



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:04 PM GMT

PDB ID : 4UTA
Title : Crystal structure of dengue 2 virus envelope glycoprotein in complex with the Fab fragment of the broadly neutralizing human antibody EDE1 C8
Authors : Rouvinski, A.; Guardado-Calvo, P.; Barba-Spaeth, G.; Duquerroy, S.; Vaney, M.C.; Rey, F.A.
Deposited on : 2014-07-18
Resolution : 3.00 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

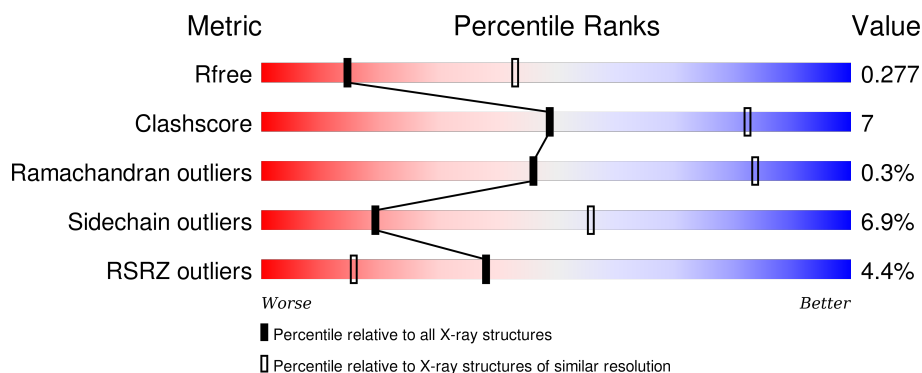
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	425	<div> <div>2%</div> <div>69% 17% • 12%</div> </div>
1	B	425	<div> <div>2%</div> <div>68% 20% • 9%</div> </div>
2	H	272	<div> <div>%</div> <div>68% 13% • 19%</div> </div>
2	I	272	<div> <div>7%</div> <div>68% 9% • 22%</div> </div>
3	L	217	<div> <div>2%</div> <div>81% 17% ••</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M	217	<div><div></div><div>12%</div><div></div><div>79%</div><div></div><div>18%</div><div>..</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12683 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 ENVELOPE GLYCOPROTEIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2898	1831	498	545	24			
1	B	386	Total	C	N	O	S	0	0	0
			3009	1897	520	568	24			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	LEU	-	EXPRESSION TAG	UNP Q68Y26
A	393	ARG	-	EXPRESSION TAG	UNP Q68Y26
A	394	PRO	-	EXPRESSION TAG	UNP Q68Y26
A	395	LEU	-	EXPRESSION TAG	UNP Q68Y26
A	396	GLU	-	EXPRESSION TAG	UNP Q68Y26
A	397	SER	-	EXPRESSION TAG	UNP Q68Y26
A	398	ARG	-	EXPRESSION TAG	UNP Q68Y26
A	399	GLY	-	EXPRESSION TAG	UNP Q68Y26
A	400	PRO	-	EXPRESSION TAG	UNP Q68Y26
A	401	PHE	-	EXPRESSION TAG	UNP Q68Y26
A	402	GLU	-	EXPRESSION TAG	UNP Q68Y26
A	403	GLY	-	EXPRESSION TAG	UNP Q68Y26
A	404	LYS	-	EXPRESSION TAG	UNP Q68Y26
A	405	PRO	-	EXPRESSION TAG	UNP Q68Y26
A	406	ILE	-	EXPRESSION TAG	UNP Q68Y26
A	407	PRO	-	EXPRESSION TAG	UNP Q68Y26
A	408	ASN	-	EXPRESSION TAG	UNP Q68Y26
A	409	PRO	-	EXPRESSION TAG	UNP Q68Y26
A	410	LEU	-	EXPRESSION TAG	UNP Q68Y26
A	411	LEU	-	EXPRESSION TAG	UNP Q68Y26
A	412	GLY	-	EXPRESSION TAG	UNP Q68Y26
A	413	LEU	-	EXPRESSION TAG	UNP Q68Y26
A	414	ASP	-	EXPRESSION TAG	UNP Q68Y26
A	415	SER	-	EXPRESSION TAG	UNP Q68Y26
A	416	THR	-	EXPRESSION TAG	UNP Q68Y26

