



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 03:18 AM BST

PDB ID : 4UF7
Title : Ghanaian henipavirus (Gh-M74a) attachment glycoprotein in complex with human ephrinB2
Authors : Lee, B.; Pernet, O.; Ahmed, A.A.; Zeltina, A.; Beaty, S.M.; Bowden, T.A.
Deposited on : 2015-03-13
Resolution : 1.70 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

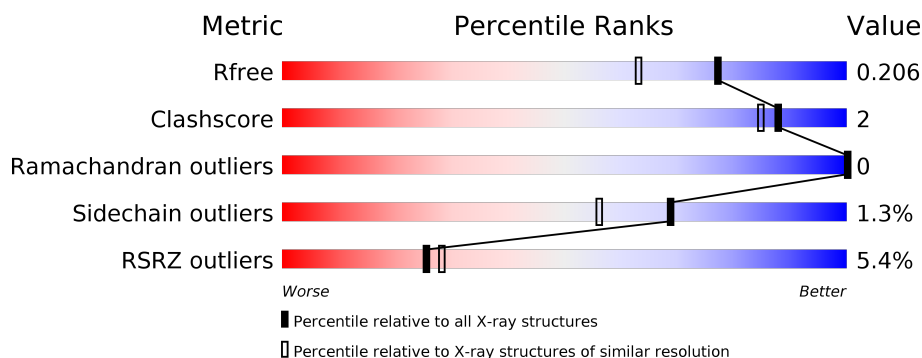
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	454	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	454	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>9%</div> </div> </div>
2	C	153	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>• •</div> <div>10%</div> </div> </div>
2	E	153	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>•</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10304 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 GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	6	0
			3409	2179	565	643	22			
1	B	412	Total	C	N	O	S	0	5	0
			3375	2158	558	637	22			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	GLU	-	expression tag	UNP I0E093
A	197	THR	-	expression tag	UNP I0E093
A	198	GLY	-	expression tag	UNP I0E093
A	633	PRO	-	expression tag	UNP I0E093
A	634	TYR	-	expression tag	UNP I0E093
A	635	ASP	-	expression tag	UNP I0E093
A	636	VAL	-	expression tag	UNP I0E093
A	637	PRO	-	expression tag	UNP I0E093
A	638	ASP	-	expression tag	UNP I0E093
A	639	TYR	-	expression tag	UNP I0E093
A	640	ALA	-	expression tag	UNP I0E093
A	641	GLY	-	expression tag	UNP I0E093
A	642	THR	-	expression tag	UNP I0E093
A	643	LYS	-	expression tag	UNP I0E093
A	644	HIS	-	expression tag	UNP I0E093
A	645	HIS	-	expression tag	UNP I0E093
A	646	HIS	-	expression tag	UNP I0E093
A	647	HIS	-	expression tag	UNP I0E093
A	648	HIS	-	expression tag	UNP I0E093
A	649	HIS	-	expression tag	UNP I0E093
B	196	GLU	-	expression tag	UNP I0E093
B	197	THR	-	expression tag	UNP I0E093
B	198	GLY	-	expression tag	UNP I0E093
B	633	PRO	-	expression tag	UNP I0E093
B	634	TYR	-	expression tag	UNP I0E093

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Chain	Residue	Modelled	Actual	Comment	Reference
B	635	ASP	-	expression tag	UNP I0E093
B	636	VAL	-	expression tag	UNP I0E093
B	637	PRO	-	expression tag	UNP I0E093
B	638	ASP	-	expression tag	UNP I0E093
B	639	TYR	-	expression tag	UNP I0E093
B	640	ALA	-	expression tag	UNP I0E093
B	641	GLY	-	expression tag	UNP I0E093
B	642	THR	-	expression tag	UNP I0E093
B	643	LYS	-	expression tag	UNP I0E093
B	644	HIS	-	expression tag	UNP I0E093
B	645	HIS	-	expression tag	UNP I0E093
B	646	HIS	-	expression tag	UNP I0E093
B	647	HIS	-	expression tag	UNP I0E093
B	648	HIS	-	expression tag	UNP I0E093
B	649	HIS	-	expression tag	UNP I0E093

