



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:02 AM BST

PDB ID : 6MEJ
Title : Crystal structure of Hepatitis C virus envelope glycoprotein E2 ectodomain in complex with human antibodies HEPC3 and HEPC46
Authors : Flyak, A.I.; Bjorkman, P.J.
Deposited on : 2018-09-06
Resolution : 2.80 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

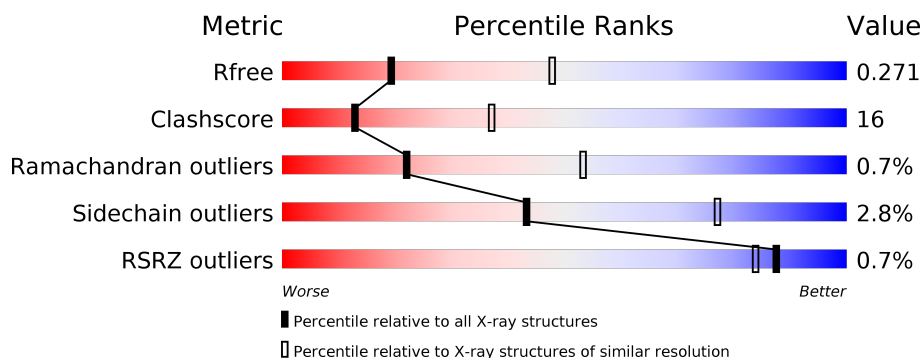
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



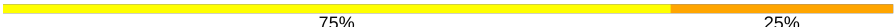
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	
2	B	217	
3	C	262	
4	H	241	
5	L	214	
6	D	5	

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Mol	Chain	Length	Quality of chain
7	E	4	 75% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8500 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 antibody HEPC46 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1610	1013	275	315	7			

- Molecule 2 is a protein called antibody HEPC46 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1577	988	264	321	4			

- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	234	Total	C	N	O	S	0	0	0
			1830	1162	325	324	19			

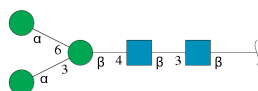
- Molecule 4 is a protein called antibody HEPC3 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	225	Total	C	N	O	S	0	0	0
			1680	1056	282	334	8			

- Molecule 5 is a protein called antibody HEPC3 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	213	Total	C	N	O	S	0	0	0
			1636	1017	281	333	5			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



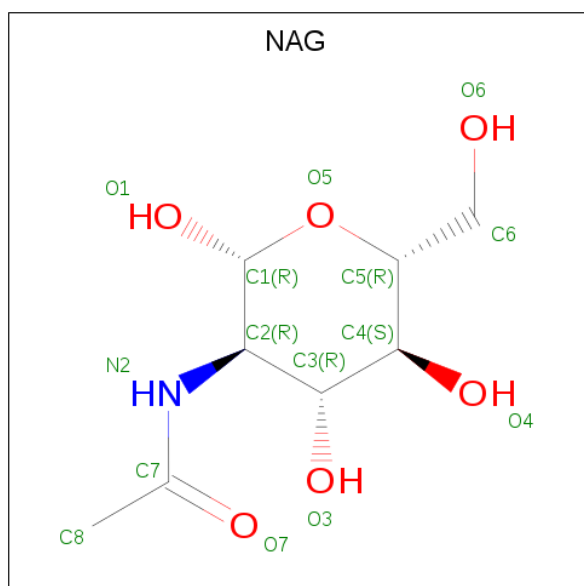
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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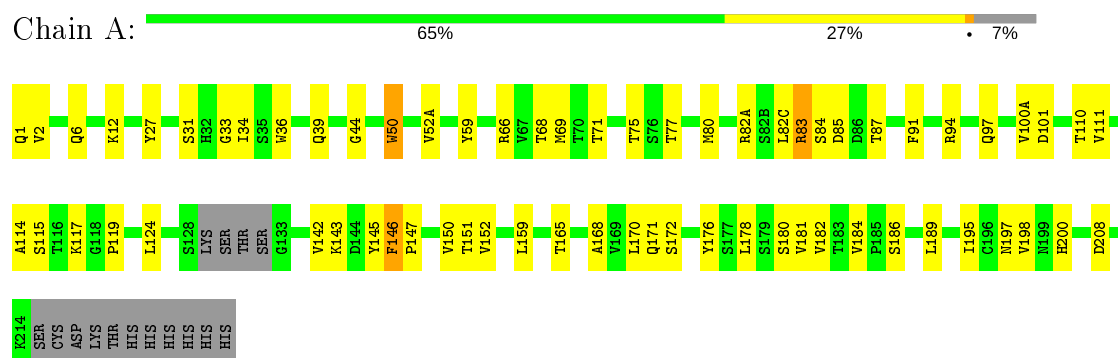
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		

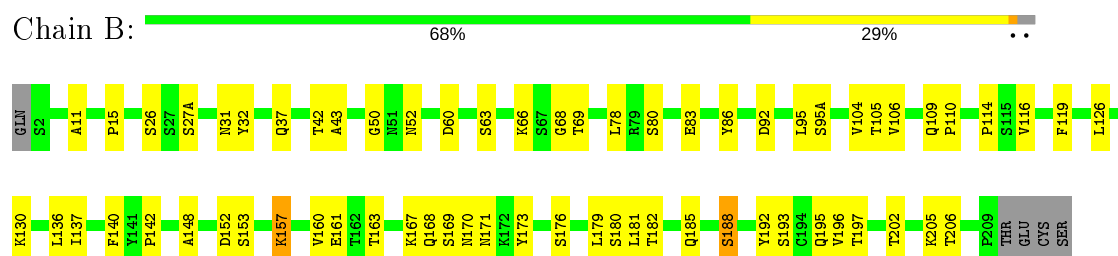
3 Residue-property plots

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.