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	ARG	-	EXPRESSION TAG	UNP Q68Y26
A	418	THR	-	EXPRESSION TAG	UNP Q68Y26
A	419	GLY	-	EXPRESSION TAG	UNP Q68Y26
A	420	HIS	-	EXPRESSION TAG	UNP Q68Y26
A	421	HIS	-	EXPRESSION TAG	UNP Q68Y26
A	422	HIS	-	EXPRESSION TAG	UNP Q68Y26
A	423	HIS	-	EXPRESSION TAG	UNP Q68Y26
A	424	HIS	-	EXPRESSION TAG	UNP Q68Y26
A	425	HIS	-	EXPRESSION TAG	UNP Q68Y26
A	118	LYS	MET	CONFLICT	UNP Q68Y26
B	392	LEU	-	EXPRESSION TAG	UNP Q68Y26
B	393	ARG	-	EXPRESSION TAG	UNP Q68Y26
B	394	PRO	-	EXPRESSION TAG	UNP Q68Y26
B	395	LEU	-	EXPRESSION TAG	UNP Q68Y26
B	396	GLU	-	EXPRESSION TAG	UNP Q68Y26
B	397	SER	-	EXPRESSION TAG	UNP Q68Y26
B	398	ARG	-	EXPRESSION TAG	UNP Q68Y26
B	399	GLY	-	EXPRESSION TAG	UNP Q68Y26
B	400	PRO	-	EXPRESSION TAG	UNP Q68Y26
B	401	PHE	-	EXPRESSION TAG	UNP Q68Y26
B	402	GLU	-	EXPRESSION TAG	UNP Q68Y26
B	403	GLY	-	EXPRESSION TAG	UNP Q68Y26
B	404	LYS	-	EXPRESSION TAG	UNP Q68Y26
B	405	PRO	-	EXPRESSION TAG	UNP Q68Y26
B	406	ILE	-	EXPRESSION TAG	UNP Q68Y26
B	407	PRO	-	EXPRESSION TAG	UNP Q68Y26
B	408	ASN	-	EXPRESSION TAG	UNP Q68Y26
B	409	PRO	-	EXPRESSION TAG	UNP Q68Y26
B	410	LEU	-	EXPRESSION TAG	UNP Q68Y26
B	411	LEU	-	EXPRESSION TAG	UNP Q68Y26
B	412	GLY	-	EXPRESSION TAG	UNP Q68Y26
B	413	LEU	-	EXPRESSION TAG	UNP Q68Y26
B	414	ASP	-	EXPRESSION TAG	UNP Q68Y26
B	415	SER	-	EXPRESSION TAG	UNP Q68Y26
B	416	THR	-	EXPRESSION TAG	UNP Q68Y26
B	417	ARG	-	EXPRESSION TAG	UNP Q68Y26
B	418	THR	-	EXPRESSION TAG	UNP Q68Y26
B	419	GLY	-	EXPRESSION TAG	UNP Q68Y26
B	420	HIS	-	EXPRESSION TAG	UNP Q68Y26
B	421	HIS	-	EXPRESSION TAG	UNP Q68Y26
B	422	HIS	-	EXPRESSION TAG	UNP Q68Y26
B	423	HIS	-	EXPRESSION TAG	UNP Q68Y26

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	424	HIS	-	EXPRESSION TAG	UNP Q68Y26
B	425	HIS	-	EXPRESSION TAG	UNP Q68Y26
B	118	LYS	MET	CONFLICT	UNP Q68Y26

- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1656	1047	271	331	7			
2	I	211	Total	C	N	O	S	0	0	0
			1594	1011	260	316	7			

- Molecule 3 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	1	0
			1675	1054	284	333	4			
3	M	213	Total	C	N	O	S	0	1	0
			1665	1049	282	330	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	18	Total	O	0	0
			18	18		

Continued on next page...

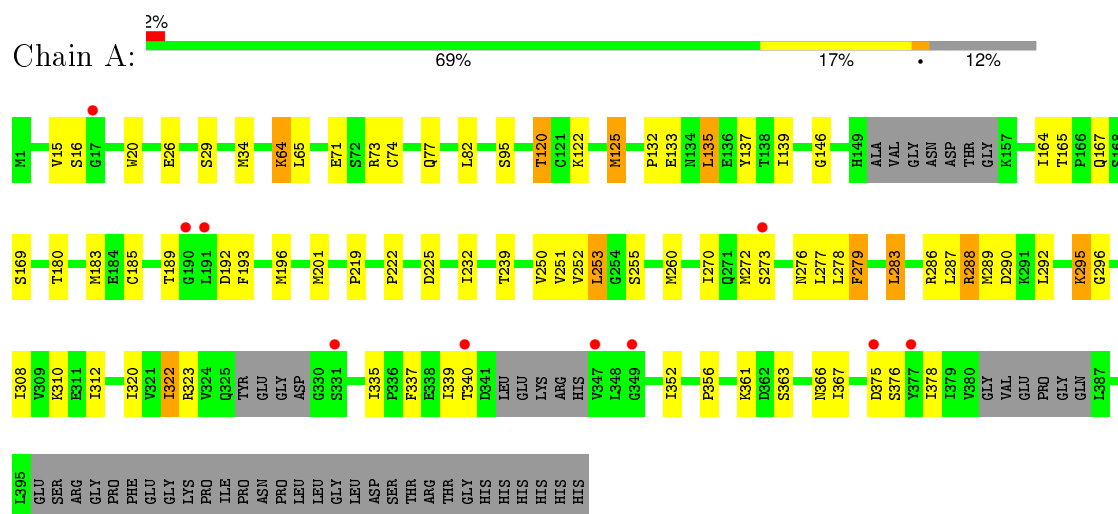
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	10	Total 10	O 10	0	0
6	I	3	Total 3	O 3	0	0
6	L	1	Total 1	O 1	0	0
6	M	3	Total 3	O 3	0	0

