



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:57 AM BST

PDB ID : 3S88
Title : Crystal structure of Sudan Ebolavirus Glycoprotein (strain Gulu) bound to 16F6
Authors : Sapphire, E.O.; Dias, J.M.; Bale, S.
Deposited on : 2011-05-27
Resolution : 3.35 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 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

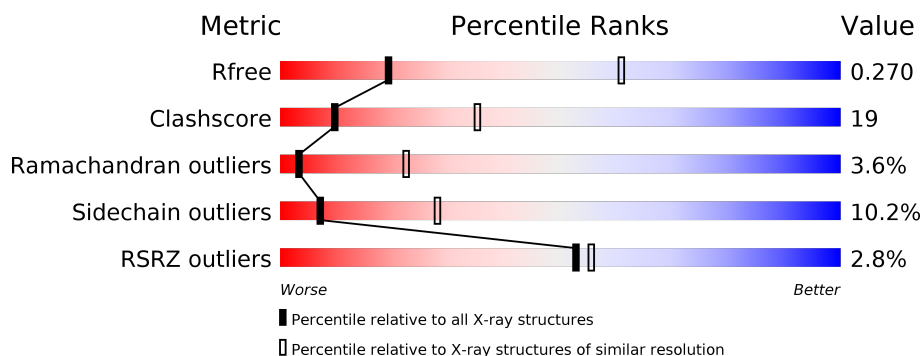
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	H	220	<div> <div></div> <div>64% 30% 5%</div> </div>
2	I	298	<div> <div>5%</div> <div>52% 28% 16%</div> </div>
3	J	167	<div> <div>2%</div> <div>35% 24% 37%</div> </div>
4	L	212	<div> <div>%</div> <div>63% 33%</div> </div>
5	A	2	<div> <div></div> <div>100%</div> </div>
5	B	2	<div> <div></div> <div>100%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6040 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 16F6 - Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	0	0
			1660	1055	273	324	8			

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	249	Total	C	N	O	S	0	0	0
			1859	1180	318	355	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	16	TYR	-	expression tag	UNP Q7T9D9
I	17	PRO	-	expression tag	UNP Q7T9D9
I	18	TYR	-	expression tag	UNP Q7T9D9
I	19	ASP	-	expression tag	UNP Q7T9D9
I	20	VAL	-	expression tag	UNP Q7T9D9
I	21	PRO	-	expression tag	UNP Q7T9D9
I	22	ASP	-	expression tag	UNP Q7T9D9
I	23	TYR	-	expression tag	UNP Q7T9D9
I	24	ALA	-	expression tag	UNP Q7T9D9
I	25	ILE	-	expression tag	UNP Q7T9D9
I	26	GLU	-	expression tag	UNP Q7T9D9
I	27	GLY	-	expression tag	UNP Q7T9D9
I	28	ARG	-	expression tag	UNP Q7T9D9
I	29	GLY	-	expression tag	UNP Q7T9D9
I	30	ALA	-	expression tag	UNP Q7T9D9
I	31	ARG	-	expression tag	UNP Q7T9D9

- Molecule 3 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	106	Total	C	N	O	S	0	0	0
			817	514	149	148	6			

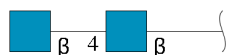
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	631	VAL	ILE	engineered mutation	UNP Q7T9D9
J	638	VAL	GLN	engineered mutation	UNP Q7T9D9

- Molecule 4 is a protein called 16F6 - Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1648	1030	281	330	7			