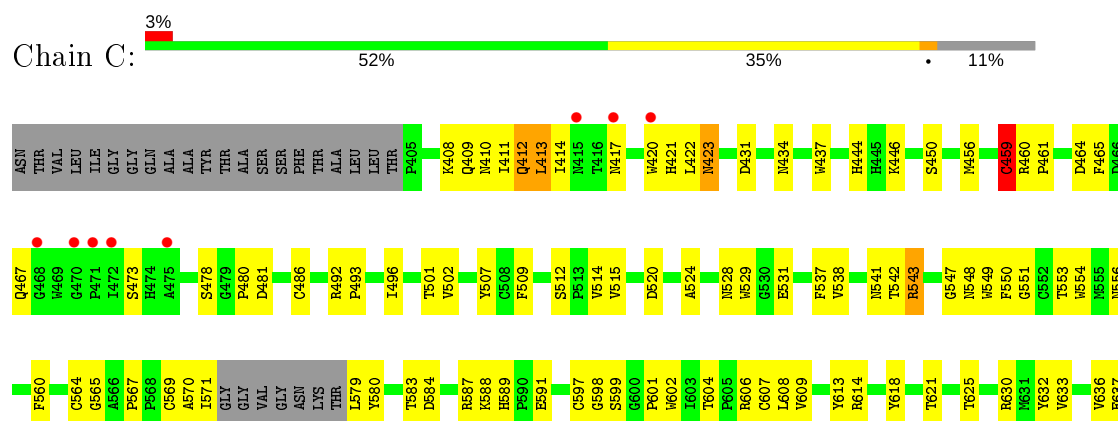
• Molecule 1: antibody HEPC46 Heavy Chain



• Molecule 2: antibody HEPC46 Light Chain



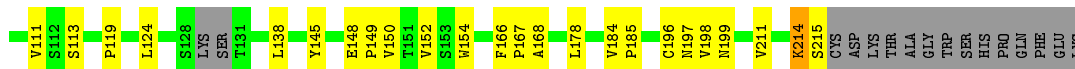
• Molecule 3: E2 glycoprotein





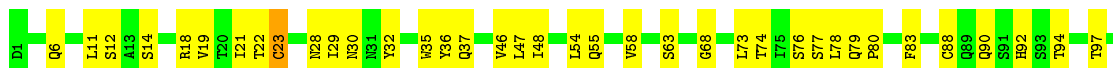
• Molecule 4: antibody HEPC3 Heavy Chain

Chain H: 68% 24% 7%



• Molecule 5: antibody HEPC3 Light Chain

Chain L: 68% 30%



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 60% 40%



• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.44Å 76.64Å 118.26Å 90.00° 106.33° 90.00°	Depositor
Resolution (Å)	78.27 – 2.80 78.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (78.27-2.80) 99.7 (78.27-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.198 , 0.271 0.198 , 0.271	Depositor DCC
R_{free} test set	1806 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.6	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	0.94	EDS
Total number of atoms	8500	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: 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	0.52	1/1647 (0.1%)	0.64	0/2245
2	B	0.46	0/1620	0.63	0/2216
3	C	0.56	1/1899 (0.1%)	0.75	2/2602 (0.1%)
4	H	0.48	0/1720	0.66	1/2345 (0.0%)
5	L	0.50	1/1669 (0.1%)	0.70	1/2265 (0.0%)
All	All	0.50	3/8555 (0.0%)	0.68	4/11673 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
4	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	564	CYS	CB-SG	-7.36	1.69	1.82
1	A	50	TRP	CB-CG	-5.81	1.39	1.50
5	L	23	CYS	CB-SG	-5.35	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	543	ARG	NE-CZ-NH1	-8.56	116.02	120.30
4	H	101	ASP	C-N-CD	-5.91	107.59	120.60
3	C	459	CYS	CA-CB-SG	-5.45	104.18	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	154	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	409	GLN	Peptide
4	H	101	ASP	Peptide

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	1610	0	1582	49	0
2	B	1577	0	1509	47	1
3	C	1830	0	1695	88	0
4	H	1680	0	1638	45	0
5	L	1636	0	1589	58	1
6	D	61	0	52	1	0
7	E	50	0	43	1	0
8	C	56	0	52	1	0
All	All	8500	0	8160	274	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 16.