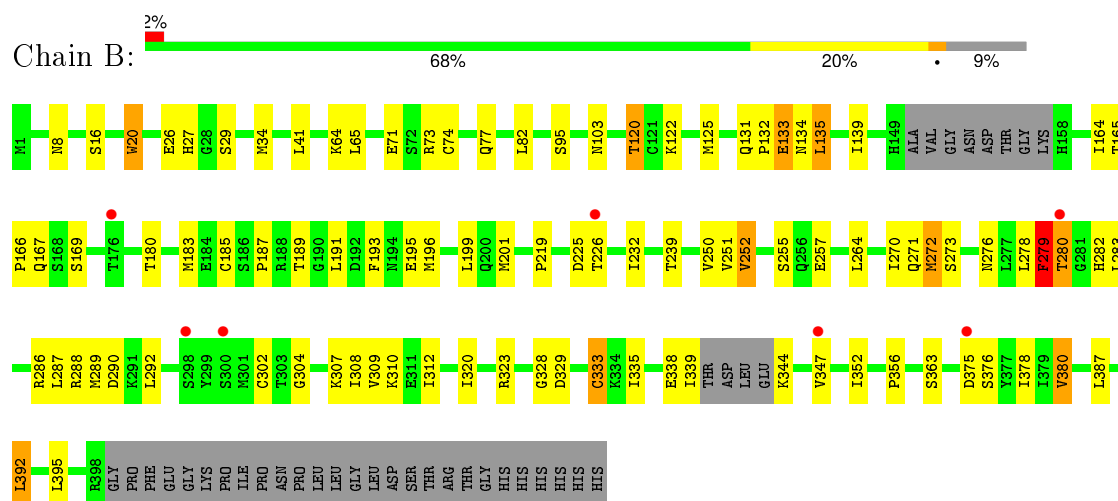
3 Residue-property plots

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: ENVELOPE GLYCOPROTEIN E

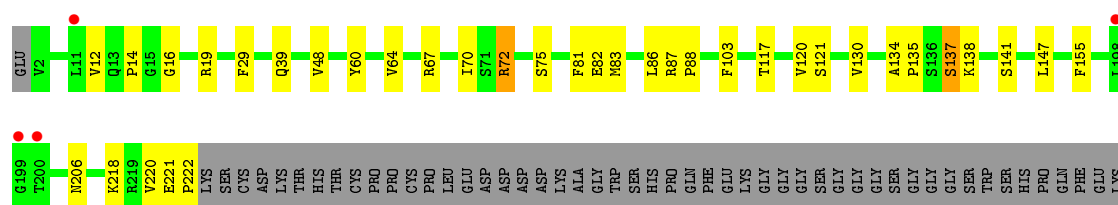


• Molecule 1: ENVELOPE GLYCOPROTEIN E

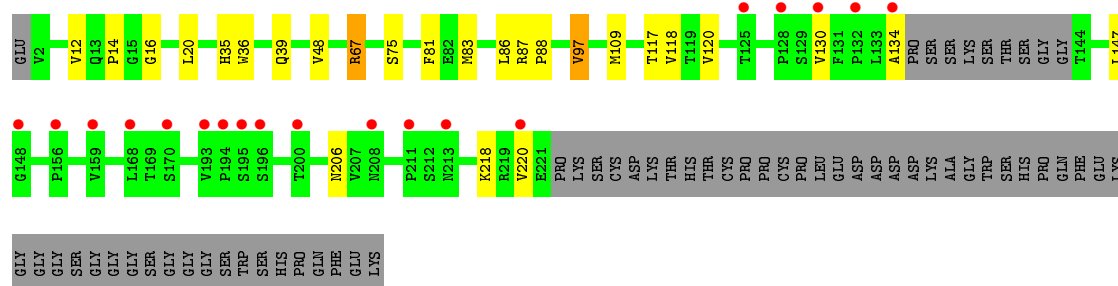


• Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8 HEAVY CHAIN

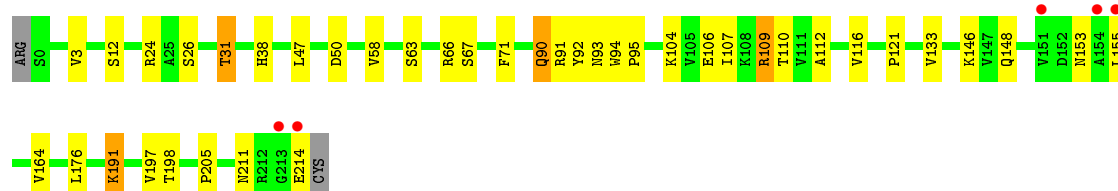
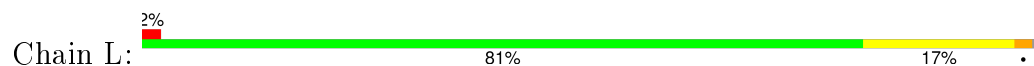




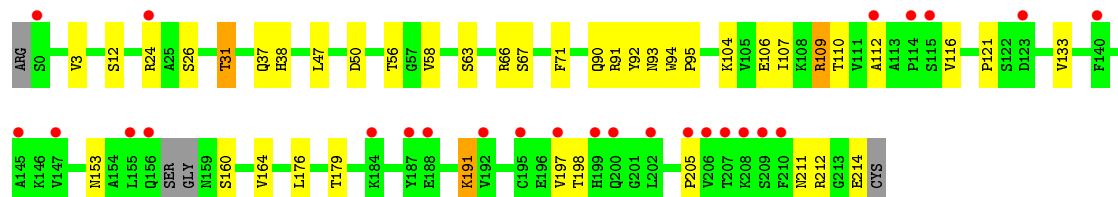
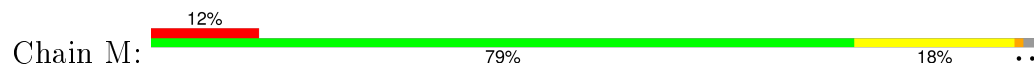
• Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8 HEAVY CHAIN



• Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8 LIGHT CHAIN



• Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8 LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.66Å 191.34Å 203.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.00 29.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.97-3.00) 95.5 (29.75-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.00Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.213 , 0.248 0.234 , 0.277	Depositor DCC
R_{free} test set	2310 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 45584 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12683	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FUC, BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/2952	0.78	1/3984 (0.0%)
1	B	0.60	0/3069	0.81	2/4145 (0.0%)
2	H	0.52	0/1699	0.73	0/2316
2	I	0.46	0/1634	0.72	0/2226
3	L	0.47	0/1719	0.72	0/2340
3	M	0.43	0/1708	0.70	0/2324
All	All	0.52	0/12781	0.76	3/17335 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	225	ASP	C-N-CA	6.05	136.82	121.70
1	B	279	PHE	C-N-CA	5.69	135.92	121.70
1	A	279	PHE	C-N-CA	5.26	134.84	121.70

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	2898	0	2907	45	0
1	B	3009	0	3012	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1656	0	1589	24	0
2	I	1594	0	1528	18	0
3	L	1675	0	1630	26	0
3	M	1665	0	1621	26	0
4	A	49	0	43	0	0
5	B	71	0	61	1	0
6	A	31	0	0	0	0
6	B	18	0	0	0	0
6	H	10	0	0	0	0
6	I	3	0	0	0	0
6	L	1	0	0	0	0
6	M	3	0	0	0	0
All	All	12683	0	12391	181	0

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 7.