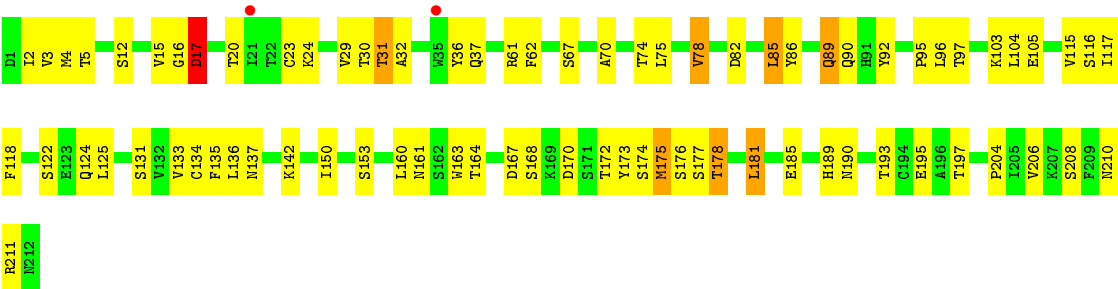
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	B	2	Total	C	N	O	0	0	0
			28	16	2	10			



• Molecule 4: 16F6 - Light chain



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	193.59Å 193.59Å 193.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.63 – 3.35 45.63 – 3.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.63-3.35) 97.2 (45.63-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.222 , 0.278 0.216 , 0.270	Depositor DCC
R_{free} test set	864 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	104.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6040	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	H	0.72	0/1704	0.74	0/2326
2	I	0.56	0/1904	0.68	0/2593
3	J	0.62	0/838	0.70	0/1144
4	L	0.64	0/1687	0.74	0/2295
All	All	0.64	0/6133	0.72	0/8358

There are no bond length outliers.

There are no bond angle outliers.

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	H	1660	0	1615	64	0
2	I	1859	0	1709	70	0
3	J	817	0	756	40	0
4	L	1648	0	1588	68	0
5	A	28	0	25	0	0
5	B	28	0	25	2	0
All	All	6040	0	5718	227	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 19.