All (274) 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)
3:C:422:LEU:HD12	3:C:529:TRP:CH2	1.84	1.12
4:H:2:VAL:HG23	4:H:102:PRO:HG2	1.48	0.95
1:A:87:THR:HG23	1:A:110:THR:HA	1.49	0.93
3:C:465:PHE:HB3	3:C:588:LYS:HG3	1.52	0.89
5:L:106:ILE:HD11	5:L:171:SER:OG	1.73	0.86
1:A:146:PHE:HD1	1:A:147:PRO:HA	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:422:LEU:HD12	3:C:529:TRP:HH2	1.41	0.85
1:A:146:PHE:CD1	1:A:147:PRO:HA	2.12	0.83
4:H:34:ILE:HG13	4:H:78:THR:HG21	1.61	0.81
4:H:61:GLN:HA	4:H:64:GLN:HG3	1.63	0.79
3:C:422:LEU:O	3:C:422:LEU:HD13	1.83	0.78
3:C:496:ILE:O	3:C:496:ILE:HD12	1.84	0.78
5:L:80:PRO:HA	5:L:83:PHE:CZ	2.20	0.77
3:C:604:THR:HG22	3:C:606:ARG:H	1.49	0.76
5:L:54:LEU:HD13	5:L:58:VAL:HG12	1.68	0.74
3:C:422:LEU:CD1	3:C:529:TRP:CH2	2.68	0.74
3:C:414:ILE:O	3:C:414:ILE:HD12	1.88	0.74
2:B:163:THR:CG2	2:B:176:SER:H	2.01	0.74
3:C:423:ASN:OD1	3:C:423:ASN:N	2.18	0.73
1:A:171:GLN:HA	2:B:161:GLU:OE2	1.88	0.73
3:C:431:ASP:HA	3:C:437:TRP:HE1	1.53	0.73
5:L:149:LYS:NZ	5:L:195:GLU:OE2	2.21	0.73
3:C:608:LEU:HD21	3:C:621:THR:HG21	1.70	0.72
3:C:467:GLN:NE2	3:C:587:ARG:O	2.23	0.71
5:L:14:SER:OG	5:L:107:LYS:NZ	2.19	0.71
3:C:434:ASN:HD21	4:H:102:PRO:HD2	1.57	0.70
3:C:434:ASN:ND2	4:H:102:PRO:HD2	2.07	0.70
2:B:116:VAL:HG11	2:B:196:VAL:HG11	1.74	0.69
3:C:553:THR:HG21	3:C:618:TYR:OH	1.92	0.69
1:A:142:VAL:HG11	1:A:150:VAL:HG11	1.75	0.69
4:H:2:VAL:CG2	4:H:102:PRO:HG2	2.23	0.69
5:L:28:ASN:ND2	5:L:68:GLY:HA2	2.09	0.68
5:L:48:ILE:HD11	5:L:54:LEU:CD2	2.24	0.68
6:D:1:NAG:O4	6:D:2:NAG:N2	2.28	0.67
2:B:181:LEU:HD23	2:B:185:GLN:HG3	1.77	0.67
3:C:422:LEU:CD1	3:C:529:TRP:CZ3	2.77	0.67
2:B:160:VAL:HG12	2:B:179:LEU:HD13	1.75	0.66
1:A:82(C):LEU:HB3	1:A:111:VAL:HG11	1.77	0.66
5:L:48:ILE:CD1	5:L:54:LEU:CD2	2.74	0.65
5:L:48:ILE:CD1	5:L:54:LEU:HD23	2.25	0.65
3:C:408:LYS:HD2	5:L:94:THR:HG21	1.78	0.65
5:L:28:ASN:HD21	5:L:68:GLY:HA2	1.61	0.64
3:C:606:ARG:NH2	3:C:645:ASN:O	2.30	0.64
3:C:608:LEU:HD11	3:C:614:ARG:HD2	1.80	0.64
2:B:83:GLU:OE2	2:B:105:THR:HG23	1.98	0.64
4:H:40:ALA:HB3	4:H:43:GLN:HG3	1.79	0.64
3:C:543:ARG:NH1	3:C:598:GLY:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:633:VAL:O	3:C:636:VAL:HG12	1.99	0.63
5:L:35:TRP:HB2	5:L:48:ILE:HB	1.81	0.63
3:C:422:LEU:HD12	3:C:529:TRP:CZ3	2.33	0.62
5:L:28:ASN:HD22	5:L:29:ILE:H	1.46	0.62
2:B:163:THR:HG22	2:B:176:SER:O	2.00	0.62
3:C:571:ILE:N	3:C:579:LEU:O	2.28	0.62
3:C:543:ARG:HH12	3:C:597:CYS:C	2.02	0.62
1:A:150:VAL:HG22	1:A:200:HIS:HB2	1.80	0.61
5:L:48:ILE:HD11	5:L:54:LEU:HD22	1.82	0.61
2:B:116:VAL:HA	2:B:136:LEU:O	2.01	0.60
3:C:496:ILE:CD1	3:C:496:ILE:O	2.49	0.60
3:C:411:ILE:C	3:C:413:LEU:H	2.04	0.60
3:C:571:ILE:HA	3:C:579:LEU:HB2	1.84	0.60
5:L:6:GLN:HA	5:L:22:THR:O	2.02	0.60
5:L:161:GLU:HB2	5:L:175:LEU:HD21	1.84	0.59
1:A:152:VAL:HG22	1:A:198:VAL:HG12	1.82	0.59
4:H:22:CYS:HB3	4:H:78:THR:HG23	1.84	0.59
3:C:556:ASN:HD22	3:C:560:PHE:HB2	1.67	0.59
3:C:548:ASN:OD1	3:C:549:TRP:N	2.33	0.59
3:C:639:ARG:HD3	3:C:639:ARG:H	1.67	0.59
2:B:167:LYS:HB2	2:B:173:TYR:CE2	2.37	0.59
2:B:27(A):SER:O	2:B:92:ASP:HA	2.03	0.58
3:C:604:THR:HB	3:C:607:CYS:HB2	1.84	0.58
2:B:182:THR:HG23	2:B:185:GLN:H	1.68	0.58
4:H:34:ILE:HG21	4:H:78:THR:HG21	1.84	0.58
3:C:478:SER:HB2	3:C:480:PRO:HD3	1.84	0.58
1:A:83:ARG:O	1:A:111:VAL:HG21	2.03	0.58
3:C:543:ARG:NH2	3:C:567:PRO:O	2.34	0.58
4:H:152:VAL:HG22	4:H:198:VAL:HG22	1.86	0.58
2:B:60:ASP:N	2:B:60:ASP:OD2	2.37	0.57
4:H:85:GLU:OE2	4:H:85:GLU:N	2.35	0.57
4:H:138:LEU:HD13	4:H:211:VAL:HG11	1.85	0.57
3:C:460:ARG:NE	3:C:464:ASP:HB2	2.19	0.57
2:B:197:THR:OG1	2:B:202:THR:HG22	2.04	0.57
4:H:95:ASP:O	4:H:100(G):ASN:ND2	2.37	0.56
5:L:175:LEU:HD23	5:L:176:SER:N	2.21	0.56
1:A:59:TYR:HE1	1:A:69:MET:HE2	1.71	0.56
5:L:6:GLN:H	5:L:100:GLN:HE22	1.52	0.56
2:B:26:SER:O	2:B:69:THR:HG23	2.06	0.56
1:A:33:GLY:O	1:A:34:ILE:HD13	2.05	0.55
1:A:68:THR:HG23	1:A:82(A):ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:THR:HG22	2:B:43:ALA:O	2.06	0.55
3:C:414:ILE:HD11	3:C:613:TYR:CZ	2.42	0.55