All (181) 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:A:295:LYS:C	1:A:296:GLY:HA3	1.74	1.08
1:B:310:LYS:HE2	3:M:31:THR:HG21	1.34	1.07
3:L:164:VAL:HG22	3:L:176:LEU:CD1	1.97	0.94
1:B:392:LEU:HG	1:B:392:LEU:O	1.68	0.93
1:A:312:ILE:HD11	1:A:320:ILE:HD13	1.51	0.91
1:B:312:ILE:HD11	1:B:320:ILE:HD13	1.54	0.90
1:A:169:SER:HB2	1:A:185:CYS:O	1.73	0.88
3:M:164:VAL:HG22	3:M:176:LEU:CD1	2.04	0.86
2:H:48:VAL:HG13	2:H:64:VAL:HG21	1.58	0.85
1:B:169:SER:HB2	1:B:185:CYS:O	1.76	0.84
3:L:164:VAL:HG22	3:L:176:LEU:HD12	1.57	0.84
1:A:337:PHE:CE2	1:A:339:ILE:HD11	2.14	0.83
3:M:164:VAL:HG22	3:M:176:LEU:HD12	1.63	0.81
1:B:304:GLY:HA3	1:B:328:GLY:HA3	1.66	0.77
1:B:380:VAL:HG13	1:B:387:LEU:HB2	1.65	0.77
1:B:191:LEU:HD21	1:B:280:THR:CG2	2.17	0.75
1:A:133:GLU:HB3	1:A:167:GLN:HG3	1.68	0.74
3:L:164:VAL:HG22	3:L:176:LEU:HD13	1.71	0.72
1:A:277:LEU:HB3	1:A:279:PHE:CE1	2.25	0.71
2:I:39:GLN:HE22	3:M:38:HIS:HE1	1.37	0.70
2:I:35:HIS:HB2	2:I:97:VAL:HG22	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:CYS:N	1:B:333:CYS:SG	2.67	0.69
3:M:164:VAL:HG22	3:M:176:LEU:HD13	1.76	0.68
2:I:67:ARG:HH12	2:I:87:ARG:NE	1.91	0.68
2:H:19:ARG:HB2	2:H:82:GLU:OE1	1.93	0.68
2:H:39:GLN:HE22	3:L:38:HIS:HE1	1.38	0.68
1:B:191:LEU:HD11	1:B:280:THR:HG23	1.76	0.67
1:A:185:CYS:HB3	1:A:283:LEU:HD22	1.75	0.67
3:L:116:VAL:HG21	3:L:197[A]:VAL:HG21	1.78	0.65
3:M:116:VAL:HG21	3:M:197[A]:VAL:HG21	1.78	0.63
3:M:90:GLN:HG2	3:M:92:TYR:H	1.63	0.63
1:A:339:ILE:HD12	1:A:378:ILE:HG12	1.81	0.63
3:L:90:GLN:HG2	3:L:92:TYR:H	1.64	0.62
1:A:64:LYS:HB3	1:A:122:LYS:HD2	1.80	0.62
1:B:64:LYS:HB3	1:B:122:LYS:HD2	1.81	0.62
2:H:121:SER:HB3	2:H:155:PHE:HZ	1.65	0.61
1:B:191:LEU:HD21	1:B:280:THR:HG23	1.82	0.60
1:A:310:LYS:HE3	3:L:31:THR:HG21	1.83	0.60
2:I:67:ARG:HH12	2:I:87:ARG:CD	2.14	0.60
3:M:211:ASN:O	3:M:214:GLU:HG2	2.02	0.59
1:B:133:GLU:HB2	1:B:167:GLN:HG3	1.83	0.59
1:A:286:ARG:HD3	1:A:288:ARG:HH21	1.66	0.59
3:L:164:VAL:CG2	3:L:176:LEU:CD1	2.78	0.59
3:L:191:LYS:HE2	3:L:211:ASN:HB3	1.84	0.59
1:B:189:THR:HG23	1:B:282:HIS:H	1.69	0.58
1:B:191:LEU:HB3	1:B:193:PHE:CE1	2.38	0.57
1:A:239:THR:HB	1:A:251:VAL:HG13	1.85	0.57
1:B:335:ILE:HD12	1:B:356:PRO:HB2	1.86	0.57
1:B:289:MET:HG2	1:B:292:LEU:HD12	1.86	0.57
5:B:569:NAG:O3	5:B:572:MAN:H2	2.05	0.57
1:B:34:MET:HE3	1:B:352:ILE:HA	1.87	0.57
1:A:335:ILE:HD12	1:A:356:PRO:HB2	1.87	0.56
3:M:3:VAL:HG22	3:M:26:SER:HB3	1.86	0.56
1:A:289:MET:HG2	1:A:292:LEU:HD12	1.86	0.56
1:B:339:ILE:HD12	1:B:378:ILE:HG13	1.87	0.56
2:H:147:LEU:HD13	2:H:220:VAL:HB	1.86	0.56
2:I:83:MET:HE1	2:I:118:VAL:HG21	1.87	0.56
2:H:121:SER:HB3	2:H:155:PHE:CZ	2.40	0.56
3:L:3:VAL:HG22	3:L:26:SER:HB3	1.88	0.56
3:L:121:PRO:HD3	3:L:133:VAL:HG22	1.88	0.56
1:B:71:GLU:HB2	1:B:82:LEU:HD21	1.87	0.55
2:I:147:LEU:HD13	2:I:220:VAL:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:SER:HB3	1:B:278:LEU:HD12	1.87	0.55
1:B:26:GLU:HG3	1:B:29:SER:HB3	1.90	0.54
1:B:191:LEU:HD21	1:B:280:THR:HG21	1.87	0.54
1:B:201:MET:HE1	1:B:257:GLU:HG3	1.89	0.54
3:L:164:VAL:CG2	3:L:176:LEU:HD12	2.33	0.53
1:A:71:GLU:HB2	1:A:82:LEU:HD21	1.91	0.53
1:B:191:LEU:HB3	1:B:193:PHE:HE1	1.73	0.53
3:M:66:ARG:HG2	3:M:67:SER:N	2.22	0.53
3:M:121:PRO:HD3	3:M:133:VAL:HG22	1.90	0.53
1:B:239:THR:HB	1:B:251:VAL:HG13	1.90	0.53
3:L:66:ARG:HG2	3:L:67:SER:N	2.23	0.53
1:B:271:GLN:H	1:B:279:PHE:HB2	1.74	0.53
1:A:310:LYS:HE3	3:L:31:THR:CG2	2.38	0.52
2:I:12:VAL:HG11	2:I:86:LEU:HD13	1.91	0.52
2:H:137:SER:HB3	2:H:222:PRO:HB3	1.92	0.52
2:H:14:PRO:C	2:H:16:GLY:H	2.13	0.52
3:M:47:LEU:HA	3:M:58:VAL:HG21	1.92	0.52
1:A:337:PHE:CZ	1:A:339:ILE:HD11	2.45	0.52
2:I:83:MET:HE3	2:I:118:VAL:HG11	1.92	0.51
1:A:74:CYS:HB2	1:A:77:GLN:HG3	1.91	0.51
1:B:65:LEU:HD13	1:B:250:VAL:HG22	1.93	0.51
1:A:133:GLU:HB3	1:A:167:GLN:CG	2.39	0.51
1:A:255:SER:HB3	1:B:255:SER:HB3	1.93	0.51
2:I:20:LEU:HD11	2:I:83:MET:CE	2.41	0.51
1:A:125:MET:HB3	1:A:201:MET:HG3	1.93	0.51
2:H:130:VAL:HG12	2:H:218:LYS:HG3	1.93	0.51
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.92	0.50
2:I:67:ARG:HH12	2:I:87:ARG:HE	1.59	0.50
3:M:191:LYS:HE2	3:M:211:ASN:HB3	1.94	0.50
1:B:166:PRO:HB3	1:B:187:PRO:HB3	1.93	0.50
2:I:109:MET:HE1	3:M:56:THR:H	1.76	0.49
1:A:137:TYR:HB2	1:A:164:ILE:HG13	1.95	0.49
3:M:212:ARG:HG2	3:M:212:ARG:O	2.11	0.49