- Molecule 2 is a protein called EPHRIN-B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	138	Total	C	N	O	S	0	5	0
			1131	727	180	217	7			
2	E	139	Total	C	N	O	S	0	2	0
			1120	719	179	215	7			

There are 24 discrepancies between the modelled and reference sequences:

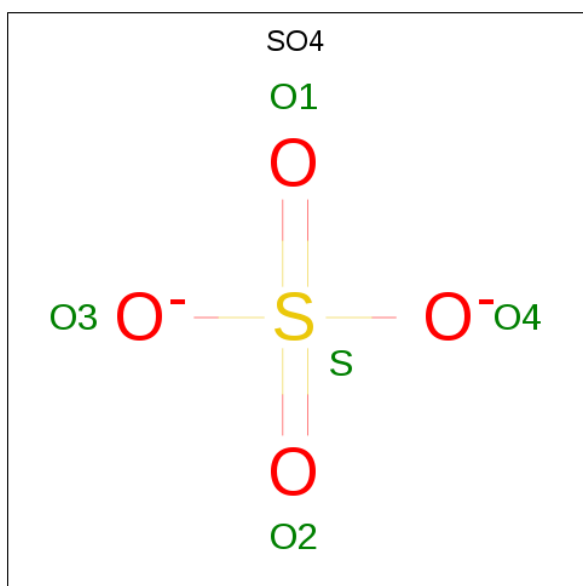
Chain	Residue	Modelled	Actual	Comment	Reference
C	27	GLU	-	expression tag	UNP P52799
C	28	THR	-	expression tag	UNP P52799
C	29	GLY	-	expression tag	UNP P52799
C	171	GLY	-	expression tag	UNP P52799
C	172	THR	-	expression tag	UNP P52799
C	173	LYS	-	expression tag	UNP P52799
C	174	HIS	-	expression tag	UNP P52799
C	175	HIS	-	expression tag	UNP P52799
C	176	HIS	-	expression tag	UNP P52799
C	177	HIS	-	expression tag	UNP P52799
C	178	HIS	-	expression tag	UNP P52799
C	179	HIS	-	expression tag	UNP P52799
E	27	GLU	-	expression tag	UNP P52799
E	28	THR	-	expression tag	UNP P52799
E	29	GLY	-	expression tag	UNP P52799

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Chain	Residue	Modelled	Actual	Comment	Reference
E	171	GLY	-	expression tag	UNP P52799
E	172	THR	-	expression tag	UNP P52799
E	173	LYS	-	expression tag	UNP P52799
E	174	HIS	-	expression tag	UNP P52799
E	175	HIS	-	expression tag	UNP P52799
E	176	HIS	-	expression tag	UNP P52799
E	177	HIS	-	expression tag	UNP P52799
E	178	HIS	-	expression tag	UNP P52799
E	179	HIS	-	expression tag	UNP P52799