5:L:6:GLN:HG2	5:L:23:CYS:SG	2.47	0.55
5:L:19:VAL:HG21	5:L:78:LEU:HD12	1.88	0.55
3:C:602:TRP:CZ2	3:C:608:LEU:HD23	2.42	0.54
5:L:106:ILE:HD11	5:L:171:SER:CB	2.38	0.54
3:C:556:ASN:HB2	3:C:560:PHE:O	2.08	0.54
2:B:31:ASN:O	2:B:66:LYS:NZ	2.41	0.54
5:L:73:LEU:HD12	5:L:74:THR:H	1.73	0.54
4:H:13:LYS:HD3	4:H:113:SER:HA	1.88	0.54
5:L:28:ASN:HD22	5:L:29:ILE:N	2.06	0.53
3:C:431:ASP:H	3:C:437:TRP:HZ2	1.54	0.53
1:A:124:LEU:HB3	2:B:119:PHE:CD1	2.43	0.53
5:L:73:LEU:HD12	5:L:74:THR:N	2.25	0.52
3:C:502:VAL:HG12	3:C:554:TRP:NE1	2.25	0.52
1:A:66:ARG:HD2	1:A:82(A):ARG:O	2.10	0.52
4:H:119:PRO:HB3	4:H:145:TYR:HB3	1.91	0.52
1:A:168:ALA:HA	1:A:178:LEU:HB3	1.91	0.52
4:H:18:VAL:HG12	4:H:82(C):LEU:HD11	1.92	0.51
5:L:77:SER:O	5:L:77:SER:OG	2.28	0.51
1:A:146:PHE:CD1	1:A:147:PRO:CA	2.90	0.51
2:B:116:VAL:O	2:B:205:LYS:HE3	2.10	0.51
5:L:28:ASN:ND2	5:L:30:ASN:H	2.08	0.51
1:A:143:LYS:NZ	2:B:130:LYS:HD3	2.26	0.51
3:C:460:ARG:HE	3:C:464:ASP:HB2	1.76	0.51
1:A:6:GLN:HE22	1:A:91:PHE:HA	1.76	0.51
2:B:105:THR:HG21	2:B:142:PRO:HB3	1.93	0.50
2:B:114:PRO:HB3	2:B:140:PHE:CD1	2.47	0.50
5:L:149:LYS:HA	5:L:154:LEU:HA	1.92	0.50
5:L:157:GLY:O	5:L:159:SER:N	2.45	0.50
3:C:434:ASN:OD1	4:H:94:ARG:NH1	2.45	0.50
3:C:431:ASP:HA	3:C:437:TRP:NE1	2.22	0.50
1:A:151:THR:O	1:A:198:VAL:HA	2.12	0.49
3:C:456:MET:HE1	3:C:486:CYS:HB2	1.95	0.49
4:H:214:LYS:HG2	4:H:215:SER:H	1.78	0.49
2:B:167:LYS:HB2	2:B:173:TYR:CZ	2.47	0.49
1:A:31:SER:O	3:C:542:THR:HB	2.12	0.49
4:H:64:GLN:C	4:H:66:ARG:H	2.16	0.49
5:L:185:ASP:HA	5:L:188:LYS:HE2	1.93	0.49
2:B:163:THR:HG22	2:B:176:SER:H	1.74	0.49
5:L:110:VAL:HG22	5:L:141:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:GLN:HG2	2:B:110:PRO:HD2	1.94	0.49
5:L:76:SER:OG	5:L:77:SER:N	2.45	0.49
1:A:168:ALA:HB2	1:A:178:LEU:HD23	1.95	0.49
1:A:186:SER:O	1:A:189:LEU:HG	2.13	0.48
4:H:84:PRO:HA	4:H:111:VAL:HG13	1.94	0.48
2:B:32:TYR:CD1	2:B:50:GLY:HA2	2.48	0.48
1:A:165:THR:HG23	1:A:180:SER:HB2	1.96	0.48
4:H:72:ASP:OD2	4:H:74:SER:HB3	2.12	0.48
5:L:108:ARG:HG2	5:L:109:THR:N	2.29	0.48
4:H:67:VAL:HB	4:H:82:LEU:HD13	1.95	0.48
3:C:501:THR:O	3:C:501:THR:HG22	2.14	0.48
3:C:502:VAL:HG21	3:C:537:PHE:CE1	2.48	0.48
2:B:181:LEU:HD21	2:B:192:TYR:CE2	2.49	0.48
2:B:193:SER:HB3	2:B:206:THR:HG23	1.95	0.48
5:L:178:THR:HG22	5:L:180:THR:HG23	1.95	0.48
1:A:159:LEU:HD21	1:A:182:VAL:HG21	1.94	0.48
4:H:148:GLU:OE2	4:H:149:PRO:HA	2.14	0.48
4:H:33:GLU:OE2	4:H:96:GLY:HA2	2.13	0.48
3:C:632:TYR:HA	3:C:636:VAL:O	2.13	0.47
2:B:114:PRO:HB3	2:B:140:PHE:HB3	1.95	0.47
2:B:163:THR:HG21	2:B:176:SER:H	1.78	0.47
3:C:411:ILE:O	3:C:413:LEU:N	2.47	0.47
4:H:2:VAL:HG23	4:H:102:PRO:CG	2.34	0.47
2:B:83:GLU:HG3	2:B:104:VAL:O	2.14	0.47
3:C:502:VAL:HG12	3:C:554:TRP:CD1	2.50	0.47
4:H:214:LYS:HG2	4:H:215:SER:N	2.29	0.47
2:B:148:ALA:O	2:B:195:GLN:HB3	2.15	0.47
3:C:502:VAL:HG21	3:C:537:PHE:HE1	1.79	0.47
4:H:124:LEU:HD22	5:L:118:PHE:HB3	1.96	0.47
5:L:47:LEU:O	5:L:48:ILE:HD13	2.15	0.47
2:B:37:GLN:HB2	2:B:86:TYR:CE1	2.50	0.47
3:C:541:ASN:HA	3:C:548:ASN:HD21	1.80	0.47
4:H:166:PHE:HB3	5:L:162:SER:OG	2.15	0.47
3:C:493:PRO:HA	3:C:565:GLY:O	2.15	0.46
1:A:97:GLN:HG2	1:A:97:GLN:O	2.16	0.46
3:C:601:PRO:O	3:C:609:VAL:HG13	2.15	0.46
5:L:12:SER:HA	5:L:105:GLU:O	2.16	0.46
1:A:50:TRP:C	1:A:69:MET:HE3	2.36	0.46
1:A:115:SER:O	1:A:146:PHE:CD2	2.69	0.46
2:B:152:ASP:O	2:B:153:SER:HB2	2.16	0.46
2:B:181:LEU:HD21	2:B:192:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:19:LYS:HE2	4:H:79:TYR:HB3	1.98	0.45
1:A:85:ASP:N	1:A:85:ASP:OD1	2.43	0.45
3:C:543:ARG:HG2	3:C:550:PHE:CD2	2.50	0.45
2:B:11:ALA:O	2:B:104:VAL:HA	2.17	0.45
2:B:69:THR:HG22	2:B:69:THR:O	2.16	0.45
4:H:100(I):PHE:HB2	5:L:36:TYR:CE2	2.51	0.45
4:H:154:TRP:CZ3	4:H:196:CYS:HB3	2.52	0.45
5:L:6:GLN:H	5:L:100:GLN:NE2	2.15	0.45
3:C:543:ARG:NH1	3:C:597:CYS:C	2.70	0.45
3:C:630:ARG:NH1	3:C:632:TYR:OH	2.49	0.45
5:L:106:ILE:HG21	5:L:106:ILE:HD13	1.77	0.45
3:C:589:HIS:CE1	3:C:591:GLU:HB2	2.52	0.45
1:A:152:VAL:HA	1:A:197:ASN:O	2.17	0.45
1:A:1:GLN:HG2	1:A:1:GLN:O	2.17	0.45
