Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 08:58 PM GMT

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 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
http://wwpdb.org/validation/2016/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:

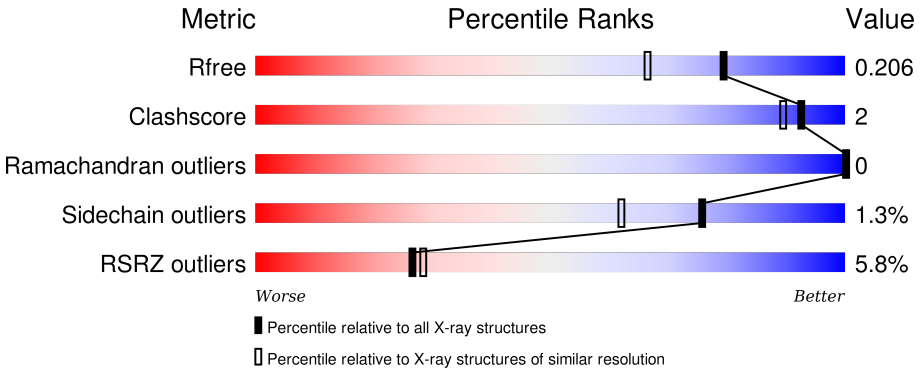
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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. 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 <=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	4% 89% • 8%
1	B	454	7% 87% • 9%
2	C	153	3% 86% • • 10%
2	E	153	4% 81% 9% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1620	-	-	-	X
3	SO4	B	1622	-	-	-	X
3	SO4	C	1172	-	-	-	X
4	ACT	A	1626	-	-	-	X
4	ACT	A	1627	-	-	-	X
4	ACT	B	1625	-	-	-	X
4	ACT	E	1173	-	-	-	X
6	NAG	A	1630	-	-	-	X
6	NAG	B	1628	-	-	-	X
6	NAG	E	1175	-	-	-	X

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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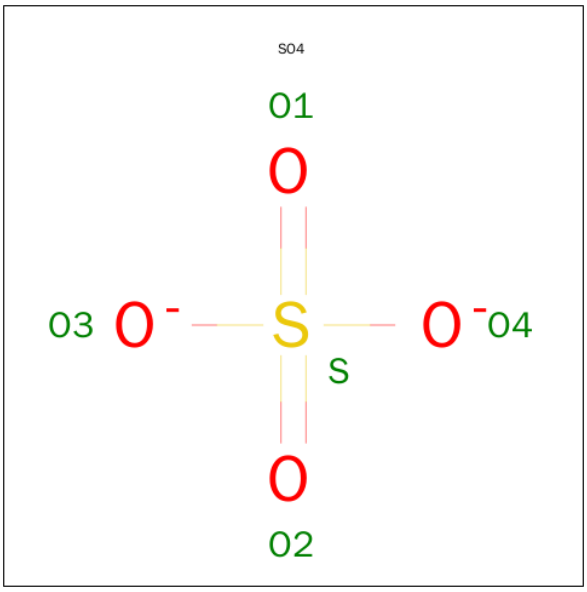
Chain	Residue	Modelled	Actual	Comment	Reference
E	171	GLY	-	EXPRESSION TAG	UNP P52799
E	172	THR	-	EXPRESSION TAG	UNP P52799
E	173	LYS	-	EXPRESSION TAG	UNP P52799
E	174	HIS	-	EXPRESSION TAG	UNP P52799
E	175	HIS	-	EXPRESSION TAG	UNP P52799
E	176	HIS	-	EXPRESSION TAG	UNP P52799
E	177	HIS	-	EXPRESSION TAG	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: O_4S).



