



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:45 PM UTC

PDB ID : 4UF7 / pdb_00004uf7
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 Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

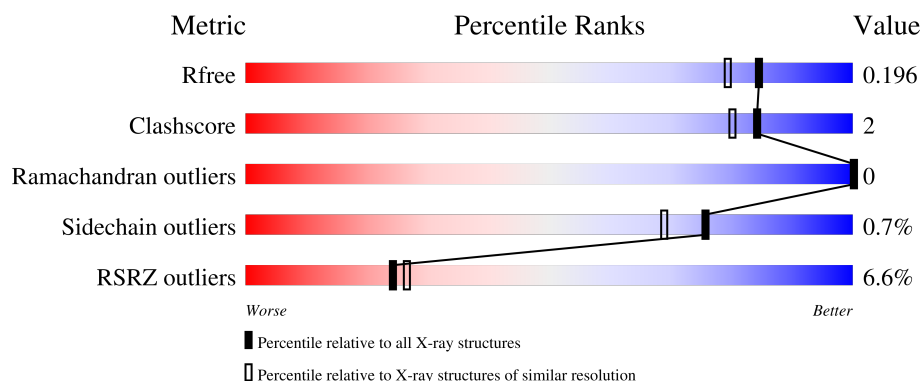
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 of 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	5% 89% 8%
1	B	454	6% 87% 9%
2	C	153	7% 86% 10%
2	E	153	8% 82% 7% 9%

2 Entry composition

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:

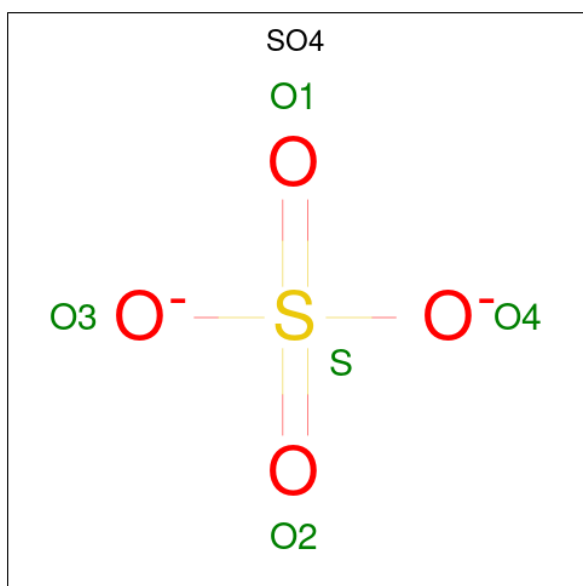
Chain	Residue	Modelled	Actual	Comment	Reference
C	27	GLU	-	expression tag	UNP P52799
C	28	THR	-	expression tag	UNP P52799
C	29	GLY	-	expression tag	UNP P52799
C	171	GLY	-	expression tag	UNP P52799
C	172	THR	-	expression tag	UNP P52799
C	173	LYS	-	expression tag	UNP P52799
C	174	HIS	-	expression tag	UNP 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 (CCD ID: SO4) (formula: O₄S).