4:H:154:TRP:CH2	4:H:196:CYS:HB3	2.52	0.45
3:C:625:THR:O	3:C:643:ALA:HA	2.17	0.45
5:L:48:ILE:CD1	5:L:54:LEU:HD22	2.44	0.44
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.52	0.44
2:B:80:SER:HA	2:B:106:VAL:HG11	1.99	0.44
3:C:639:ARG:HD3	3:C:639:ARG:N	2.33	0.44
3:C:411:ILE:C	3:C:413:LEU:N	2.70	0.44
3:C:456:MET:HE1	3:C:459:CYS:HB2	2.00	0.44
5:L:18:ARG:HG2	5:L:76:SER:HA	1.99	0.44
3:C:632:TYR:CE1	3:C:637:GLU:HB2	2.53	0.44
4:H:167:PRO:HG2	5:L:163:VAL:O	2.17	0.44
5:L:28:ASN:ND2	5:L:29:ILE:N	2.66	0.44
2:B:168:GLN:C	2:B:170:ASN:H	2.21	0.44
5:L:163:VAL:HG22	5:L:175:LEU:HG	2.00	0.44
1:A:170:LEU:HD23	1:A:176:TYR:CZ	2.53	0.44
1:A:36:TRP:HD1	1:A:69:MET:SD	2.40	0.44
3:C:520:ASP:HB2	3:C:524:ALA:HB3	2.00	0.44
3:C:542:THR:O	3:C:547:GLY:HA3	2.18	0.44
5:L:21:ILE:HD13	5:L:102:THR:HG21	1.99	0.44
5:L:37:GLN:HB3	5:L:47:LEU:HD22	1.99	0.43
2:B:15:PRO:HA	2:B:78:LEU:O	2.18	0.43
4:H:100(D):ARG:HB3	5:L:32:TYR:OH	2.18	0.43
3:C:602:TRP:CH2	3:C:608:LEU:HD23	2.53	0.43
1:A:114:ALA:O	1:A:146:PHE:HE2	2.02	0.43
2:B:180:SER:C	2:B:181:LEU:HD12	2.38	0.43
3:C:538:VAL:HG23	3:C:538:VAL:O	2.17	0.43
5:L:151:ASP:HA	5:L:191:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:32:TYR:HB2	5:L:92:HIS:HB2	1.99	0.43
1:A:184:VAL:HG21	1:A:189:LEU:HD21	2.01	0.43
7:E:3:BMA:H3	7:E:4:MAN:H2	1.53	0.43
2:B:52:ASN:N	2:B:52:ASN:OD1	2.51	0.43
3:C:417:ASN:O	3:C:515:VAL:HG21	2.19	0.43
3:C:507:TYR:HA	3:C:514:VAL:O	2.19	0.43
3:C:520:ASP:HB3	3:C:524:ALA:H	1.83	0.43
3:C:569:CYS:O	3:C:580:TYR:HA	2.18	0.43
4:H:33:GLU:CD	4:H:96:GLY:HA2	2.39	0.43
1:A:75:THR:HG22	1:A:77:THR:OG1	2.18	0.42
3:C:502:VAL:HG12	3:C:554:TRP:HE1	1.84	0.42
3:C:614:ARG:NH1	3:C:621:THR:OG1	2.52	0.42
4:H:52:THR:OG1	4:H:56:GLU:CG	2.67	0.42
1:A:52(A):VAL:HG22	1:A:71:THR:HG21	2.00	0.42
3:C:543:ARG:HG2	3:C:550:PHE:HD2	1.84	0.42
1:A:69:MET:HE2	1:A:69:MET:HB2	1.80	0.42
3:C:446:LYS:HD3	3:C:446:LYS:HA	1.87	0.42
3:C:604:THR:HG22	3:C:606:ARG:N	2.26	0.42
1:A:2:VAL:HG23	1:A:27:TYR:HD2	1.84	0.42
3:C:423:ASN:HD22	8:C:4313:NAG:C7	2.33	0.42
3:C:632:TYR:HE1	3:C:637:GLU:HB2	1.85	0.42
1:A:34:ILE:HA	1:A:34:ILE:HD13	1.75	0.42
3:C:422:LEU:C	3:C:422:LEU:HD13	2.40	0.42
3:C:528:ASN:O	3:C:531:GLU:HG3	2.19	0.42
4:H:4:LEU:HD22	4:H:22:CYS:SG	2.60	0.42
5:L:47:LEU:HA	5:L:47:LEU:HD12	1.88	0.42
1:A:181:VAL:HG21	2:B:136:LEU:CD1	2.49	0.42
4:H:184:VAL:HB	4:H:185:PRO:HD2	2.02	0.42
2:B:126:LEU:HD23	2:B:130:LYS:O	2.20	0.41
3:C:408:LYS:O	3:C:408:LYS:HG2	2.18	0.41
4:H:150:VAL:HG23	4:H:199:ASN:O	2.19	0.41
4:H:52:THR:OG1	4:H:56:GLU:HG3	2.19	0.41
1:A:84:SER:OG	1:A:172:SER:O	2.33	0.41
3:C:414:ILE:HG12	3:C:444:HIS:NE2	2.35	0.41
3:C:460:ARG:HA	3:C:461:PRO:HD3	1.97	0.41
1:A:12:LYS:O	1:A:111:VAL:HA	2.20	0.41
1:A:94:ARG:O	1:A:100(A):VAL:HA	2.20	0.41
1:A:195:ILE:HG21	1:A:208:ASP:HB3	2.01	0.41
3:C:551:GLY:HA3	3:C:599:SER:O	2.20	0.41
4:H:168:ALA:HA	4:H:178:LEU:HB3	2.03	0.41
2:B:137:ILE:N	2:B:137:ILE:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:509:PHE:CD2	3:C:609:VAL:HG21	2.56	0.41
5:L:11:LEU:HD11	5:L:19:VAL:HG13	2.03	0.41
2:B:137:ILE:HG22	2:B:140:PHE:CE1	2.56	0.41
3:C:420:TRP:O	3:C:421:HIS:ND1	2.54	0.41
2:B:95:LEU:HA	2:B:95:LEU:HD23	1.78	0.41
1:A:39:GLN:HG3	1:A:44:GLY:O	2.20	0.41
3:C:583:THR:OG1	3:C:584:ASP:N	2.53	0.41
5:L:46:VAL:HG11	5:L:55:GLN:OE1	2.20	0.41
5:L:48:ILE:HD12	5:L:54:LEU:HD23	2.01	0.41
4:H:36:TRP:HA	4:H:91:TYR:O	2.21	0.41
2:B:185:GLN:HA	2:B:188:SER:HB3	2.03	0.40
4:H:36:TRP:CE2	4:H:80:MET:HB2	2.56	0.40
5:L:125:LEU:HD23	5:L:125:LEU:HA	1.82	0.40
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.03	0.40
3:C:502:VAL:CG1	3:C:554:TRP:CD1	3.04	0.40
4:H:124:LEU:HD23	4:H:124:LEU:HA	1.72	0.40
4:H:124:LEU:HB3	5:L:118:PHE:CD2	2.56	0.40
5:L:78:LEU:HD23	5:L:79:GLN:N	2.37	0.40
5:L:90:GLN:HE21	5:L:97:THR:H	1.69	0.40
1:A:114:ALA:HB1	1:A:146:PHE:CD2	2.56	0.40
1:A:36:TRP:CD1	1:A:69:MET:SD	3.15	0.40
3:C:473:SER:OG	3:C:570:ALA:HB3	2.21	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)
2:B:60:ASP:OD1	5:L:183:LYS:NZ[2_544]	2.13	0.07