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



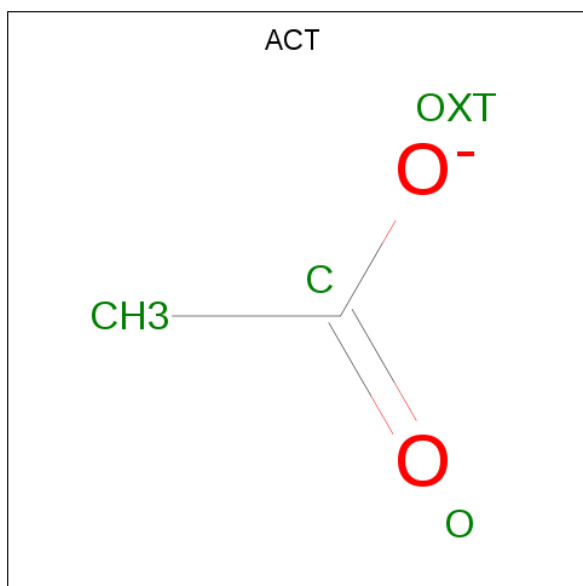
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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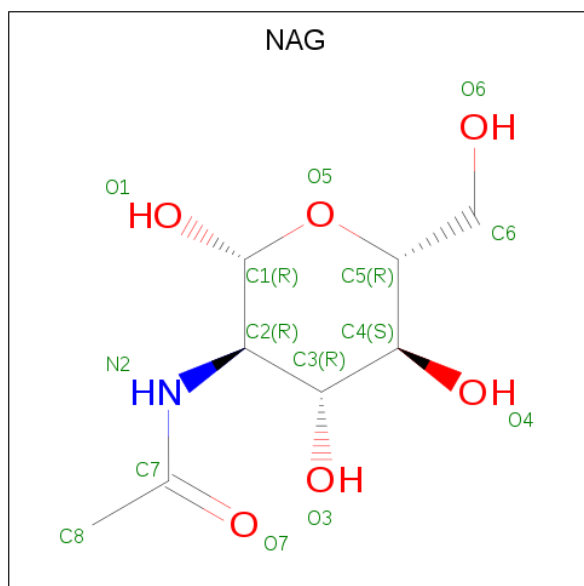
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	417	Total	O	0	0
			417	417		
7	B	344	Total	O	0	0
			344	344		
7	C	124	Total	O	0	0
			124	124		
7	E	135	Total	O	0	0
			135	135		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.22Å 152.53Å 163.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.47 – 1.70 60.72 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (111.47-1.70) 99.0 (60.72-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.175 , 0.199 0.183 , 0.206	Depositor DCC
R_{free} test set	8583 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10304	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: CL, NAG, SO4, ACT

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	0/3527	0.74	0/4810
1	B	0.56	0/3480	0.74	0/4744
2	C	0.51	0/1168	0.75	0/1575
2	E	0.53	0/1148	0.80	1/1549 (0.1%)
All	All	0.54	0/9323	0.75	1/12678 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	91	ARG	NE-CZ-NH1	5.40	123.00	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3409	0	3274	9	0
1	B	3375	0	3225	15	1
2	C	1131	0	1129	4	0
2	E	1120	0	1110	10	1
3	A	30	0	0	0	0
3	B	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
4	A	16	0	12	1	0
4	B	8	0	6	0	0
4	E	4	0	3	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	56	0	52	0	0
6	B	56	0	52	0	0
6	C	14	0	13	0	0
6	E	28	0	26	0	0
7	A	417	0	0	2	0
7	B	344	0	0	2	0
7	C	124	0	0	0	0
7	E	135	0	0	3	0
All	All	10304	0	8902	36	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 36 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:287[A]:TYR:CE1	1:B:341[A]:GLU:OE1	1.87	1.28
1:B:287[A]:TYR:CZ	1:B:341[A]:GLU:OE2	1.91	1.24
1:B:287[A]:TYR:CE2	1:B:341[A]:GLU:OE2	1.96	1.17
1:A:594:ASN:O	7:A:2404:HOH:O	1.88	0.90
1:B:287[A]:TYR:CZ	1:B:341[A]:GLU:CD	2.45	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287[A]:TYR:OH	2:E:34:GLU:CG[3_555]	1.77	0.43