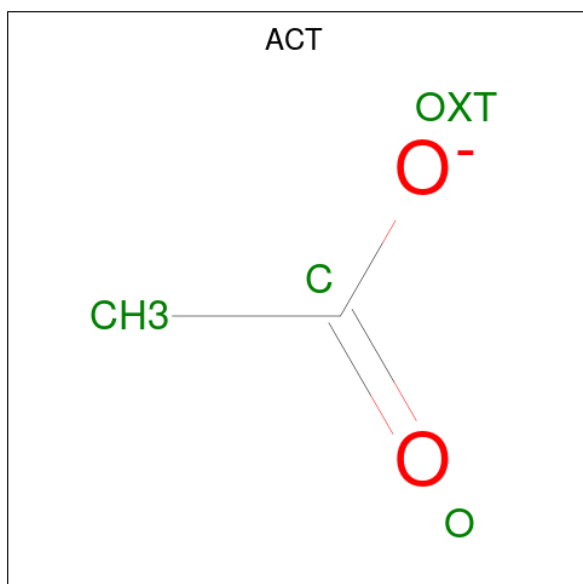
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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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	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 (CCD ID: 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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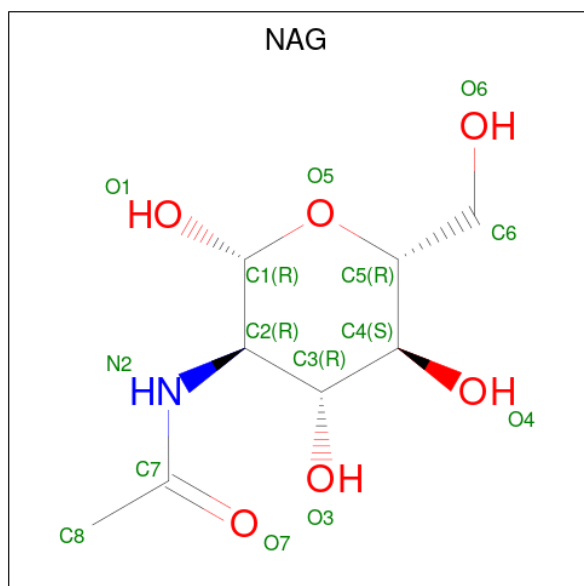
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

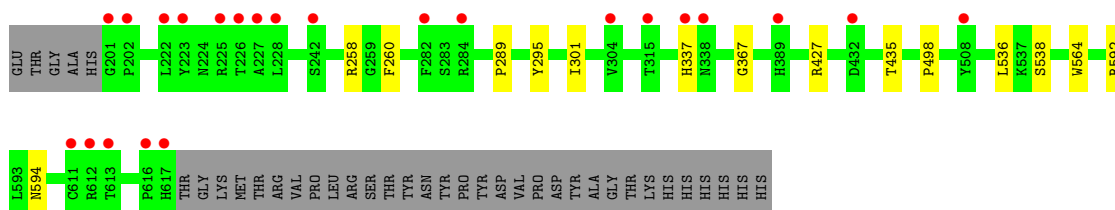
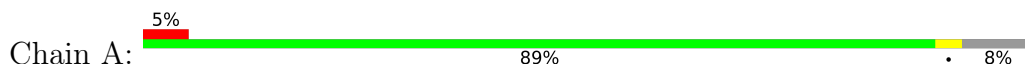
- Molecule 7 is water.

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		

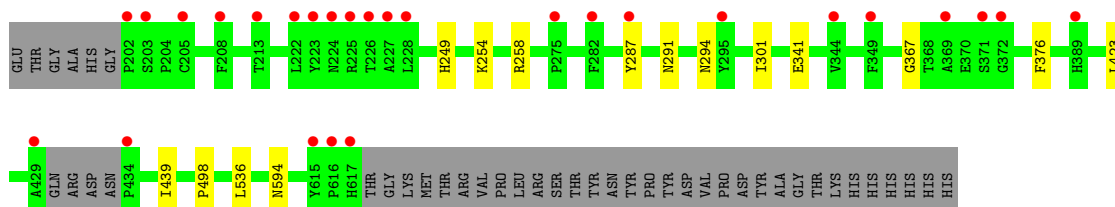
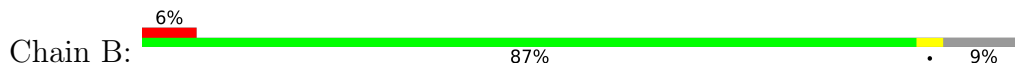
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

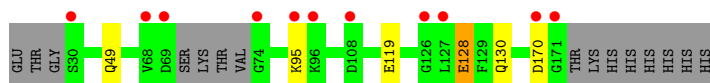
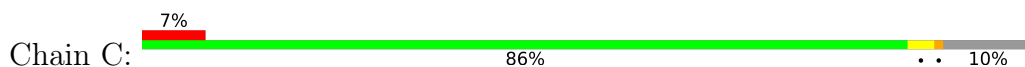
• Molecule 1: GLYCOPROTEIN