All (227) 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:H:88:SER:O	1:H:91:THR:HG22	1.47	1.13
3:J:521:GLN:HA	3:J:522:GLU:HB3	1.20	1.13
3:J:521:GLN:HA	3:J:522:GLU:CB	1.89	1.01
4:L:193:THR:HG22	4:L:208:SER:HB2	1.53	0.89
4:L:20:THR:CG2	4:L:74:THR:HG23	2.09	0.81
4:L:20:THR:HG23	4:L:74:THR:HG23	1.64	0.78
2:I:66:VAL:HG12	2:I:184:LEU:HD11	1.65	0.78
2:I:180:VAL:HG22	3:J:562:ALA:HB1	1.65	0.77
1:H:179:ASP:O	1:H:180:LEU:HD12	1.85	0.77
2:I:185:ILE:C	2:I:186:LEU:HD23	2.05	0.77
2:I:126:PRO:O	2:I:129:VAL:HG12	1.87	0.75
1:H:74:ASN:O	1:H:75:ALA:HB3	1.85	0.74
4:L:195:GLU:HG2	4:L:206:VAL:HG22	1.70	0.73
1:H:40:ASN:HD21	1:H:44:ARG:H	1.37	0.73
4:L:189:HIS:O	4:L:211:ARG:HD3	1.90	0.72
1:H:133:GLY:HA2	1:H:219:ALA:HB2	1.72	0.71
3:J:521:GLN:CA	3:J:522:GLU:HB3	2.11	0.70
1:H:133:GLY:HA2	1:H:219:ALA:CB	2.21	0.70
4:L:193:THR:HG22	4:L:208:SER:CB	2.23	0.68
3:J:573:LEU:O	3:J:576:THR:HG22	1.92	0.68
2:I:222:ILE:HG23	2:I:232:THR:HG22	1.76	0.67
1:H:74:ASN:O	1:H:75:ALA:CB	2.43	0.67
4:L:190:ASN:ND2	4:L:210:ASN:HB3	2.11	0.66
2:I:159:PHE:CZ	3:J:569:LEU:HD12	2.32	0.65
2:I:101:ALA:HB2	3:J:519:THR:HG22	1.78	0.65
3:J:563:ASN:O	3:J:566:THR:HG22	1.98	0.64
1:H:35:PHE:HE2	1:H:99:GLN:HB2	1.61	0.64
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.80	0.64
2:I:71:GLU:HA	2:I:75:VAL:HG22	1.82	0.62
4:L:29:VAL:O	4:L:29:VAL:HG12	1.98	0.62
2:I:217:TYR:O	2:I:218:LEU:HD13	1.99	0.62
2:I:234:PHE:CD1	2:I:253:LEU:HD23	2.34	0.61
2:I:236:ILE:HD12	2:I:257:ASN:HA	1.81	0.61
1:H:40:ASN:C	1:H:40:ASN:HD22	2.03	0.61
4:L:163:TRP:HE1	4:L:175:MET:CE	2.13	0.61
1:H:51:ILE:HB	1:H:70:ILE:HD13	1.82	0.61
2:I:256:LEU:HD13	2:I:256:LEU:C	2.21	0.61
2:I:66:VAL:CG1	2:I:184:LEU:HD11	2.31	0.61
3:J:549:HIS:O	3:J:550:ASN:ND2	2.34	0.60
2:I:96:VAL:HG13	3:J:580:ARG:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:62:PHE:CE1	4:L:75:LEU:HD13	2.36	0.59
2:I:138:VAL:CG2	2:I:217:TYR:CD1	2.85	0.59
1:H:131:ALA:HB2	1:H:216:ILE:CG2	2.34	0.58
2:I:52:VAL:HG13	2:I:53:CYS:O	2.03	0.58
2:I:68:LEU:HD11	3:J:558:LEU:HD12	1.86	0.58
4:L:24:LYS:NZ	4:L:70:ALA:HB2	2.19	0.58
2:I:101:ALA:CB	3:J:519:THR:HG22	2.33	0.58
4:L:161:ASN:HD22	4:L:177:SER:HA	1.68	0.58
1:H:99:GLN:HG2	1:H:100:LEU:O	2.04	0.58
4:L:142:LYS:HB2	4:L:173:TYR:CE2	2.38	0.57
2:I:236:ILE:HG23	2:I:257:ASN:OD1	2.04	0.57
2:I:68:LEU:HD11	3:J:558:LEU:CD1	2.34	0.57
4:L:136:LEU:N	4:L:136:LEU:HD12	2.20	0.57
4:L:29:VAL:HG13	4:L:92:TYR:HB2	1.85	0.57
2:I:162:TYR:CE1	2:I:176:PHE:HB3	2.39	0.57
