



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:39 AM GMT

PDB ID : 4L6T
Title : GM1 bound form of the ECX AB5 holotoxin
Authors : Littler, D.R.; Ng, N.M.; Rossjohn, J.; Beddoe, T.
Deposited on : 2013-06-12
Resolution : 1.86 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>

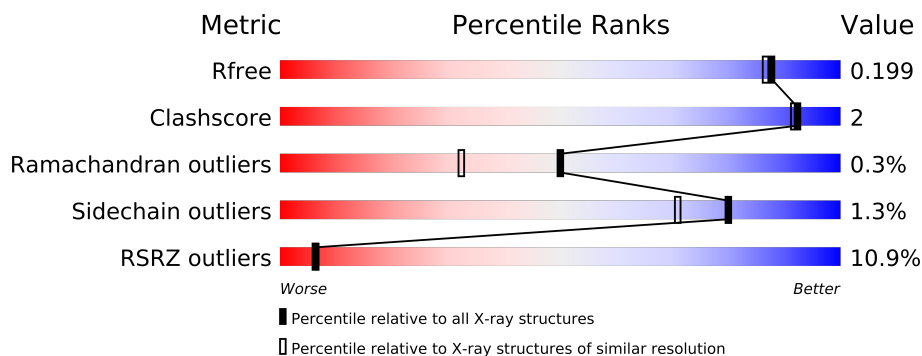
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.86 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	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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	266	
2	B	112	
2	C	112	
2	D	112	
2	E	112	
2	F	112	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7017 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 ECXA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1938	1212	347	373	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	INITIATING METHIONINE	UNP Q8GAV4

- Molecule 2 is a protein called ECXB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	105	Total	C	N	O	S	0	0	0
			825	518	140	161	6			
2	C	105	Total	C	N	O	S	0	4	0
			847	531	142	168	6			
2	D	105	Total	C	N	O	S	0	2	0
			838	525	142	165	6			
2	E	105	Total	C	N	O	S	0	1	0
			829	520	141	163	5			
2	F	105	Total	C	N	O	S	0	2	0
			836	523	143	165	5			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
B	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
B	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
B	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
C	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
C	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
C	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
D	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
D	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
D	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
E	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
E	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
E	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
F	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
F	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
F	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total C N O 68 37 2 29	0	0
4	C	5	Total C N O 68 37 2 29	0	0
4	D	5	Total C N O 68 37 2 29	0	0
4	E	5	Total C N O 68 37 2 29	0	0
4	F	5	Total C N O 68 37 2 29	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
B	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
B	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
B	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
B	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
C	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
C	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
C	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
C	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
D	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
D	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
D	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
D	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
E	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
E	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
E	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
E	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	22	MET	-	INITIATING METHIONINE	UNP Q8GAV3
F	126	LEU	-	EXPRESSION TAG	UNP Q8GAV3
F	127	GLU	-	EXPRESSION TAG	UNP Q8GAV3
F	128	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	129	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	130	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	131	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	132	HIS	-	EXPRESSION TAG	UNP Q8GAV3
F	133	HIS	-	EXPRESSION TAG	UNP Q8GAV3

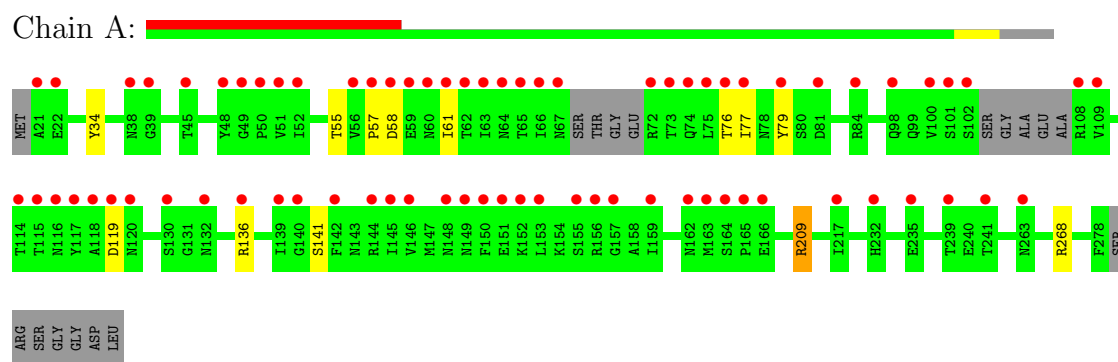
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	93	Total O 94 94	0	1
5	C	115	Total O 115 115	0	0
5	D	119	Total O 119 119	0	0
5	E	101	Total O 102 102	0	1
5	F	85	Total O 85 85	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: ECXA