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	421/454 (93%)	407 (97%)	14 (3%)	0	100	100
1	B	413/454 (91%)	399 (97%)	14 (3%)	0	100	100
2	C	139/153 (91%)	137 (99%)	2 (1%)	0	100	100
2	E	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
All	All	1110/1214 (91%)	1078 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/417 (94%)	388 (99%)	3 (1%)	81	74
1	B	386/417 (93%)	382 (99%)	4 (1%)	76	67
2	C	129/138 (94%)	126 (98%)	3 (2%)	50	33
2	E	126/138 (91%)	123 (98%)	3 (2%)	49	31
All	All	1032/1110 (93%)	1019 (99%)	13 (1%)	69	56

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	485	TYR
1	B	497	ARG
2	E	95	LYS

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Mol	Chain	Res	Type
1	B	254	LYS
2	C	128	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	291	ASN
1	B	294	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	$\# Z > 2$
4	ACT	A	1625	-	1,3,3	0.78	0	0,3,3	0.00	-
6	NAG	A	1632	1	14,14,15	0.30	0	17,19,21	1.32	3 (17%)
6	NAG	B	1630	1	14,14,15	0.27	0	17,19,21	1.18	3 (17%)
6	NAG	A	1630	1	14,14,15	0.33	0	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	1172	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	B	1619	-	4,4,4	0.33	0	6,6,6	0.15	0
6	NAG	E	1175	2	14,14,15	0.42	0	17,19,21	0.82	1 (5%)
3	SO4	A	1621	-	4,4,4	0.24	0	6,6,6	0.50	0
4	ACT	B	1625	-	1,3,3	0.48	0	0,3,3	0.00	-
6	NAG	E	1174	2	14,14,15	0.44	0	17,19,21	1.37	2 (11%)
3	SO4	A	1619	-	4,4,4	0.31	0	6,6,6	0.05	0
6	NAG	C	1173	2	14,14,15	0.38	0	17,19,21	1.43	2 (11%)
6	NAG	B	1628	1	14,14,15	0.38	0	17,19,21	0.99	2 (11%)
3	SO4	B	1618	-	4,4,4	0.35	0	6,6,6	0.23	0
3	SO4	B	1622	-	4,4,4	0.30	0	6,6,6	0.14	0
3	SO4	A	1623	-	4,4,4	0.24	0	6,6,6	0.44	0
6	NAG	A	1631	1	14,14,15	0.55	0	17,19,21	1.08	1 (5%)
3	SO4	B	1621	-	4,4,4	0.31	0	6,6,6	0.24	0
4	ACT	E	1173	-	1,3,3	0.57	0	0,3,3	0.00	-
4	ACT	A	1627	-	1,3,3	1.06	0	0,3,3	0.00	-
6	NAG	B	1627	1	14,14,15	0.46	0	17,19,21	1.11	2 (11%)
3	SO4	A	1622	-	4,4,4	0.40	0	6,6,6	0.20	0
3	SO4	B	1620	-	4,4,4	0.32	0	6,6,6	0.07	0
4	ACT	A	1624	-	1,3,3	1.26	0	0,3,3	0.00	-
3	SO4	A	1618	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SO4	B	1623	-	4,4,4	0.28	0	6,6,6	0.39	0
6	NAG	A	1629	1	14,14,15	0.29	0	17,19,21	0.95	0
6	NAG	B	1629	1	14,14,15	0.44	0	17,19,21	1.55	2 (11%)
3	SO4	A	1620	-	4,4,4	0.34	0	6,6,6	0.16	0
4	ACT	B	1624	-	1,3,3	0.49	0	0,3,3	0.00	-
4	ACT	A	1626	-	1,3,3	1.62	0	0,3,3	0.00	-

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	A	1629	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1629	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1631	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1630	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1632	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1173	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1630	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1628	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1627	1	-	2/6/23/26	0/1/1/1
6	NAG	E	1174	2	-	2/6/23/26	0/1/1/1
6	NAG	E	1175	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1629	NAG	C2-N2-C7	3.48	127.86	122.90
6	B	1629	NAG	C8-C7-N2	3.48	121.99	116.10
6	C	1173	NAG	C8-C7-N2	3.42	121.90	116.10
6	E	1174	NAG	C8-C7-N2	3.25	121.59	116.10
6	C	1173	NAG	C2-N2-C7	3.24	127.51	122.90

