	A	1408	11/12	0.33	-	82,84,86,87	0
6	BMA	A	1413	11/12	0.18	-	79,81,81,82	0
5	NAG	A	1410	14/15	0.36	-	73,77,80,83	0
4	BMA	B	1421	11/12	0.38	-	81,84,84,85	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	A	1404	14/15	0.31	18.46	60,68,70,73	0
3	NAG	A	1403	14/15	0.29	12.67	57,64,65,65	0
7	GOL	B	1412	6/6	0.32	12.37	60,61,64,65	0
3	NAG	B	1422	14/15	0.37	10.44	61,69,72,73	0
3	NAG	B	1418	14/15	0.26	3.68	58,64,69,69	0
3	NAG	A	1405	14/15	0.22	2.51	56,63,67,69	0
3	NAG	B	1423	14/15	0.30	0.50	60,69,71,72	0
2	K	A	1402	1/1	0.14	0.35	49,49,49,49	0
7	GOL	B	1413	6/6	0.16	-0.14	81,82,82,82	0
2	K	B	1411	1/1	0.13	-0.14	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.