• Molecule 2: ECXB



• Molecule 2: ECXB



• Molecule 2: ECXB



• Molecule 2: ECXB



- Molecule 2: ECXB

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.44Å 120.44Å 273.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.82 – 1.86 29.82 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.82-1.86) 99.3 (29.82-1.86)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.178 , 0.198 0.178 , 0.199	Depositor DCC
R_{free} test set	4899 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 98568 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: GAL, ZN, BGC, NGA, SIA

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	0.27	0/1975	0.45	0/2675
2	B	0.46	0/838	0.56	0/1132
2	C	0.42	0/866	0.58	0/1170
2	D	0.43	0/851	0.57	0/1150
2	E	0.39	0/842	0.53	0/1139
2	F	0.38	0/849	0.51	0/1148
All	All	0.38	0/6221	0.52	0/8414

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	1938	0	0	5	0
2	B	825	0	0	2	0
2	C	847	0	0	1	0
2	D	838	0	0	2	0
2	E	829	0	0	2	0
2	F	836	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	B	68	0	58	0	0
4	C	68	0	58	0	0
4	D	68	0	58	0	0
4	E	68	0	58	0	0
4	F	68	0	58	0	0
5	A	48	0	0	1	0
5	B	94	0	0	1	0
5	C	115	0	0	0	0
5	D	119	0	0	1	0
5	E	102	0	0	0	0
5	F	85	0	0	0	0
All	All	7017	0	290	12	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 (12) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:48[B]:THR:OG1	2:C:63:SER:OG	2.27	0.53
2:B:40:TYR:OH	2:B:116:ASN:OD1	2.33	0.47
2:E:48[B]:THR:OG1	2:E:63:SER:OG	2.34	0.46
1:A:268:ARG:NH2	5:A:439:HOH:O	2.47	0.46
1:A:61:ILE:N	1:A:77:ILE:O	2.49	0.46
1:A:119:ASP:OD2	1:A:141:SER:OG	2.36	0.43
2:B:43:ASN:ND2	5:B:371:HOH:O	2.50	0.43
1:A:119:ASP:N	1:A:119:ASP:OD2	2.50	0.43
2:D:43:ASN:ND2	5:D:309:HOH:O	2.53	0.42
2:D:45:GLU:OE1	2:D:45:GLU:N	2.54	0.40
1:A:209:ARG:NH2	2:E:99:PHE:O	2.54	0.40
2:F:48:THR:OG1	2:F:63[B]:SER:OG	2.39	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	243/266 (91%)	232 (96%)	9 (4%)	2 (1%)	27	10
2	B	103/112 (92%)	102 (99%)	1 (1%)	0	100	100
2	C	107/112 (96%)	107 (100%)	0	0	100	100
2	D	105/112 (94%)	105 (100%)	0	0	100	100
2	E	104/112 (93%)	104 (100%)	0	0	100	100
2	F	105/112 (94%)	105 (100%)	0	0	100	100
All	All	767/826 (93%)	755 (98%)	10 (1%)	2 (0%)	50	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	57	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/228 (92%)	205 (97%)	6 (3%)	56	37
2	B	93/100 (93%)	93 (100%)	0	100	100
2	C	97/100 (97%)	97 (100%)	0	100	100
2	D	95/100 (95%)	94 (99%)	1 (1%)	84	77
2	E	93/100 (93%)	91 (98%)	2 (2%)	64	48
2	F	94/100 (94%)	94 (100%)	0	100	100
All	All	683/728 (94%)	674 (99%)	9 (1%)	80	71

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

Mol	Chain	Res	Type
1	A	34	TYR
1	A	55	THR

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Mol	Chain	Res	Type
1	A	76	THR
1	A	79	TYR
1	A	136	ARG
1	A	209	ARG
2	D	31	CYS
2	E	31	CYS
2	E	102	ILE