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

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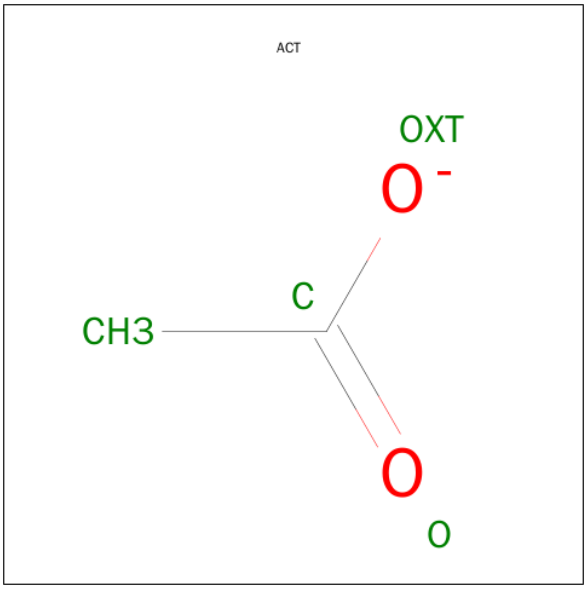
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- 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 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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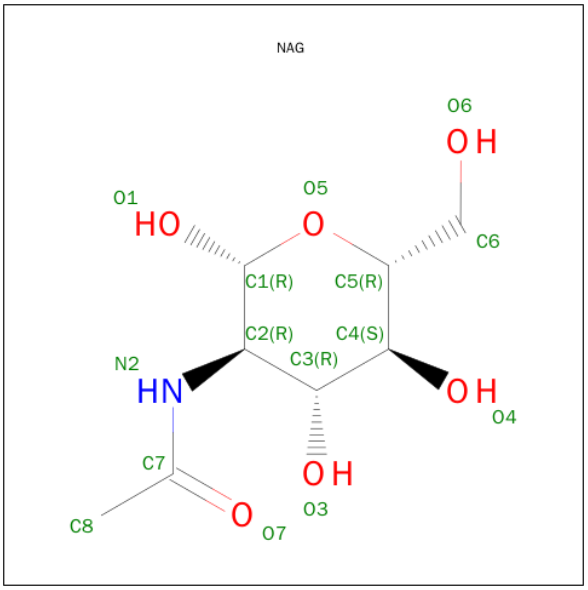
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0

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

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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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.

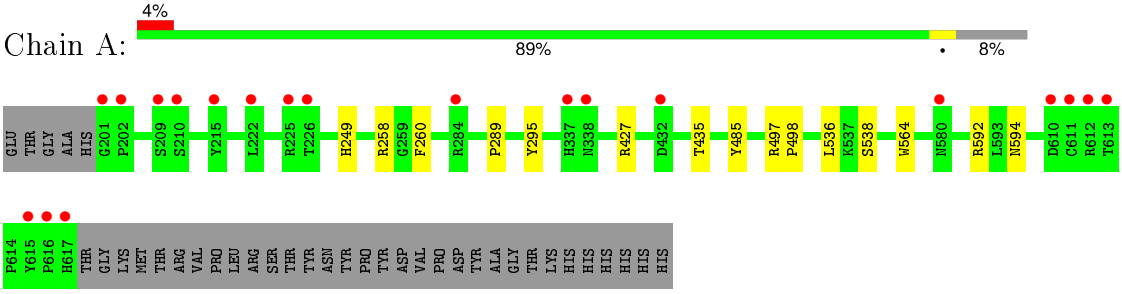
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	417	Total	O	0	0
			417	417		
7	B	344	Total	O	0	0
			344	344		
7	C	124	Total	O	0	0
			124	124		
7	E	135	Total	O	0	0
			135	135		

3 Residue-property plots (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.

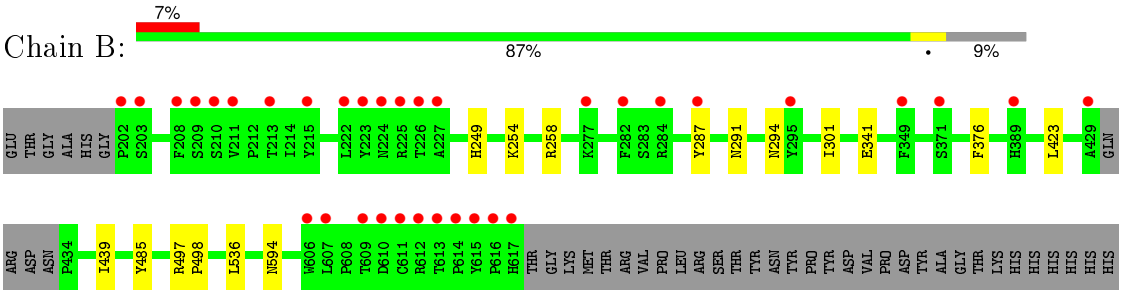
- Molecule 1: GLYCOPROTEIN

Chain A:



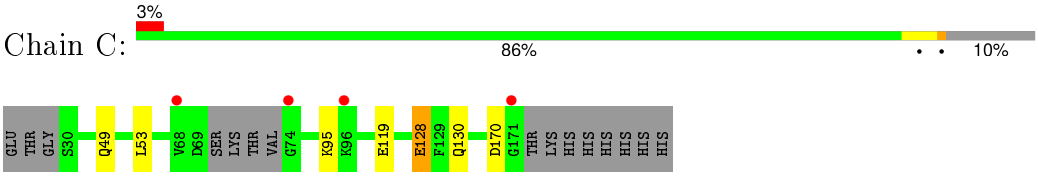
- Molecule 1: GLYCOPROTEIN

Chain B:



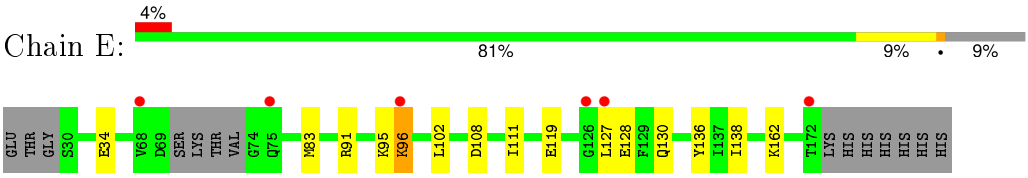
- Molecule 2: EPHRIN-B2

Chain C:



- Molecule 2: EPHRIN-B2

Chain E:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	8584 reflections (5.27%)	DCC
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 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 171423 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

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.

All (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
1:B:287[A]:TYR:CE1	1:B:341[A]:GLU:CD	2.51	0.82
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
1:B:287[A]:TYR:CD2	1:B:341[A]:GLU:OE2	2.52	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:83:MET:HE1	7:E:2047:HOH:O	2.12	0.48
2:C:128:GLU:OE2	2:C:130[B]:GLN:HG3	2.14	0.47
2:C:49[B]:GLN:HA	2:C:49[B]:GLN:HE21	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: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
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
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: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 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	86	79
1	B	386/417 (93%)	382 (99%)	4 (1%)	82	72
2	C	129/138 (94%)	126 (98%)	3 (2%)	58	37
2	E	126/138 (91%)	123 (98%)	3 (2%)	57	36
All	All	1032/1110 (93%)	1019 (99%)	13 (1%)	76	62

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

Mol	Chain	Res	Type
1	A	249	HIS
1	A	485	TYR
1	A	497	ARG
1	B	249	HIS
1	B	254	LYS
1	B	485	TYR
1	B	497	ARG
2	C	53	LEU
2	C	95	LYS
2	C	128	GLU
2	E	95	LYS
2	E	96	LYS
2	E	108	ASP