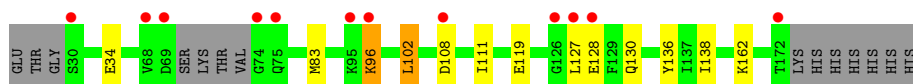
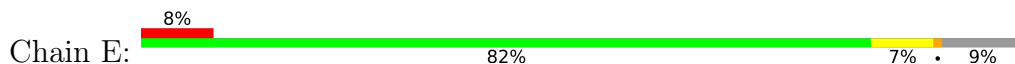
• Molecule 1: GLYCOPROTEIN



• Molecule 2: EPHRIN-B2



• Molecule 2: EPHRIN-B2



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 – 1.70 111.47 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (111.47-1.70) 95.0 (111.47-1.70)	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 (Not available) , 0.196	Depositor DCC
R_{free} test set	8584 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 , 34.9	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: SO4, NAG, ACT, CL

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	0.67	0/3527	0.77	1/4810 (0.0%)
1	B	0.66	0/3480	0.77	0/4744
2	C	0.63	0/1168	0.80	0/1575
2	E	0.68	0/1148	0.84	0/1549
All	All	0.66	0/9323	0.78	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(°)
1	A	337	HIS	N-CA-C	5.10	116.53	111.07

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	10	0
1	B	3375	0	3225	17	1
2	C	1131	0	1129	5	0
2	E	1120	0	1110	11	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	4	0
All	All	10304	0	8902	41	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.

All (41) 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:B:287[A]:TYR:CZ	1:B:341[A]:GLU:CD	2.45	0.94
1:A:594:ASN:O	7:A:2404:HOH:O	1.88	0.90
1:B:287[A]:TYR:CE1	1:B:341[A]:GLU:CD	2.51	0.87
1:B:287[A]:TYR:CZ	1:B:341[A]:GLU:OE1	2.38	0.76
1:B:423:LEU:HD11	1:B:439:ILE:HD12	1.71	0.72
1:B:258:ARG:NH2	2:C:119:GLU:OE2	2.30	0.64
1:A:258:ARG:NH2	2:E:119:GLU:OE2	2.31	0.64
1:B:594:ASN:O	7:B:2336:HOH:O	2.15	0.63
7:A:2365:HOH:O	4:E:1173:ACT:H2	2.01	0.61
1:B:287[A]:TYR:CD1	1:B:341[A]:GLU:OE1	2.50	0.60
2:E:83:MET:HE1	7:E:2047:HOH:O	2.02	0.59
1:B:287[A]:TYR:CD2	1:B:341[A]:GLU:OE2	2.52	0.58
2:E:83:MET:HE3	7:E:2049:HOH:O	2.04	0.57
1:B:291:ASN:HB2	7:B:2065:HOH:O	2.06	0.55
1:A:427:ARG:HB2	1:A:435[B]:THR:CG2	2.38	0.53
2:E:128:GLU:OE2	2:E:130:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ASN:OD1	1:B:294:ASN:ND2	2.42	0.51
1:A:260:PHE:HB2	2:C:170:ASP:OD1	2.12	0.49
2:C:128:GLU:OE2	2:C:130[B]:GLN:HG3	2.14	0.47
2:C:49[B]:GLN:HE21	2:C:49[B]:GLN:HA	1.81	0.45
2:E:138:ILE:HG22	2:E:162:LYS:HB2	1.98	0.45
2:E:102[B]:LEU:CD2	2:E:111:ILE:HG22	2.46	0.45
2:C:128:GLU:CD	2:C:128:GLU:C	2.85	0.45
2:E:127:LEU:HG	7:E:2077:HOH:O	2.16	0.45
1:A:427:ARG:HB2	1:A:435[B]:THR:HG22	2.00	0.44
1:A:564:TRP:CZ3	1:A:592:ARG:HD3	2.53	0.43
1:B:301:ILE:HG12	1:B:367:GLY:C	2.43	0.43
2:E:136:TYR:OH	7:E:2096:HOH:O	2.19	0.43
2:E:96:LYS:N	2:E:96:LYS:HD3	2.34	0.43
1:B:301:ILE:HD12	1:B:376:PHE:CZ	2.54	0.43
1:A:538:SER:N	4:A:1625:ACT:H2	2.34	0.42
1:A:301:ILE:HG12	1:A:367:GLY:C	2.45	0.42
2:E:102[B]:LEU:HD22	2:E:111:ILE:HG22	2.01	0.42
2:E:96:LYS:HD3	2:E:96:LYS:H	1.86	0.41
1:B:498:PRO:HD3	1:B:536:LEU:HB2	2.02	0.41
1:A:498:PRO:HD3	1:A:536:LEU:HB2	2.03	0.40
1:B:287[A]:TYR:CD1	1:B:341[A]:GLU:CD	2.97	0.40
1:A:289:PRO:HG3	1:A:295[B]:TYR:CG	2.57	0.40