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	GAL	B	201	4	10,11,12	0.64	0	11,15,17	0.85	1 (9%)
4	NGA	B	202	4	12,14,15	0.36	0	15,19,21	0.90	1 (6%)
4	GAL	B	203	4	10,11,12	0.44	0	11,15,17	1.63	2 (18%)
4	SIA	B	204	4	20,20,21	3.79	4 (20%)	23,28,31	2.71	2 (8%)
4	BGC	B	205	4	12,12,12	0.41	0	17,17,17	0.82	0
4	GAL	C	201	4	10,11,12	0.54	0	11,15,17	0.71	0
4	NGA	C	202	4	12,14,15	0.49	0	15,19,21	1.32	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GAL	C	203	4	10,11,12	0.43	0	11,15,17	1.58	1 (9%)
4	SIA	C	204	4	20,20,21	3.60	4 (20%)	23,28,31	2.75	2 (8%)
4	BGC	C	205	4	12,12,12	0.38	0	17,17,17	0.87	1 (5%)
4	GAL	D	201	4	10,11,12	0.53	0	11,15,17	0.77	0
4	NGA	D	202	4	12,14,15	0.41	0	15,19,21	1.22	2 (13%)
4	GAL	D	203	4	10,11,12	0.48	0	11,15,17	1.30	1 (9%)
4	SIA	D	204	4	20,20,21	3.69	4 (20%)	23,28,31	2.66	2 (8%)
4	BGC	D	205	4	12,12,12	0.40	0	17,17,17	0.94	1 (5%)
4	GAL	E	201	4	10,11,12	0.55	0	11,15,17	0.95	0
4	NGA	E	202	4	12,14,15	0.42	0	15,19,21	1.13	1 (6%)
4	GAL	E	203	4	10,11,12	0.50	0	11,15,17	1.44	2 (18%)
4	SIA	E	204	4	20,20,21	4.05	3 (15%)	23,28,31	2.55	1 (4%)
4	BGC	E	205	4	12,12,12	0.45	0	17,17,17	1.01	0
4	GAL	F	201	4	10,11,12	0.49	0	11,15,17	0.57	0
4	NGA	F	202	4	12,14,15	0.43	0	15,19,21	1.49	2 (13%)
4	GAL	F	203	4	10,11,12	0.43	0	11,15,17	1.26	2 (18%)
4	SIA	F	204	4	20,20,21	3.91	3 (15%)	23,28,31	2.80	2 (8%)
4	BGC	F	205	4	12,12,12	0.43	0	17,17,17	1.16	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
4	GAL	B	201	4	-	0/2/19/22	0/1/1/1
4	NGA	B	202	4	-	0/6/23/26	0/1/1/1
4	GAL	B	203	4	-	0/2/19/22	0/1/1/1
4	SIA	B	204	4	-	0/15/34/38	0/1/1/1
4	BGC	B	205	4	-	0/2/22/22	0/1/1/1
4	GAL	C	201	4	-	0/2/19/22	0/1/1/1
4	NGA	C	202	4	-	0/6/23/26	0/1/1/1
4	GAL	C	203	4	-	0/2/19/22	0/1/1/1
4	SIA	C	204	4	-	0/15/34/38	0/1/1/1
4	BGC	C	205	4	-	0/2/22/22	0/1/1/1
4	GAL	D	201	4	-	0/2/19/22	0/1/1/1
4	NGA	D	202	4	-	0/6/23/26	0/1/1/1
4	GAL	D	203	4	-	0/2/19/22	0/1/1/1
4	SIA	D	204	4	-	0/15/34/38	0/1/1/1
4	BGC	D	205	4	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	E	201	4	-	0/2/19/22	0/1/1/1
4	NGA	E	202	4	-	0/6/23/26	0/1/1/1
4	GAL	E	203	4	-	0/2/19/22	0/1/1/1
4	SIA	E	204	4	-	0/15/34/38	0/1/1/1
4	BGC	E	205	4	-	0/2/22/22	0/1/1/1
4	GAL	F	201	4	-	0/2/19/22	0/1/1/1
4	NGA	F	202	4	-	0/6/23/26	0/1/1/1
4	GAL	F	203	4	-	0/2/19/22	0/1/1/1
4	SIA	F	204	4	-	0/15/34/38	0/1/1/1
4	BGC	F	205	4	-	0/2/22/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	204	SIA	O6-C2	17.36	1.44	1.28
4	F	204	SIA	O6-C2	16.73	1.43	1.28
4	B	204	SIA	O6-C2	16.11	1.43	1.28