1:H:177:GLN:NE2	4:L:160:LEU:HD11	2.19	0.57
1:H:40:ASN:ND2	1:H:44:ARG:H	2.02	0.57
4:L:75:LEU:CD2	4:L:78:VAL:HG22	2.35	0.56
1:H:142:VAL:HG22	1:H:143:THR:N	2.20	0.56
1:H:194:ARG:HD2	1:H:195:PRO:HA	1.88	0.56
2:I:184:LEU:N	2:I:184:LEU:HD12	2.21	0.56
2:I:52:VAL:O	2:I:55:ASP:OD1	2.23	0.56
2:I:79:ILE:HG21	2:I:220:TYR:CE1	2.41	0.56
1:H:176:LEU:HD13	1:H:181:TYR:CD1	2.40	0.55
4:L:75:LEU:HD23	4:L:78:VAL:HG22	1.87	0.55
3:J:583:THR:O	3:J:583:THR:HG22	2.06	0.55
5:B:1:NAG:O4	5:B:2:NAG:H83	2.07	0.55
2:I:138:VAL:HG21	2:I:217:TYR:CD1	2.41	0.55
2:I:97:VAL:HG12	3:J:581:THR:HB	1.88	0.55
3:J:561:LEU:O	3:J:565:THR:HG23	2.05	0.55
2:I:103:GLU:O	2:I:104:TRP:C	2.44	0.54
2:I:131:GLY:HA2	2:I:174:VAL:HG12	1.89	0.54
4:L:15:VAL:HG13	4:L:15:VAL:O	2.06	0.54
2:I:234:PHE:CG	2:I:253:LEU:HD23	2.42	0.54
2:I:154:HIS:NE2	2:I:178:GLU:OE1	2.30	0.54
4:L:181:LEU:N	4:L:181:LEU:HD12	2.22	0.54
4:L:30:THR:OG1	4:L:31:THR:N	2.39	0.54
4:L:20:THR:HG22	4:L:74:THR:HG23	1.87	0.54
1:H:131:ALA:HB2	1:H:216:ILE:HG22	1.90	0.54
2:I:79:ILE:O	2:I:83:THR:OG1	2.25	0.54
2:I:144:THR:O	2:I:224:ASN:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:ASN:ND2	1:H:165:LEU:HD12	2.23	0.53
4:L:115:VAL:HG22	4:L:136:LEU:HG	1.90	0.53
4:L:16:GLY:O	4:L:17:ASP:O	2.26	0.53
3:J:558:LEU:C	3:J:558:LEU:HD12	2.29	0.53
2:I:127:ASP:O	3:J:580:ARG:NH2	2.42	0.53
4:L:96:LEU:HD22	4:L:96:LEU:H	1.74	0.53
1:H:35:PHE:CE2	1:H:99:GLN:HB2	2.44	0.53
4:L:135:PHE:C	4:L:136:LEU:HD12	2.29	0.53
4:L:163:TRP:HE1	4:L:175:MET:HE2	1.73	0.53
1:H:208:SER:HB3	1:H:210:THR:HG23	1.91	0.52
2:I:110:ASN:HD22	2:I:175:ASN:HD22	1.55	0.52
3:J:529:ILE:HG22	3:J:529:ILE:O	2.10	0.52
3:J:549:HIS:O	3:J:550:ASN:CG	2.48	0.52
3:J:583:THR:HA	3:J:586:ASN:ND2	2.25	0.52
2:I:46:THR:OG1	2:I:47:GLU:N	2.43	0.51
2:I:219:GLU:C	2:I:220:TYR:CD2	2.83	0.51
4:L:197:THR:HG22	4:L:204:PRO:HG3	1.92	0.51
1:H:36:TRP:O	1:H:48:VAL:HG22	2.10	0.51
2:I:186:LEU:HD23	2:I:186:LEU:N	2.25	0.51
2:I:68:LEU:CD1	3:J:559:ARG:HA	2.40	0.51
3:J:550:ASN:OD1	3:J:551:GLN:N	2.44	0.51
1:H:52:ASN:O	1:H:55:GLY:N	2.40	0.51
4:L:124:GLN:HE22	4:L:131:SER:CB	2.25	0.50
4:L:163:TRP:NE1	4:L:175:MET:CE	2.73	0.50
4:L:2:ILE:HD12	4:L:2:ILE:H	1.76	0.50
4:L:117:ILE:HD13	4:L:208:SER:HA	1.93	0.50
4:L:85:LEU:HD11	4:L:103:LYS:HG2	1.93	0.50
2:I:48:ILE:HD12	2:I:49:ASP:H	1.77	0.50
2:I:126:PRO:O	2:I:129:VAL:CG1	2.60	0.49
1:H:40:ASN:C	1:H:40:ASN:ND2	2.66	0.49
1:H:60:TYR:OH	1:H:70:ILE:HG22	2.12	0.49