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

There are no RNA molecules 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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	SO4	A	1618	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SO4	A	1619	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	A	1620	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	A	1621	-	4,4,4	0.21	0	6,6,6	0.45	0
3	SO4	A	1622	-	4,4,4	0.48	0	6,6,6	0.33	0
3	SO4	A	1623	-	4,4,4	0.37	0	6,6,6	0.35	0
4	ACT	A	1624	-	1,3,3	1.10	0	0,3,3	0.00	-
4	ACT	A	1625	-	1,3,3	0.79	0	0,3,3	0.00	-
4	ACT	A	1626	-	1,3,3	1.43	0	0,3,3	0.00	-
4	ACT	A	1627	-	1,3,3	0.91	0	0,3,3	0.00	-
6	NAG	A	1629	1	14,14,15	0.28	0	15,19,21	0.97	0
6	NAG	A	1630	1	14,14,15	0.32	0	15,19,21	0.97	1 (6%)
6	NAG	A	1631	1	14,14,15	0.53	0	15,19,21	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	1632	1	14,14,15	0.28	0	15,19,21	1.25	2 (13%)
3	SO4	B	1618	-	4,4,4	0.37	0	6,6,6	0.28	0
3	SO4	B	1619	-	4,4,4	0.43	0	6,6,6	0.14	0
3	SO4	B	1620	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	B	1621	-	4,4,4	0.32	0	6,6,6	0.23	0
3	SO4	B	1622	-	4,4,4	0.31	0	6,6,6	0.13	0
3	SO4	B	1623	-	4,4,4	0.30	0	6,6,6	0.66	0
4	ACT	B	1624	-	1,3,3	0.38	0	0,3,3	0.00	-
4	ACT	B	1625	-	1,3,3	0.38	0	0,3,3	0.00	-
6	NAG	B	1627	1	14,14,15	0.48	0	15,19,21	1.04	1 (6%)
6	NAG	B	1628	1	14,14,15	0.37	0	15,19,21	0.93	1 (6%)
6	NAG	B	1629	1	14,14,15	0.42	0	15,19,21	1.48	2 (13%)
6	NAG	B	1630	1	14,14,15	0.26	0	15,19,21	1.09	2 (13%)
3	SO4	C	1172	-	4,4,4	0.33	0	6,6,6	0.12	0
6	NAG	C	1173	2	14,14,15	0.37	0	15,19,21	1.41	2 (13%)
4	ACT	E	1173	-	1,3,3	0.46	0	0,3,3	0.00	-
6	NAG	E	1174	2	14,14,15	0.44	0	15,19,21	1.37	2 (13%)
6	NAG	E	1175	2	14,14,15	0.42	0	15,19,21	0.75	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	SO4	A	1618	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1619	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1620	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1621	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1622	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1623	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1624	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1625	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1626	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1627	-	-	0/0/0/0	0/0/0/0
6	NAG	A	1629	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	1631	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1632	1	-	0/6/23/26	0/1/1/1
3	SO4	B	1618	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1619	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	1620	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1621	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1622	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1623	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1624	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1625	-	-	0/0/0/0	0/0/0/0
6	NAG	B	1627	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1628	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1629	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1630	1	-	0/6/23/26	0/1/1/1
3	SO4	C	1172	-	-	0/0/0/0	0/0/0/0
6	NAG	C	1173	2	-	0/6/23/26	0/1/1/1
4	ACT	E	1173	-	-	0/0/0/0	0/0/0/0
6	NAG	E	1174	2	-	0/6/23/26	0/1/1/1
6	NAG	E	1175	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1628	NAG	C1-O5-C5	2.15	114.98	112.25
6	B	1630	NAG	C8-C7-N2	2.22	120.36	116.11
6	A	1632	NAG	C8-C7-N2	2.36	120.63	116.11
6	B	1630	NAG	C2-N2-C7	2.59	126.37	123.04
6	A	1632	NAG	C2-N2-C7	2.73	126.55	123.04
6	E	1174	NAG	C8-C7-N2	2.87	121.59	116.11
6	A	1630	NAG	C1-O5-C5	2.99	116.04	112.25
6	C	1173	NAG	C8-C7-N2	3.03	121.90	116.11
6	B	1629	NAG	C8-C7-N2	3.07	121.99	116.11
6	B	1627	NAG	C2-N2-C7	3.29	127.26	123.04
6	E	1174	NAG	C2-N2-C7	3.36	127.36	123.04
6	C	1173	NAG	C2-N2-C7	3.48	127.51	123.04
6	B	1629	NAG	C2-N2-C7	3.76	127.86	123.04

There are no chirality outliers.

There are no torsion outliers.