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 ⓘ

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	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 ⓘ

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%)	391 (100%)	0	100	100
1	B	386/417 (93%)	384 (100%)	2 (0%)	81	76
2	C	129/138 (94%)	127 (98%)	2 (2%)	55	41
2	E	126/138 (91%)	122 (97%)	4 (3%)	34	17
All	All	1032/1110 (93%)	1024 (99%)	8 (1%)	76	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	249	HIS
1	B	254	LYS
2	C	95	LYS
2	C	128	GLU
2	E	96	LYS
2	E	102[A]	LEU
2	E	102[B]	LEU
2	E	108	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	A	486	GLN
1	B	291	ASN
1	B	294	ASN
1	B	355	GLN
1	B	412	GLN

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 oligosaccharides 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	1627	-	3,3,3	0.76	0	3,3,3	1.07	0
3	SO4	A	1618	-	4,4,4	0.43	0	6,6,6	0.07	0
3	SO4	B	1618	-	4,4,4	0.45	0	6,6,6	0.25	0
6	NAG	A	1630	1	14,14,15	0.34	0	17,19,21	1.02	1 (5%)
4	ACT	A	1624	-	3,3,3	0.82	0	3,3,3	0.79	0
3	SO4	A	1623	-	4,4,4	0.33	0	6,6,6	0.39	0
6	NAG	A	1632	1	14,14,15	0.30	0	17,19,21	1.34	3 (17%)
3	SO4	B	1623	-	4,4,4	0.39	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1629	1	14,14,15	0.29	0	17,19,21	0.96	0
3	SO4	B	1620	-	4,4,4	0.42	0	6,6,6	0.08	0
3	SO4	A	1621	-	4,4,4	0.35	0	6,6,6	0.49	0
4	ACT	B	1625	-	3,3,3	0.75	0	3,3,3	1.36	0
4	ACT	E	1173	-	3,3,3	0.83	0	3,3,3	0.57	0
6	NAG	B	1630	1	14,14,15	0.27	0	17,19,21	1.21	3 (17%)
4	ACT	B	1624	-	3,3,3	0.76	0	3,3,3	0.98	0
3	SO4	B	1622	-	4,4,4	0.41	0	6,6,6	0.15	0
4	ACT	A	1626	-	3,3,3	0.77	0	3,3,3	0.94	0
3	SO4	A	1619	-	4,4,4	0.42	0	6,6,6	0.06	0
3	SO4	A	1620	-	4,4,4	0.44	0	6,6,6	0.14	0
6	NAG	A	1631	1	14,14,15	0.55	0	17,19,21	1.05	1 (5%)
6	NAG	B	1629	1	14,14,15	0.44	0	17,19,21	1.57	2 (11%)
3	SO4	B	1621	-	4,4,4	0.41	0	6,6,6	0.24	0
3	SO4	B	1619	-	4,4,4	0.42	0	6,6,6	0.17	0
6	NAG	E	1174	2	14,14,15	0.47	0	17,19,21	1.40	2 (11%)
6	NAG	E	1175	2	14,14,15	0.45	0	17,19,21	0.74	0
6	NAG	C	1173	2	14,14,15	0.40	0	17,19,21	1.47	2 (11%)
4	ACT	A	1625	-	3,3,3	0.83	0	3,3,3	0.86	0
3	SO4	A	1622	-	4,4,4	0.50	0	6,6,6	0.24	0
3	SO4	C	1172	-	4,4,4	0.41	0	6,6,6	0.11	0
6	NAG	B	1627	1	14,14,15	0.46	0	17,19,21	1.16	2 (11%)
6	NAG	B	1628	1	14,14,15	0.40	0	17,19,21	0.89	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1627	1	-	2/6/23/26	0/1/1/1
6	NAG	E	1175	2	-	0/6/23/26	0/1/1/1