4:L:4:MET:CE	4:L:23:CYS:SG	3.01	0.49
4:L:36:TYR:OH	4:L:89:GLN:NE2	2.46	0.49
4:L:181:LEU:HD23	4:L:185:GLU:HG2	1.94	0.49
1:H:158:VAL:HG21	1:H:183:LEU:HD11	1.95	0.49
2:I:126:PRO:HD2	2:I:129:VAL:HG11	1.95	0.49
3:J:550:ASN:O	3:J:551:GLN:C	2.51	0.49
4:L:2:ILE:N	4:L:2:ILE:HD12	2.28	0.49
1:H:18:LEU:CD2	1:H:115:LEU:HD23	2.42	0.48
2:I:86:TRP:HB2	2:I:153:PHE:O	2.13	0.48
4:L:82:ASP:O	4:L:86:TYR:OH	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:139:HIS:N	2:I:139:HIS:ND1	2.61	0.48
1:H:193:PRO:O	1:H:194:ARG:CB	2.61	0.48
1:H:151:TYR:OH	1:H:183:LEU:HD23	2.14	0.48
4:L:163:TRP:HE1	4:L:175:MET:HE1	1.79	0.48
4:L:29:VAL:CG1	4:L:29:VAL:O	2.62	0.48
4:L:170:ASP:O	4:L:172:THR:HG23	2.14	0.47
4:L:4:MET:HE3	4:L:23:CYS:SG	2.54	0.47
4:L:24:LYS:HZ3	4:L:70:ALA:HB2	1.78	0.47
1:H:132:PRO:O	1:H:219:ALA:HB3	2.13	0.47
1:H:179:ASP:C	1:H:180:LEU:HD12	2.34	0.47
2:I:65:SER:OG	2:I:100:GLU:HG3	2.14	0.47
1:H:143:THR:C	1:H:144:LEU:HD13	2.34	0.47
2:I:35:LEU:HD12	2:I:183:PHE:O	2.14	0.47
1:H:205:HIS:CE1	1:H:208:SER:HG	2.30	0.47
1:H:172:PHE:CD1	4:L:164:THR:HG23	2.50	0.47
1:H:144:LEU:HB3	1:H:216:ILE:HG21	1.97	0.47
1:H:103:ASN:HD21	3:J:553:ALA:HA	1.79	0.47
4:L:137:ASN:HB3	4:L:174:SER:HB3	1.97	0.47
1:H:161:ASN:HD22	1:H:165:LEU:HD12	1.80	0.46
1:H:176:LEU:HD13	1:H:181:TYR:CE1	2.50	0.46
1:H:149:LYS:HA	1:H:182:THR:HG23	1.95	0.46
4:L:134:CYS:SG	4:L:136:LEU:HD11	2.55	0.46
2:I:138:VAL:CG2	2:I:217:TYR:HD1	2.28	0.46
4:L:163:TRP:NE1	4:L:175:MET:HE2	2.31	0.46
1:H:22:CYS:HB3	1:H:79:LEU:HB3	1.98	0.46
3:J:603:ILE:O	3:J:605:GLY:N	2.49	0.46
1:H:130:LEU:HB3	4:L:118:PHE:CD2	2.52	0.45
1:H:177:GLN:HA	1:H:177:GLN:OE1	2.17	0.45
4:L:95:PRO:O	4:L:97:THR:HG23	2.16	0.45
2:I:256:LEU:HD13	2:I:256:LEU:O	2.16	0.45
3:J:566:THR:HG21	5:B:1:NAG:H82	1.98	0.45
1:H:179:ASP:OD1	1:H:179:ASP:N	2.49	0.45
3:J:517:TYR:CZ	3:J:546:GLY:HA3	2.52	0.45
1:H:183:LEU:HD12	1:H:184:SER:N	2.31	0.45
4:L:2:ILE:CG2	4:L:3:VAL:N	2.80	0.45
1:H:133:GLY:CA	1:H:219:ALA:CB	2.93	0.44
2:I:138:VAL:HG21	2:I:217:TYR:HD1	1.80	0.44
2:I:223:GLU:HA	2:I:224:ASN:OD1	2.16	0.44
4:L:86:TYR:CE2	4:L:104:LEU:HD22	2.52	0.44
2:I:113:ILE:HG22	2:I:121:CYS:SG	2.57	0.44
4:L:29:VAL:CG1	4:L:32:ALA:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:ASN:HD21	1:H:199:VAL:HA	1.82	0.44
2:I:52:VAL:HG22	2:I:53:CYS:N	2.33	0.44
2:I:68:LEU:HD13	3:J:559:ARG:HG2	2.00	0.44
3:J:554:LEU:O	3:J:554:LEU:HD23	2.17	0.44
1:H:107:ASP:N	1:H:107:ASP:OD1	2.44	0.44
4:L:15:VAL:CG1	4:L:15:VAL:O	2.65	0.44