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	211/230 (92%)	201 (95%)	9 (4%)	1 (0%)	29	61
2	B	210/217 (97%)	188 (90%)	18 (9%)	4 (2%)	8	26
3	C	230/262 (88%)	202 (88%)	27 (12%)	1 (0%)	34	66
4	H	221/241 (92%)	202 (91%)	18 (8%)	1 (0%)	29	61
5	L	211/214 (99%)	193 (92%)	17 (8%)	1 (0%)	29	61
All	All	1083/1164 (93%)	986 (91%)	89 (8%)	8 (1%)	22	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	102	PRO
5	L	158	ASN
2	B	171	ASN
2	B	188	SER
3	C	412	GLN
2	B	157	LYS
1	A	146	PHE
2	B	68	GLY

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	180/195 (92%)	177 (98%)	3 (2%)	60	87
2	B	176/181 (97%)	172 (98%)	4 (2%)	50	82
3	C	197/216 (91%)	185 (94%)	12 (6%)	18	48
4	H	189/203 (93%)	186 (98%)	3 (2%)	62	88
5	L	187/188 (100%)	183 (98%)	4 (2%)	53	84
All	All	929/983 (94%)	903 (97%)	26 (3%)	43	77

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	101	ASP
1	A	117	LYS
2	B	63	SER
2	B	95(A)	SER
2	B	157	LYS
2	B	169	SER
3	C	410	ASN
3	C	412	GLN
3	C	413	LEU
3	C	423	ASN
3	C	450	SER
3	C	459	CYS
3	C	481	ASP
3	C	492	ARG
3	C	512	SER
3	C	638	HIS
3	C	639	ARG
3	C	640	LEU
4	H	83	ARG
4	H	197	ASN
4	H	214	LYS
5	L	63	SER
5	L	88	CYS
5	L	176	SER
5	L	194	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	H	61	GLN
4	H	171	GLN
5	L	28	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 ⓘ