3:L:106:GLU:HG2	3:L:107:ILE:N	2.28	0.49
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.95	0.49
1:B:27:HIS:CE1	1:B:278:LEU:HD22	2.47	0.49
1:B:139:ILE:HD11	1:B:283:LEU:HD23	1.95	0.49
1:A:295:LYS:C	1:A:296:GLY:CA	2.66	0.48
1:A:34:MET:HE3	1:A:352:ILE:HA	1.95	0.48
2:H:39:GLN:HE22	3:L:38:HIS:CE1	2.26	0.48
2:H:134:ALA:HA	2:H:220:VAL:HG12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:164:VAL:CG2	3:M:176:LEU:CD1	2.86	0.48
1:B:132:PRO:O	1:B:135:LEU:HB2	2.13	0.47
2:I:134:ALA:HA	2:I:220:VAL:HG12	1.95	0.47
1:A:65:LEU:HD13	1:A:250:VAL:HG22	1.97	0.47
1:B:125:MET:HB3	1:B:201:MET:HG3	1.97	0.47
3:M:198:THR:HG22	3:M:205:PRO:HG3	1.97	0.47
2:I:14:PRO:C	2:I:16:GLY:H	2.18	0.47
3:L:198:THR:HG22	3:L:205:PRO:HG3	1.95	0.47
3:L:66:ARG:HG3	3:L:71:PHE:CE2	2.49	0.47
1:B:73:ARG:HA	3:L:93:ASN:HD21	1.79	0.47
1:A:277:LEU:CB	1:A:279:PHE:CE1	2.97	0.46
1:B:133:GLU:CB	1:B:167:GLN:HG3	2.46	0.46
3:M:37:GLN:HB2	3:M:47:LEU:HD11	1.97	0.46
3:M:94:TRP:CD1	3:M:95:PRO:HD2	2.51	0.46
1:A:73:ARG:HA	3:M:93:ASN:HD21	1.80	0.46
1:A:146:GLY:HA2	1:A:366:ASN:O	2.16	0.46
2:H:135:PRO:HG3	2:H:147:LEU:CD2	2.46	0.46
3:L:94:TRP:CD1	3:L:95:PRO:HD2	2.50	0.46
3:L:191:LYS:CE	3:L:211:ASN:HB3	2.44	0.46
1:A:26:GLU:HG3	1:A:29:SER:HB3	1.98	0.46
2:H:12:VAL:HG13	2:H:120:VAL:HG13	1.98	0.46
1:A:273:SER:H	1:A:278:LEU:HD13	1.80	0.45
1:A:132:PRO:O	1:A:135:LEU:HB2	2.16	0.45
3:M:164:VAL:CG2	3:M:176:LEU:HD12	2.40	0.45
1:B:219:PRO:HA	1:B:232:ILE:O	2.16	0.45
1:A:286:ARG:HD3	1:A:288:ARG:NH2	2.30	0.45
2:H:135:PRO:HG3	2:H:147:LEU:HD23	1.98	0.45
1:B:74:CYS:HB2	1:B:77:GLN:HG3	1.98	0.45
1:A:20:TRP:HA	1:A:287:LEU:O	2.17	0.45
2:I:130:VAL:HG12	2:I:218:LYS:HG3	1.99	0.45
3:M:106:GLU:HG2	3:M:107:ILE:N	2.31	0.45
1:A:64:LYS:HG2	1:A:120:THR:HB	1.97	0.44
1:A:201:MET:CE	1:A:260:MET:HB3	2.47	0.44
1:B:309:VAL:HG22	1:B:323:ARG:O	2.17	0.44
1:B:304:GLY:HA3	1:B:328:GLY:CA	2.44	0.44
1:B:286:ARG:HD3	1:B:288:ARG:HH22	1.82	0.44
2:H:48:VAL:HG13	2:H:64:VAL:CG2	2.36	0.44
1:B:41:LEU:HD11	1:B:292:LEU:HD11	2.00	0.44
1:A:337:PHE:HE2	1:A:339:ILE:HD11	1.74	0.44
2:H:121:SER:CB	2:H:155:PHE:HZ	2.30	0.43
3:L:146:LYS:HB2	3:L:198:THR:OG1	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:HIS:HE1	1:B:278:LEU:HD22	1.82	0.43
2:I:36:TRP:O	2:I:48:VAL:HG22	2.18	0.43
1:B:131:GLN:HB2	1:B:134:ASN:HD22	1.82	0.43
2:H:135:PRO:HD2	2:H:221:GLU:C	2.39	0.43
2:H:121:SER:CB	2:H:155:PHE:CZ	3.01	0.43
1:A:132:PRO:HG3	1:A:193:PHE:HB2	2.00	0.43
1:B:309:VAL:HG23	1:B:323:ARG:HB3	2.00	0.43
1:A:253:LEU:HD22	1:A:253:LEU:HA	1.87	0.43
1:A:322:ILE:HD12	1:A:367:ILE:O	2.19	0.43
3:L:109:ARG:HH21	3:L:112:ALA:HB2	1.84	0.43
1:A:272:MET:HA	1:A:276:ASN:O	2.19	0.43
1:B:65:LEU:HD12	1:B:252:VAL:HG22	2.01	0.42
2:H:88:PRO:HA	2:H:120:VAL:HB	2.01	0.42
3:M:66:ARG:HG3	3:M:71:PHE:CE2	2.54	0.42
2:I:12:VAL:HG13	2:I:120:VAL:HG13	2.02	0.42
1:B:272:MET:HA	1:B:276:ASN:O	2.20	0.42
1:B:64:LYS:HG2	1:B:120:THR:HB	2.01	0.42
2:H:138:LYS:HG2	2:H:138:LYS:H	1.60	0.42
3:M:109:ARG:HH21	3:M:112:ALA:HB2	1.84	0.42
3:L:148:GLN:HB3	3:L:155:LEU:CD1	2.50	0.41
1:B:132:PRO:HG3	1:B:193:PHE:HB2	2.02	0.41
2:I:88:PRO:HA	2:I:120:VAL:HB	2.02	0.41
1:A:219:PRO:HA	1:A:232:ILE:O	2.20	0.41
1:B:20:TRP:HA	1:B:287:LEU:O	2.20	0.41
3:L:90:GLN:HE21	3:L:90:GLN:HB3	1.64	0.41
1:B:199:LEU:HD23	1:B:264:LEU:HD21	2.03	0.41
1:B:103:ASN:HB2	2:H:103:PHE:CD2	2.54	0.41
1:B:309:VAL:HG22	1:B:323:ARG:C	2.40	0.41
1:B:8:ASN:ND2	1:B:29:SER:HB2	2.36	0.41
2:H:29:PHE:O	2:H:72:ARG:NH2	2.54	0.41
1:A:222:PRO:HD2	1:A:225:ASP:HB3	2.03	0.41
1:A:339:ILE:HD12	1:A:378:ILE:CG1	2.48	0.40
1:A:139:ILE:HD11	1:A:283:LEU:HD13	2.03	0.40
3:M:160:SER:HA	3:M:179:THR:O	2.20	0.40
2:H:60:TYR:CE1	2:H:70:ILE:HG22	2.56	0.40
1:A:277:LEU:CB	1:A:279:PHE:HE1	2.34	0.40
2:I:39:GLN:HE22	3:M:38:HIS:CE1	2.27	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	361/425 (85%)	339 (94%)	21 (6%)	1 (0%)	46	84
1	B	380/425 (89%)	359 (94%)	18 (5%)	3 (1%)	24	66
2	H	219/272 (80%)	205 (94%)	14 (6%)	0	100	100
2	I	207/272 (76%)	194 (94%)	13 (6%)	0	100	100
3	L	214/217 (99%)	207 (97%)	7 (3%)	0	100	100
3	M	210/217 (97%)	201 (96%)	9 (4%)	0	100	100
All	All	1591/1828 (87%)	1505 (95%)	82 (5%)	4 (0%)	46	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	226	THR
1	B	280	THR
1	B	16	SER
1	A	16	SER