2:I:58:ALA:HB3	2:I:62:GLN:OE1	2.17	0.43
2:I:138:VAL:HG22	2:I:217:TYR:CD1	2.53	0.43
4:L:31:THR:O	4:L:31:THR:OG1	2.33	0.43
1:H:91:THR:HB	1:H:117:VAL:H	1.82	0.43
2:I:110:ASN:HD22	2:I:175:ASN:ND2	2.16	0.43
4:L:150:ILE:HG21	4:L:189:HIS:CD2	2.53	0.43
1:H:132:PRO:O	1:H:219:ALA:CB	2.67	0.43
4:L:122:SER:HA	4:L:125:LEU:HD23	2.01	0.43
4:L:37:GLN:HG3	4:L:86:TYR:CE1	2.53	0.43
3:J:579:LEU:HD12	3:J:579:LEU:H	1.83	0.43
1:H:113:THR:HG23	1:H:113:THR:O	2.18	0.43
2:I:160:PHE:CE1	2:I:170:ILE:HD11	2.54	0.43
4:L:170:ASP:OD1	4:L:172:THR:HG23	2.19	0.43
1:H:136:ALA:O	1:H:137:ALA:HB3	2.18	0.42
1:H:177:GLN:O	1:H:179:ASP:N	2.48	0.42
2:I:102:GLY:HA3	3:J:518:TRP:CZ2	2.53	0.42
4:L:133:VAL:HG22	4:L:178:THR:HB	2.01	0.42
4:L:36:TYR:HE1	4:L:89:GLN:HE21	1.66	0.42
2:I:251:GLN:OE1	2:I:251:GLN:N	2.47	0.42
2:I:57:LEU:C	2:I:57:LEU:HD13	2.39	0.42
3:J:590:ILE:O	3:J:591:ASP:C	2.57	0.42
1:H:156:VAL:HG12	1:H:157:THR:N	2.32	0.42
2:I:284:ASP:O	2:I:285:ILE:CB	2.67	0.42
2:I:117:ASP:N	2:I:117:ASP:OD2	2.50	0.42
3:J:601:CYS:SG	3:J:609:CYS:O	2.78	0.42
1:H:208:SER:O	1:H:210:THR:HG23	2.19	0.42
2:I:93:PRO:HA	2:I:94:PRO:HD3	1.92	0.42
1:H:142:VAL:CG2	1:H:143:THR:N	2.83	0.42
2:I:113:ILE:HD13	2:I:225:PHE:CG	2.55	0.42
3:J:525:ASN:O	3:J:526:ALA:HB3	2.20	0.42
3:J:513:PRO:HB2	3:J:552:ASN:OD1	2.19	0.42
1:H:47:TRP:O	1:H:61:PRO:HG3	2.19	0.42
3:J:569:LEU:HD22	3:J:569:LEU:HA	1.85	0.42
4:L:2:ILE:HG22	4:L:3:VAL:N	2.35	0.42
2:I:189:PRO:CB	2:I:190:LYS:CB	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:ALA:O	1:H:133:GLY:N	2.53	0.41
2:I:217:TYR:N	2:I:217:TYR:CD2	2.88	0.41
2:I:223:GLU:HA	2:I:224:ASN:HA	1.81	0.41
3:J:569:LEU:O	3:J:573:LEU:HD13	2.19	0.41
4:L:190:ASN:HD21	4:L:210:ASN:HB3	1.84	0.41
3:J:554:LEU:C	3:J:554:LEU:HD23	2.40	0.41
4:L:96:LEU:HD22	4:L:96:LEU:N	2.35	0.41
1:H:133:GLY:O	1:H:219:ALA:CB	2.69	0.41
2:I:113:ILE:CG2	2:I:114:LYS:N	2.83	0.41
2:I:47:GLU:O	2:I:48:ILE:C	2.59	0.41
4:L:85:LEU:HD21	4:L:103:LYS:HE2	2.03	0.41
4:L:85:LEU:HD13	4:L:85:LEU:HA	1.91	0.41
3:J:583:THR:O	3:J:583:THR:CG2	2.67	0.41
4:L:4:MET:HE2	4:L:23:CYS:SG	2.61	0.41
1:H:52:ASN:HD22	1:H:56:GLY:H	1.68	0.41
2:I:169:VAL:HG12	2:I:170:ILE:N	2.34	0.41
4:L:161:ASN:HB2	4:L:163:TRP:CH2	2.56	0.41
1:H:113:THR:CG2	1:H:113:THR:O	2.69	0.41
2:I:145:GLY:N	2:I:225:PHE:HZ	2.18	0.40
4:L:16:GLY:O	4:L:17:ASP:C	2.60	0.40
1:H:79:LEU:HD12	1:H:80:PHE:H	1.86	0.40
1:H:68:PHE:N	1:H:68:PHE:CD1	2.89	0.40
1:H:27:PHE:CE1	1:H:29:PHE:HA	2.56	0.40