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1632	NAG	C8-C7-N2-C2
6	A	1632	NAG	O7-C7-N2-C2
6	B	1630	NAG	C8-C7-N2-C2
6	B	1630	NAG	O7-C7-N2-C2
6	E	1174	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1625	ACT	1	0
4	E	1173	ACT	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	417/454 (91%)	-0.00	17 (4%) 37 41	15, 28, 61, 102	0
1	B	412/454 (90%)	0.18	33 (8%) 12 14	19, 32, 63, 107	0
2	C	138/153 (90%)	-0.18	4 (2%) 51 56	21, 31, 54, 86	0
2	E	139/153 (90%)	-0.09	6 (4%) 35 39	18, 30, 55, 89	0
All	All	1106/1214 (91%)	0.03	60 (5%) 25 28	15, 30, 61, 107	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	617	HIS	7.0
1	A	612	ARG	6.4
1	B	612	ARG	6.3
1	B	617	HIS	6.2
1	B	616	PRO	5.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	ACT	A	1627	4/4	0.72	0.24	33,37,40,40	0
4	ACT	E	1173	4/4	0.74	0.26	49,51,52,54	0
4	ACT	A	1626	4/4	0.78	0.17	54,54,55,56	0
6	NAG	B	1630	14/15	0.79	0.34	70,77,81,83	0
6	NAG	B	1629	14/15	0.79	0.22	46,54,57,58	0
6	NAG	A	1632	14/15	0.79	0.38	73,80,82,83	0
6	NAG	E	1174	14/15	0.80	0.28	44,50,54,57	0
3	SO4	A	1620	5/5	0.80	0.21	88,93,96,97	0
6	NAG	C	1173	14/15	0.80	0.25	53,59,64,64	0
4	ACT	B	1625	4/4	0.81	0.24	52,53,53,56	0
6	NAG	E	1175	14/15	0.82	0.34	55,63,67,67	0
3	SO4	C	1172	5/5	0.82	0.29	114,114,115,116	0
6	NAG	A	1629	14/15	0.82	0.25	46,53,57,60	0
4	ACT	B	1624	4/4	0.84	0.18	60,62,63,65	0
4	ACT	A	1625	4/4	0.84	0.24	50,50,51,52	0
6	NAG	B	1628	14/15	0.85	0.23	51,55,58,59	0
3	SO4	A	1619	5/5	0.85	0.33	115,118,120,120	0
3	SO4	B	1622	5/5	0.87	0.29	89,95,95,96	0
6	NAG	A	1630	14/15	0.87	0.20	48,51,56,57	0
6	NAG	B	1627	14/15	0.89	0.10	28,30,35,37	0
6	NAG	A	1631	14/15	0.89	0.11	30,35,40,44	0
4	ACT	A	1624	4/4	0.90	0.10	64,64,64,64	0
3	SO4	B	1620	5/5	0.90	0.16	79,83,85,87	0
3	SO4	A	1622	5/5	0.91	0.10	40,44,51,51	0
3	SO4	B	1618	5/5	0.95	0.10	60,62,63,65	0
3	SO4	A	1623	5/5	0.97	0.11	28,29,32,32	0
3	SO4	B	1619	5/5	0.97	0.14	46,46,48,48	0
3	SO4	B	1621	5/5	0.97	0.17	49,51,54,54	0
5	CL	B	1626	1/1	0.97	0.06	34,34,34,34	0
3	SO4	A	1618	5/5	0.97	0.08	56,57,58,58	0
3	SO4	B	1623	5/5	0.97	0.11	31,32,35,37	0
3	SO4	A	1621	5/5	0.98	0.09	36,39,43,44	0
5	CL	A	1628	1/1	0.99	0.06	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.