6	NAG	B	1630	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1173	2	-	2/6/23/26	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	E	1174	2	-	2/6/23/26	0/1/1/1
6	NAG	A	1631	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1629	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1628	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1629	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1629	NAG	C2-N2-C7	3.70	127.86	122.90
6	B	1629	NAG	C8-C7-N2	3.54	121.99	116.12
6	C	1173	NAG	C8-C7-N2	3.48	121.90	116.12
6	C	1173	NAG	C2-N2-C7	3.44	127.51	122.90
6	E	1174	NAG	C2-N2-C7	3.33	127.36	122.90
6	E	1174	NAG	C8-C7-N2	3.30	121.59	116.12
6	B	1627	NAG	C2-N2-C7	3.25	127.26	122.90
6	A	1630	NAG	C1-O5-C5	2.88	116.04	112.19
6	A	1632	NAG	C2-N2-C7	2.72	126.55	122.90
6	A	1632	NAG	C8-C7-N2	2.72	120.63	116.12
6	B	1630	NAG	C2-N2-C7	2.59	126.37	122.90
6	B	1630	NAG	C8-C7-N2	2.56	120.36	116.12
6	A	1631	NAG	O5-C1-C2	-2.55	107.35	111.29
6	B	1627	NAG	O5-C1-C2	-2.20	107.88	111.29
6	A	1632	NAG	O5-C1-C2	-2.18	107.92	111.29
6	B	1630	NAG	O5-C1-C2	-2.13	107.99	111.29
6	B	1628	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (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	1627	NAG	C8-C7-N2-C2
6	B	1627	NAG	O7-C7-N2-C2
6	B	1629	NAG	C8-C7-N2-C2
6	B	1629	NAG	O7-C7-N2-C2
6	B	1630	NAG	C8-C7-N2-C2
6	B	1630	NAG	O7-C7-N2-C2
6	C	1173	NAG	C8-C7-N2-C2
6	C	1173	NAG	O7-C7-N2-C2
6	E	1174	NAG	C8-C7-N2-C2
6	E	1174	NAG	O7-C7-N2-C2
6	B	1628	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	1629	NAG	O5-C5-C6-O6
6	B	1629	NAG	C4-C5-C6-O6
6	B	1628	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/454 (91%)	0.19	23 (5%) 30 34	13, 28, 61, 102	6 (1%)
1	B	412/454 (90%)	0.46	27 (6%) 24 26	12, 32, 63, 107	5 (1%)
2	C	138/153 (90%)	0.31	11 (7%) 18 19	15, 31, 53, 86	5 (3%)
2	E	139/153 (90%)	0.38	12 (8%) 16 17	14, 30, 55, 89	2 (1%)
All	All	1106/1214 (91%)	0.33	73 (6%) 24 26	12, 30, 61, 107	18 (1%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	429	ALA	8.0
2	E	68	VAL	4.8
1	B	226	THR	4.5
2	E	126	GLY	4.5
1	B	434	PRO	4.4
1	A	227	ALA	4.4
1	A	223	TYR	4.3
2	C	171	GLY	4.3
2	C	68	VAL	4.1
1	B	202	PRO	4.0
1	B	617	HIS	3.9
2	C	69	ASP	3.8
2	C	127	LEU	3.7
1	A	613	THR	3.7
1	B	223	TYR	3.7
1	B	282	PHE	3.7
1	A	202	PRO	3.6
1	A	617	HIS	3.5
2	E	127	LEU	3.5
1	B	287[A]	TYR	3.4
1	A	338	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	616	PRO	3.4
1	A	201	GLY	3.3