There are no symmetry-related clashes.

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	H	218/220 (99%)	200 (92%)	11 (5%)	7 (3%)	4	24
2	I	243/298 (82%)	196 (81%)	37 (15%)	10 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	104/167 (62%)	88 (85%)	7 (7%)	9 (9%)	1	5
4	L	210/212 (99%)	191 (91%)	17 (8%)	2 (1%)	15	49
All	All	775/897 (86%)	675 (87%)	72 (9%)	28 (4%)	3	22

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	194	ARG
2	I	225	PHE
2	I	274	ILE
3	J	522	GLU
3	J	604	LEU
3	J	605	GLY
4	L	17	ASP
1	H	75	ALA
2	I	190	LYS
4	L	78	VAL
1	H	18	LEU
1	H	29	PHE
2	I	278	ASP
2	I	285	ILE
3	J	608	CYS
3	J	610	ILE
1	H	53	SER
2	I	41	SER
2	I	53	CYS
2	I	229	HIS
3	J	526	ALA
1	H	30	ASN
2	I	310	ALA
3	J	511	CYS
3	J	527	ALA
1	H	132	PRO
2	I	307	SER
3	J	606	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	183/183 (100%)	166 (91%)	17 (9%)	9	32
2	I	186/256 (73%)	164 (88%)	22 (12%)	5	21
3	J	80/142 (56%)	72 (90%)	8 (10%)	7	29
4	L	187/187 (100%)	169 (90%)	18 (10%)	8	30
All	All	636/768 (83%)	571 (90%)	65 (10%)	7	28