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	325/369 (88%)	298 (92%)	27 (8%)	14	46
1	B	337/369 (91%)	308 (91%)	29 (9%)	13	44
2	H	186/226 (82%)	176 (95%)	10 (5%)	27	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	178/226 (79%)	172 (97%)	6 (3%)	44	81
3	L	189/190 (100%)	176 (93%)	13 (7%)	19	56
3	M	188/190 (99%)	177 (94%)	11 (6%)	24	63
All	All	1403/1570 (89%)	1307 (93%)	96 (7%)	19	56

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	64	LYS
1	A	95	SER
1	A	120	THR
1	A	125	MET
1	A	135	LEU
1	A	165	THR
1	A	180	THR
1	A	183	MET
1	A	189	THR
1	A	192	ASP
1	A	196	MET
1	A	252	VAL
1	A	253	LEU
1	A	270	ILE
1	A	283	LEU
1	A	288	ARG
1	A	290	ASP
1	A	295	LYS
1	A	308	ILE
1	A	322	ILE
1	A	323	ARG
1	A	340	THR
1	A	361	LYS
1	A	363	SER
1	A	375	ASP
1	A	376	SER
1	B	20	TRP
1	B	95	SER
1	B	120	THR
1	B	133	GLU
1	B	135	LEU
1	B	164	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	165	THR
1	B	180	THR
1	B	183	MET
1	B	195	GLU
1	B	196	MET
1	B	252	VAL
1	B	270	ILE
1	B	272	MET
1	B	279	PHE
1	B	290	ASP
1	B	307	LYS
1	B	308	ILE
1	B	329	ASP
1	B	333	CYS
1	B	338	GLU
1	B	344	LYS
1	B	347	VAL
1	B	363	SER
1	B	375	ASP
1	B	376	SER
1	B	380	VAL
1	B	392	LEU
1	B	395	LEU
2	H	67	ARG
2	H	72	ARG
2	H	75	SER
2	H	81	PHE
2	H	83	MET
2	H	87	ARG
2	H	117	THR
2	H	137	SER
2	H	141	SER
2	H	206	ASN
2	I	67	ARG
2	I	75	SER
2	I	81	PHE
2	I	97	VAL
2	I	117	THR
2	I	206	ASN
3	L	12	SER
3	L	24	ARG
3	L	31	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	50	ASP
3	L	63	SER
3	L	90	GLN
3	L	91	ARG
3	L	104	LYS
3	L	109	ARG
3	L	110	THR
3	L	153	ASN
3	L	191	LYS
3	L	214	GLU
3	M	12	SER
3	M	24	ARG
3	M	31	THR
3	M	50	ASP
3	M	63	SER
3	M	91	ARG
3	M	104	LYS
3	M	109	ARG
3	M	110	THR
3	M	153	ASN
3	M	191	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	134	ASN
1	A	158	HIS
1	A	200	GLN
1	B	27	HIS
1	B	124	ASN
1	B	134	ASN
1	B	386	GLN
3	L	38	HIS
3	L	90	GLN
3	M	38	HIS