9 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$
6	NAG	D	1	3,6	14,14,15	0.66	0	17,19,21	2.54	6 (35%)
6	NAG	D	2	6	14,14,15	0.56	0	17,19,21	1.91	5 (29%)
6	BMA	D	3	6	11,11,12	1.08	1 (9%)	15,15,17	1.03	1 (6%)
6	MAN	D	4	6	11,11,12	0.64	0	15,15,17	1.22	2 (13%)
6	MAN	D	5	6	11,11,12	0.61	0	15,15,17	1.03	1 (6%)
7	NAG	E	1	3,7	14,14,15	0.41	0	17,19,21	1.06	1 (5%)
7	NAG	E	2	7	14,14,15	0.44	0	17,19,21	1.22	2 (11%)
7	BMA	E	3	7	11,11,12	1.22	2 (18%)	15,15,17	1.01	0
7	MAN	E	4	7	11,11,12	0.58	0	15,15,17	0.81	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
6	NAG	D	1	3,6	-	3/6/23/26	0/1/1/1
6	NAG	D	2	6	-	3/6/23/26	0/1/1/1
6	BMA	D	3	6	-	1/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5	6	-	0/2/19/22	0/1/1/1
7	NAG	E	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	E	2	7	-	4/6/23/26	0/1/1/1
7	BMA	E	3	7	-	1/2/19/22	0/1/1/1
7	MAN	E	4	7	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	3	BMA	C4-C5	2.67	1.58	1.53
7	E	3	BMA	C4-C3	2.50	1.58	1.52
6	D	3	BMA	C1-C2	2.28	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1	NAG	C1-C2-N2	-6.17	99.94	110.49
6	D	1	NAG	C2-N2-C7	5.01	130.04	122.90
6	D	2	NAG	C2-N2-C7	4.34	129.08	122.90
6	D	1	NAG	O3-C3-C4	-3.07	103.25	110.35
6	D	2	NAG	C4-C3-C2	3.01	115.43	111.02
7	E	1	NAG	C2-N2-C7	-2.76	118.98	122.90
7	E	2	NAG	C2-N2-C7	-2.75	118.99	122.90
6	D	4	MAN	C1-C2-C3	-2.51	106.58	109.67
6	D	1	NAG	O3-C3-C2	-2.48	104.34	109.47
6	D	1	NAG	O5-C5-C6	-2.41	103.42	107.20
6	D	2	NAG	O7-C7-N2	2.30	126.18	121.95
6	D	2	NAG	C6-C5-C4	2.21	118.18	113.00
7	E	2	NAG	O5-C1-C2	-2.17	107.86	111.29
6	D	1	NAG	C3-C4-C5	2.14	114.06	110.24
6	D	3	BMA	O2-C2-C3	-2.10	105.93	110.14
6	D	5	MAN	O5-C5-C6	2.05	110.41	107.20
6	D	4	MAN	C1-O5-C5	-2.02	109.46	112.19
6	D	2	NAG	C3-C4-C5	-2.01	106.65	110.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C3-C2-N2-C7
6	D	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
7	E	3	BMA	O5-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6
7	E	2	NAG	O5-C5-C6-O6
6	D	3	BMA	O5-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
7	E	1	NAG	C4-C5-C6-O6
7	E	2	NAG	C8-C7-N2-C2
6	D	2	NAG	C3-C2-N2-C7
7	E	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	E	1	NAG	O5-C5-C6-O6
6	D	2	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	3	BMA	1	0
6	D	2	NAG	1	0
7	E	4	MAN	1	0
6	D	1	NAG	1	0