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 (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, 95^{th} 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%)	0.06	20 (4%)	34	38	15, 28, 61, 102	0
1	B	412/454 (90%)	0.24	34 (8%)	14	16	19, 32, 63, 107	0
2	C	138/153 (90%)	-0.13	4 (2%)	55	59	21, 31, 54, 86	0
2	E	139/153 (90%)	-0.04	6 (4%)	39	43	18, 30, 55, 89	0
All	All	1106/1214 (91%)	0.09	64 (5%)	26	28	15, 30, 61, 107	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	617	HIS	7.1
1	A	612	ARG	6.5
1	B	612	ARG	6.3
1	B	617	HIS	6.2
1	B	616	PRO	6.1
1	B	226	THR	5.7
1	B	615	TYR	5.7
1	A	616	PRO	5.6
1	B	429	ALA	5.5
1	B	613	THR	5.5
1	A	226	THR	5.3
1	B	211	VAL	4.9
1	B	202	PRO	4.9
1	B	210	SER	4.8
1	A	611	CYS	4.2
1	A	613	THR	4.2
1	B	215	TYR	4.1
2	E	68	VAL	3.7
1	A	202	PRO	3.7
1	B	287[A]	TYR	3.7
1	B	611	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	172	THR	3.6
2	E	75	GLN	3.6
1	B	349	PHE	3.4
2	C	68	VAL	3.3
1	B	223	TYR	3.3
1	A	338	ASN	3.3
1	B	227	ALA	3.3
2	C	74	GLY	3.2
1	B	614	PRO	3.0
1	B	282	PHE	3.0
1	B	610	ASP	3.0
1	A	201	GLY	3.0
1	B	209	SER	2.9
1	A	337	HIS	2.9
1	B	606	TRP	2.7
1	B	609	THR	2.7
1	A	209	SER	2.7
1	B	222	LEU	2.7
1	A	284	ARG	2.6
1	B	208	PHE	2.6
1	A	225	ARG	2.6
1	B	225	ARG	2.6
1	B	371	SER	2.6
1	B	277	LYS	2.5
1	B	213	THR	2.5
1	A	210	SER	2.5
2	E	126	GLY	2.4
1	B	203	SER	2.4
1	A	580[A]	ASN	2.4
2	C	171	GLY	2.4
1	A	610	ASP	2.4
1	A	432	ASP	2.4
1	B	295	TYR	2.4
1	B	284	ARG	2.3
2	E	127	LEU	2.2
2	E	96	LYS	2.2
1	B	224	ASN	2.2
1	B	607	LEU	2.1
2	C	96	LYS	2.1
1	B	389	HIS	2.1
1	A	222	LEU	2.0
1	A	215	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	615	TYR	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 carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	1622	5/5	0.87	0.30	6.86	89,95,95,96	0
6	NAG	B	1628	14/15	0.85	0.23	6.81	51,55,58,59	0
4	ACT	A	1627	4/4	0.71	0.24	6.62	33,37,40,40	0
6	NAG	A	1630	14/15	0.86	0.21	6.45	48,51,56,57	0
4	ACT	E	1173	4/4	0.74	0.26	4.95	49,51,52,54	0
4	ACT	A	1626	4/4	0.77	0.17	3.90	54,54,55,56	0
3	SO4	A	1620	5/5	0.80	0.21	2.75	88,93,96,97	0
3	SO4	C	1172	5/5	0.81	0.29	2.52	114,114,115,116	0
4	ACT	B	1625	4/4	0.81	0.24	2.19	52,53,53,56	0
6	NAG	E	1175	14/15	0.81	0.34	2.15	55,63,67,67	0
3	SO4	B	1618	5/5	0.95	0.11	1.99	60,62,63,65	0
6	NAG	B	1629	14/15	0.79	0.23	1.52	46,54,57,58	0
3	SO4	A	1623	5/5	0.97	0.11	1.35	28,29,32,32	0
3	SO4	B	1623	5/5	0.97	0.11	0.86	31,32,35,37	0
5	CL	A	1628	1/1	0.99	0.07	0.08	27,27,27,27	0
6	NAG	B	1627	14/15	0.89	0.10	0.04	28,30,35,37	0
3	SO4	B	1620	5/5	0.90	0.16	-0.04	79,83,85,87	0
6	NAG	A	1631	14/15	0.89	0.11	-0.04	30,35,40,44	0
3	SO4	A	1622	5/5	0.91	0.10	-0.20	40,44,51,51	0
3	SO4	A	1618	5/5	0.97	0.08	-0.45	56,57,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	1619	5/5	0.97	0.14	-0.50	46,46,48,48	0
5	CL	B	1626	1/1	0.97	0.06	-0.73	34,34,34,34	0
4	ACT	A	1624	4/4	0.90	0.10	-0.97	64,64,64,64	0
6	NAG	A	1632	14/15	0.78	0.39	-	73,80,82,83	0
6	NAG	E	1174	14/15	0.79	0.28	-	44,50,54,57	0
3	SO4	B	1621	5/5	0.97	0.17	-	49,51,54,54	0
3	SO4	A	1619	5/5	0.85	0.34	-	115,118,120,120	0
6	NAG	A	1629	14/15	0.82	0.26	-	46,53,57,60	0
6	NAG	C	1173	14/15	0.79	0.25	-	53,59,64,64	0
6	NAG	B	1630	14/15	0.78	0.34	-	70,77,81,83	0
4	ACT	A	1625	4/4	0.84	0.24	-	50,50,51,52	0
4	ACT	B	1624	4/4	0.85	0.18	-	60,62,63,65	0
3	SO4	A	1621	5/5	0.98	0.09	-	36,39,43,44	0

6.5 Other polymers

There are no such residues in this entry.