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 ⓘ

10 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	A	567	1,4	14,14,15	0.42	0	15,19,21	1.01	1 (6%)
4	FUC	A	568	4	10,10,11	0.50	0	14,14,16	1.66	2 (14%)
4	NAG	A	569	4	14,14,15	0.32	0	15,19,21	0.97	1 (6%)
4	BMA	A	570	4	11,11,12	0.28	0	14,15,17	0.70	1 (7%)
5	NAG	B	567	1,5	14,14,15	0.39	0	15,19,21	0.92	0
5	FUC	B	568	5	10,10,11	0.54	0	14,14,16	1.68	3 (21%)
5	NAG	B	569	5	14,14,15	0.34	0	15,19,21	1.09	1 (6%)
5	BMA	B	570	5	11,11,12	0.31	0	14,15,17	0.82	1 (7%)
5	MAN	B	571	5	11,11,12	0.53	0	14,15,17	1.40	2 (14%)
5	MAN	B	572	5	11,11,12	0.49	0	14,15,17	1.61	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	567	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	568	4	-	0/0/17/20	0/1/1/1
4	NAG	A	569	4	-	0/6/23/26	0/1/1/1
4	BMA	A	570	4	-	0/2/19/22	0/1/1/1
5	NAG	B	567	1,5	-	0/6/23/26	0/1/1/1
5	FUC	B	568	5	-	0/0/17/20	0/1/1/1
5	NAG	B	569	5	-	0/6/23/26	0/1/1/1
5	BMA	B	570	5	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	B	571	5	-	0/2/19/22	0/1/1/1
5	MAN	B	572	5	-	0/2/19/22	1/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	567	NAG	C1-O5-C5	-2.33	109.29	112.25
5	B	571	MAN	C1-C2-C3	2.00	111.91	109.54
4	A	570	BMA	C1-O5-C5	2.10	114.91	112.25
5	B	572	MAN	C1-C2-C3	2.15	112.09	109.54
5	B	570	BMA	C1-O5-C5	2.43	115.33	112.25
4	A	568	FUC	C1-O5-C5	2.84	116.76	112.38
5	B	568	FUC	C1-C2-C3	3.07	113.17	109.54
5	B	568	FUC	C1-O5-C5	3.21	117.34	112.38
5	B	568	FUC	C3-C4-C5	3.29	115.26	109.72
4	A	569	NAG	C1-O5-C5	3.49	116.68	112.25
5	B	569	NAG	C1-O5-C5	3.65	116.88	112.25
4	A	568	FUC	C3-C4-C5	4.11	116.65	109.72
5	B	571	MAN	C1-O5-C5	4.15	117.52	112.25
5	B	572	MAN	C1-O5-C5	5.24	118.90	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	572	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	569	NAG	1	0
5	B	572	MAN	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	373/425 (87%)	-0.05	10 (2%) 58 28	42, 74, 130, 141	0
1	B	386/425 (90%)	-0.22	7 (1%) 71 43	36, 69, 121, 131	0
2	H	221/272 (81%)	0.04	4 (1%) 71 43	39, 83, 119, 138	0
2	I	211/272 (77%)	0.49	19 (9%) 12 4	45, 105, 152, 160	0
3	L	215/217 (99%)	-0.08	5 (2%) 64 33	50, 73, 118, 155	0
3	M	213/217 (98%)	0.64	26 (12%) 5 2	58, 117, 164, 175	0
All	All	1619/1828 (88%)	0.08	71 (4%) 38 16	36, 85, 142, 175	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	187	TYR	5.1
3	M	206	VAL	4.9
2	I	200	THR	4.8
3	M	209	SER	4.8
3	M	197[A]	VAL	4.2
3	M	207	THR	3.9
1	A	191	LEU	3.8
3	M	0	SER	3.8
1	A	347	VAL	3.7
2	I	196	SER	3.6
3	M	115	SER	3.6
2	I	168	LEU	3.5
3	M	208	LYS	3.4
2	I	193	VAL	3.4
2	I	125	THR	3.3
3	M	205	PRO	3.2
1	A	331	SER	3.2
2	I	195	SER	3.2
2	I	156	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	154	ALA	3.2
2	I	194	PRO	3.1
3	M	156	GLN	3.0
1	A	375	ASP	3.0
1	A	377	TYR	2.9
1	B	300	SER	2.9
3	M	210	PHE	2.8
2	I	134	ALA	2.8
2	I	213	ASN	2.8
3	M	192	VAL	2.6
3	M	184	LYS	2.6
3	M	114	PRO	2.5
3	L	155	LEU	2.5
2	H	11	LEU	2.5
2	I	132	PRO	2.4
3	M	112	ALA	2.4
3	M	155	LEU	2.4
3	L	151	VAL	2.4
1	A	340	THR	2.3
3	M	202	LEU	2.3
3	L	213	GLY	2.3
1	B	280	THR	2.3
2	I	148	GLY	2.2
2	I	170	SER	2.2
2	I	208	ASN	2.2
2	H	199	GLY	2.2
3	M	188	GLU	2.2
3	M	199	HIS	2.2
3	M	24	ARG	2.2
1	A	190	GLY	2.2
3	L	214	GLU	2.1
3	M	145	ALA	2.1
3	M	195	CYS	2.1
1	B	226	THR	2.1
2	H	200	THR	2.1
3	M	140	PHE	2.1
3	M	200	GLN	2.1
3	M	123	ASP	2.1
2	H	198	LEU	2.1
2	I	130	VAL	2.1
1	B	298	SER	2.1
1	A	349	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	220	VAL	2.1
1	A	273	SER	2.0
1	B	176	THR	2.0
2	I	159	VAL	2.0
2	I	211	PRO	2.0
1	A	17	GLY	2.0
2	I	128	PRO	2.0
1	B	375	ASP	2.0
3	M	147	VAL	2.0
1	B	347	VAL	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](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	567	14/15	0.92	0.18	0.03	96,102,108,114	0
5	NAG	B	567	14/15	0.94	0.16	-0.41	75,81,88,92	0
5	MAN	B	571	11/12	0.93	0.41	-	123,129,131,132	0
5	MAN	B	572	11/12	0.70	0.28	-	151,154,156,157	0
5	FUC	B	568	10/11	0.94	0.20	-	82,87,89,89	0
4	FUC	A	568	10/11	0.82	0.27	-	111,112,116,119	0
4	NAG	A	569	14/15	0.86	0.29	-	121,124,127,128	0
4	BMA	A	570	11/12	0.84	0.28	-	122,129,130,131	0
5	BMA	B	570	11/12	0.82	0.31	-	122,129,137,143	0
5	NAG	B	569	14/15	0.86	0.28	-	90,103,107,115	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.