4	D	204	SIA	O6-C2	15.65	1.42	1.28
4	C	204	SIA	O6-C2	15.35	1.42	1.28
4	E	204	SIA	O1A-C1	3.53	1.33	1.23
4	D	204	SIA	O1A-C1	3.36	1.33	1.23
4	F	204	SIA	O1A-C1	3.32	1.33	1.23
4	B	204	SIA	O1A-C1	3.30	1.33	1.23
4	C	204	SIA	O1A-C1	3.15	1.32	1.23
4	C	204	SIA	O1B-C1	-2.44	1.22	1.30
4	F	204	SIA	O1B-C1	-2.32	1.23	1.30
4	E	204	SIA	O1B-C1	-2.29	1.23	1.30
4	B	204	SIA	C3-C2	2.27	1.54	1.46
4	D	204	SIA	C3-C2	2.27	1.54	1.46
4	D	204	SIA	O1B-C1	-2.21	1.23	1.30
4	B	204	SIA	O1B-C1	-2.10	1.23	1.30
4	C	204	SIA	C3-C2	2.02	1.53	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	204	SIA	O6-C2-C3	-12.83	108.15	124.91
4	C	204	SIA	O6-C2-C3	-12.39	108.72	124.91
4	B	204	SIA	O6-C2-C3	-12.31	108.83	124.91
4	D	204	SIA	O6-C2-C3	-12.03	109.19	124.91
4	E	204	SIA	O6-C2-C3	-11.53	109.85	124.91
4	C	203	GAL	O3-C3-C2	-4.18	102.30	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	202	NGA	O5-C5-C6	3.91	111.09	106.98
4	C	202	NGA	O5-C5-C6	3.79	110.96	106.98
4	B	203	GAL	O5-C5-C6	3.46	110.61	106.98
4	D	203	GAL	O3-C3-C2	-3.37	103.78	109.94
4	D	202	NGA	O5-C5-C6	3.17	110.31	106.98
4	B	203	GAL	O3-C3-C2	-3.16	104.16	109.94
4	E	203	GAL	O3-C3-C2	-3.05	104.36	109.94
4	E	203	GAL	O5-C5-C6	2.71	109.82	106.98
4	F	203	GAL	O3-C3-C2	-2.69	105.01	109.94
4	E	202	NGA	O5-C5-C6	2.66	109.77	106.98
4	F	203	GAL	O5-C5-C6	2.64	109.75	106.98
4	D	202	NGA	C3-C2-N2	-2.32	108.23	111.76
4	F	202	NGA	C3-C2-N2	-2.16	108.47	111.76
4	B	202	NGA	C3-C2-N2	-2.14	108.50	111.76
4	D	204	SIA	O1B-C1-O1A	-2.12	118.53	123.35
4	C	204	SIA	O1B-C1-O1A	-2.12	118.53	123.35
4	F	204	SIA	O1B-C1-O1A	-2.11	118.57	123.35
4	B	204	SIA	O1B-C1-O1A	-2.10	118.58	123.35
4	D	205	BGC	O4-C4-C3	-2.10	105.64	110.35
4	B	201	GAL	O5-C5-C6	2.09	109.18	106.98
4	C	205	BGC	O5-C1-C2	-2.05	106.69	109.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	249/266 (93%)	1.37	74 (29%) 1 1	23, 67, 112, 134	0
2	B	105/112 (93%)	-0.31	1 (0%) 79 78	16, 25, 41, 56	0
2	C	105/112 (93%)	-0.22	3 (2%) 49 45	13, 18, 34, 90	0
2	D	105/112 (93%)	-0.35	2 (1%) 64 63	12, 17, 30, 78	0
2	E	105/112 (93%)	-0.28	3 (2%) 49 45	14, 20, 36, 87	0
2	F	105/112 (93%)	-0.15	3 (2%) 49 45	16, 29, 45, 93	0
All	All	774/826 (93%)	0.26	86 (11%) 6 6	12, 28, 100, 134	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ASP	8.6
2	F	126	LEU	7.5
2	B	126	LEU	7.4
1	A	57	PRO	7.3
2	C	126	LEU	7.2
1	A	66	ILE	6.3
1	A	79	TYR	6.1
1	A	49	GLY	5.9
1	A	67	ASN	5.8
1	A	61	ILE	5.5
1	A	155	SER	5.5
1	A	77	ILE	5.3
1	A	144	ARG	5.3
1	A	65	THR	5.3
2	D	22	MET	5.2
1	A	165	PRO	5.0