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	20	LEU
1	H	21	SER
1	H	40	ASN
1	H	81	LEU
1	H	88	SER
1	H	98	ARG
1	H	99	GLN
1	H	116	THR
1	H	117	VAL
1	H	144	LEU
1	H	157	THR
1	H	175	VAL
1	H	179	ASP
1	H	188	THR
1	H	197	GLU
1	H	220	ASP
2	I	32	SER
2	I	44	GLU
2	I	48	ILE
2	I	51	LEU
2	I	55	ASP
2	I	61	ASP
2	I	65	SER
2	I	89	ARG
2	I	95	LYS
2	I	122	LEU
2	I	127	ASP
2	I	136	ARG
2	I	139	HIS

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Mol	Chain	Res	Type
2	I	155	LYS
2	I	175	ASN
2	I	184	LEU
2	I	186	LEU
2	I	213	TYR
2	I	218	LEU
2	I	246	ARG
2	I	248	HIS
2	I	254	PHE
3	J	521	GLN
3	J	524	HIS
3	J	545	GLU
3	J	548	MET
3	J	560	GLN
3	J	569	LEU
3	J	601	CYS
3	J	609	CYS
4	L	5	THR
4	L	12	SER
4	L	17	ASP
4	L	31	THR
4	L	61	ARG
4	L	67	SER
4	L	85	LEU
4	L	89	GLN
4	L	90	GLN
4	L	105	GLU
4	L	116	SER
4	L	153	SER
4	L	167	ASP
4	L	168	SER
4	L	175	MET
4	L	176	SER
4	L	178	THR
4	L	181	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	40	ASN
1	H	52	ASN
1	H	161	ASN

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Mol	Chain	Res	Type
2	I	175	ASN
2	I	265	GLN
3	J	586	ASN
4	L	6	GLN
4	L	89	GLN
4	L	124	GLN
4	L	138	ASN
4	L	161	ASN
4	L	189	HIS
4	L	190	ASN
4	L	210	ASN
4	L	212	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](#)

4 monosaccharides 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	$\# Z > 2$
5	NAG	A	1	2,5	14,14,15	0.51	0	17,19,21	0.88	0
5	NAG	A	2	5	14,14,15	0.56	0	17,19,21	0.92	0
5	NAG	B	1	3,5	14,14,15	0.57	0	17,19,21	1.80	4 (23%)
5	NAG	B	2	5	14,14,15	0.48	0	17,19,21	1.82	3 (17%)

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
5	NAG	A	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	O5-C1-C2	-4.56	104.09	111.29
5	B	2	NAG	C4-C3-C2	-3.58	105.77	111.02
5	B	2	NAG	O5-C1-C2	-3.42	105.88	111.29
5	B	2	NAG	C1-O5-C5	3.33	116.70	112.19
5	B	1	NAG	C3-C4-C5	-3.28	104.39	110.24
5	B	1	NAG	O6-C6-C5	-2.69	102.07	111.29
5	B	1	NAG	C2-N2-C7	-2.41	119.48	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2	NAG	C4-C5-C6-O6
5	B	2	NAG	O5-C5-C6-O6
5	B	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2	NAG	1	0
5	B	1	NAG	2	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	220/220 (100%)	-0.21	1 (0%) 91 93	62, 93, 130, 162	0
2	I	249/298 (83%)	0.21	16 (6%) 19 21	81, 144, 248, 271	0
3	J	106/167 (63%)	0.24	3 (2%) 53 55	78, 121, 229, 260	0
4	L	212/212 (100%)	-0.16	2 (0%) 84 87	67, 104, 145, 165	0
All	All	787/897 (87%)	-0.00	22 (2%) 53 55	62, 111, 229, 271	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	287	GLU	5.1
2	I	87	GLY	4.0
1	H	134	SER	3.4
2	I	222	ILE	3.2
2	I	86	TRP	3.2
2	I	226	GLY	3.1
2	I	244	LEU	3.0
2	I	286	GLY	2.9
2	I	285	ILE	2.5
3	J	600	THR	2.5
2	I	221	GLU	2.4
2	I	142	GLN	2.4
2	I	301	LEU	2.4
3	J	524	HIS	2.3
4	L	21	ILE	2.3
2	I	300	GLN	2.2
2	I	112	GLU	2.2
2	I	231	THR	2.2
4	L	35	TRP	2.2
2	I	284	ASP	2.0
3	J	525	ASN	2.0
2	I	267	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](#)

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
5	NAG	A	2	14/15	0.77	0.39	202,206,212,213	0
5	NAG	A	1	14/15	0.82	0.32	190,198,203,203	0
5	NAG	B	2	14/15	0.92	0.21	156,162,165,165	0
5	NAG	B	1	14/15	0.94	0.20	129,136,143,150	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.