5.6 Ligand geometry

4 ligands 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
8	NAG	C	4313	3	14,14,15	0.49	0	17,19,21	1.04	1 (5%)
8	NAG	C	4312	3	14,14,15	0.67	0	17,19,21	0.94	1 (5%)
8	NAG	C	4301	3	14,14,15	0.53	0	17,19,21	0.90	0
8	NAG	C	4311	3	14,14,15	0.62	0	17,19,21	1.82	5 (29%)

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
8	NAG	C	4313	3	-	0/6/23/26	0/1/1/1
8	NAG	C	4312	3	-	0/6/23/26	0/1/1/1
8	NAG	C	4301	3	-	6/6/23/26	0/1/1/1
8	NAG	C	4311	3	-	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(°)
8	C	4311	NAG	C6-C5-C4	-3.44	104.94	113.00
8	C	4311	NAG	O5-C1-C2	-2.99	106.57	111.29
8	C	4311	NAG	C4-C3-C2	-2.99	106.64	111.02
8	C	4311	NAG	C1-O5-C5	2.49	115.57	112.19
8	C	4311	NAG	O7-C7-N2	2.36	126.30	121.95
8	C	4312	NAG	C1-O5-C5	2.23	115.22	112.19
8	C	4313	NAG	O5-C5-C6	2.08	110.47	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	4301	NAG	C1-C2-N2-C7
8	C	4301	NAG	C8-C7-N2-C2
8	C	4301	NAG	O7-C7-N2-C2
8	C	4311	NAG	C8-C7-N2-C2
8	C	4311	NAG	O7-C7-N2-C2
8	C	4311	NAG	O5-C5-C6-O6
8	C	4301	NAG	O5-C5-C6-O6
8	C	4311	NAG	C4-C5-C6-O6
8	C	4301	NAG	C4-C5-C6-O6
8	C	4301	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	4313	NAG	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	215/230 (93%)	-0.17	0	100 100	45, 70, 99, 128	0
2	B	212/217 (97%)	-0.04	0	100 100	42, 77, 106, 136	0
3	C	234/262 (89%)	0.24	8 (3%)	45 35	43, 70, 132, 180	0
4	H	225/241 (93%)	-0.05	0	100 100	40, 63, 94, 140	0
5	L	213/214 (99%)	-0.06	0	100 100	44, 72, 103, 124	0
All	All	1099/1164 (94%)	-0.01	8 (0%)	87 84	40, 70, 108, 180	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	417	ASN	4.6
3	C	468	GLY	4.4
3	C	415	ASN	3.8
3	C	471	PRO	3.0
3	C	472	ILE	2.9
3	C	470	GLY	2.7
3	C	420	TRP	2.7
3	C	475	ALA	2.1

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
6	BMA	D	3	11/12	0.67	0.27	127,136,147,151	0
6	MAN	D	4	11/12	0.70	0.31	118,140,145,145	0
7	BMA	E	3	11/12	0.74	0.18	126,134,141,143	0
7	MAN	E	4	11/12	0.75	0.25	104,132,139,141	0
6	NAG	D	2	14/15	0.83	0.21	70,87,108,116	0
6	MAN	D	5	11/12	0.90	0.27	117,122,125,126	0
7	NAG	E	2	14/15	0.93	0.14	88,99,102,117	0
6	NAG	D	1	14/15	0.96	0.15	56,67,88,91	0
7	NAG	E	1	14/15	0.97	0.12	31,53,63,72	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	C	4312	14/15	0.81	0.27	92,101,105,111	0
8	NAG	C	4311	14/15	0.86	0.15	58,76,104,108	0
8	NAG	C	4313	14/15	0.87	0.18	91,107,120,125	0
8	NAG	C	4301	14/15	0.90	0.15	86,92,99,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.