1	A	109	VAL	5.0
2	D	126	LEU	4.9
1	A	72	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	126	LEU	4.7
1	A	59	GLU	4.6
1	A	150	PHE	4.5
1	A	50	PRO	4.5
1	A	152	LYS	4.4
1	A	60	ASN	4.4
1	A	148	ASN	4.4
1	A	21	ALA	4.3
1	A	100	VAL	4.3
1	A	232	HIS	4.1
1	A	119	ASP	4.1
1	A	156	ARG	4.0
1	A	162	ASN	3.9
1	A	64	ASN	3.8
1	A	73	THR	3.8
1	A	118	ALA	3.7
1	A	101	SER	3.7
1	A	117	TYR	3.7
1	A	38	ASN	3.6
1	A	163	MET	3.6
1	A	56	VAL	3.5
2	F	125	ASN	3.4
1	A	145	ILE	3.4
1	A	84	ARG	3.3
1	A	149	ASN	3.3
1	A	52	ILE	3.2
2	C	22	MET	3.1
2	E	22	MET	3.1
1	A	39	GLY	3.1
1	A	263	ASN	3.1
2	E	125	ASN	3.0
1	A	120	ASN	3.0
1	A	116	ASN	3.0
1	A	102	SER	2.8
1	A	62	THR	2.8
1	A	74	GLN	2.8
1	A	241	THR	2.8
1	A	130	SER	2.8
1	A	132	ASN	2.7
1	A	239	THR	2.7
1	A	22	GLU	2.7
1	A	63	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	22	MET	2.5
1	A	157	GLY	2.5
1	A	164	SER	2.5
1	A	75	LEU	2.5
1	A	45	THR	2.4
1	A	151	GLU	2.4
1	A	235	GLU	2.4
1	A	76	THR	2.4
1	A	81	ASP	2.3
1	A	142	PHE	2.3
2	C	23	THR	2.3
1	A	153	LEU	2.3
1	A	108	ARG	2.3
1	A	115	THR	2.3
1	A	217	ILE	2.3
1	A	114	THR	2.3
1	A	51	VAL	2.3
1	A	159	ILE	2.3
1	A	48	TYR	2.2
1	A	140	GLY	2.2
1	A	139	ILE	2.2
1	A	146	VAL	2.2
1	A	166	GLU	2.2
1	A	98	GLN	2.2
1	A	136	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NGA	C	202	14/15	0.10	1.48	15,21,29,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GAL	B	203	11/12	0.12	0.89	20,23,30,42	0
4	GAL	B	201	11/12	0.08	0.68	16,19,25,25	0
4	SIA	C	204	20/21	0.08	0.46	17,21,23,24	0
4	SIA	F	204	20/21	0.10	0.42	23,29,37,38	0
4	GAL	F	201	11/12	0.08	0.00	23,28,33,33	0
4	NGA	E	202	14/15	0.08	-0.02	18,24,30,39	0
4	GAL	E	201	11/12	0.07	-0.06	15,18,22,22	0
4	GAL	D	201	11/12	0.07	-0.15	14,15,17,17	0
4	BGC	B	205	12/12	0.12	-0.17	25,31,40,45	0
4	NGA	D	202	14/15	0.07	-0.25	17,20,27,35	0
4	NGA	F	202	14/15	0.10	-0.40	29,31,39,48	0
4	SIA	B	204	20/21	0.07	-0.46	20,25,31,31	0
4	SIA	E	204	20/21	0.07	-0.57	19,24,27,27	0
4	SIA	D	204	20/21	0.06	-0.57	17,21,24,24	0
4	NGA	B	202	14/15	0.07	-0.81	22,26,31,31	0
4	GAL	C	201	11/12	0.06	-0.89	14,16,17,18	0
4	GAL	D	203	11/12	0.10	-	18,23,29,35	0
4	BGC	C	205	12/12	0.31	-	35,48,52,61	0
4	GAL	F	203	11/12	0.13	-	30,36,43,43	0
4	BGC	F	205	12/12	0.32	-	51,62,70,75	0
4	BGC	E	205	12/12	0.21	-	40,50,53,61	0
4	GAL	C	203	11/12	0.13	-	20,23,27,34	0
4	GAL	E	203	11/12	0.10	-	20,26,30,37	0
4	BGC	D	205	12/12	0.34	-	31,44,59,62	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	ZN	A	301	1/1	0.05	-2.99	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.