2	E	96	LYS	3.3
2	E	172	THR	3.3
1	A	222	LEU	3.2
2	C	30	SER	3.2
1	A	284	ARG	3.2
1	B	295	TYR	3.2
2	E	69	ASP	3.1
1	B	222	LEU	3.1
1	A	226	THR	3.1
2	C	126	GLY	3.1
1	A	611	CYS	3.1
2	E	128	GLU	3.1
1	B	371	SER	3.0
1	A	337	HIS	2.9
2	E	74	GLY	2.8
1	B	227	ALA	2.7
1	B	616	PRO	2.7
1	B	228	LEU	2.7
1	A	508	TYR	2.7
2	C	96	LYS	2.6
1	A	304	VAL	2.6
1	B	389	HIS	2.5
1	B	344	VAL	2.5
2	E	108	ASP	2.5
1	A	432	ASP	2.4
1	B	224	ASN	2.4
1	B	349	PHE	2.4
1	B	203	SER	2.3
1	B	615	TYR	2.3
2	C	108[A]	ASP	2.3
1	B	275	PRO	2.2
1	A	225	ARG	2.2
1	B	225	ARG	2.2
1	A	228	LEU	2.2
2	E	30	SER	2.2
1	B	208	PHE	2.2
1	A	315	THR	2.2
2	E	95	LYS	2.2
1	A	282	PHE	2.2
1	A	612	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	95	LYS	2.2
1	B	205	CYS	2.1
2	C	74	GLY	2.1
1	B	213	THR	2.1
2	C	170	ASP	2.1
1	B	372	GLY	2.0
2	E	75	GLN	2.0
1	A	389	HIS	2.0
1	B	369	ALA	2.0
1	A	242	SER	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	C	1172	5/5	0.49	0.16	114,114,115,116	0
6	NAG	A	1632	14/15	0.61	0.14	73,80,82,83	0
6	NAG	E	1175	14/15	0.64	0.17	55,63,67,67	0
6	NAG	B	1630	14/15	0.65	0.16	70,77,81,83	0
4	ACT	A	1626	4/4	0.69	0.21	54,54,55,56	0
4	ACT	A	1624	4/4	0.73	0.21	64,64,64,64	0
6	NAG	C	1173	14/15	0.74	0.13	53,59,64,64	0
4	ACT	B	1625	4/4	0.74	0.27	52,53,53,56	0
6	NAG	B	1629	14/15	0.76	0.16	46,54,57,58	0
3	SO4	A	1620	5/5	0.77	0.18	88,93,96,97	0
6	NAG	A	1629	14/15	0.78	0.13	46,53,57,60	0
6	NAG	E	1174	14/15	0.80	0.12	44,50,54,57	0
6	NAG	A	1630	14/15	0.80	0.13	48,51,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	1627	4/4	0.81	0.21	33,37,40,40	0
4	ACT	E	1173	4/4	0.81	0.21	49,51,52,54	0
3	SO4	B	1620	5/5	0.82	0.11	79,83,85,87	0
3	SO4	B	1622	5/5	0.83	0.16	89,95,95,96	0
6	NAG	B	1628	14/15	0.86	0.12	51,55,58,59	0
4	ACT	B	1624	4/4	0.87	0.23	60,62,63,65	0
3	SO4	A	1619	5/5	0.87	0.14	115,118,120,120	0
3	SO4	A	1622	5/5	0.88	0.11	40,44,51,51	0
6	NAG	A	1631	14/15	0.88	0.11	30,35,40,44	0
4	ACT	A	1625	4/4	0.88	0.24	50,50,51,52	0
3	SO4	B	1619	5/5	0.89	0.10	46,46,48,48	0
6	NAG	B	1627	14/15	0.89	0.11	28,30,35,37	0
3	SO4	B	1618	5/5	0.93	0.09	60,62,63,65	0
3	SO4	B	1621	5/5	0.94	0.08	49,51,54,54	0
3	SO4	A	1618	5/5	0.95	0.06	56,57,58,58	0
3	SO4	A	1621	5/5	0.96	0.06	36,39,43,44	0
3	SO4	B	1623	5/5	0.96	0.12	31,32,35,37	0
3	SO4	A	1623	5/5	0.96	0.14	28,29,32,32	0
5	CL	B	1626	1/1	0.98	0.06	34,34,34,34	0
5	CL	A	1628	1/1	0.98	0.05	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.