Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 06:13 PM EDT

PDB ID	:	4XI5
Title	:	gHgL of varicella-zoster virus in complex with human neutralizing antibodies
Authors	:	Xing, Y.
Deposited on	:	2015-01-06
Resolution	:	3.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

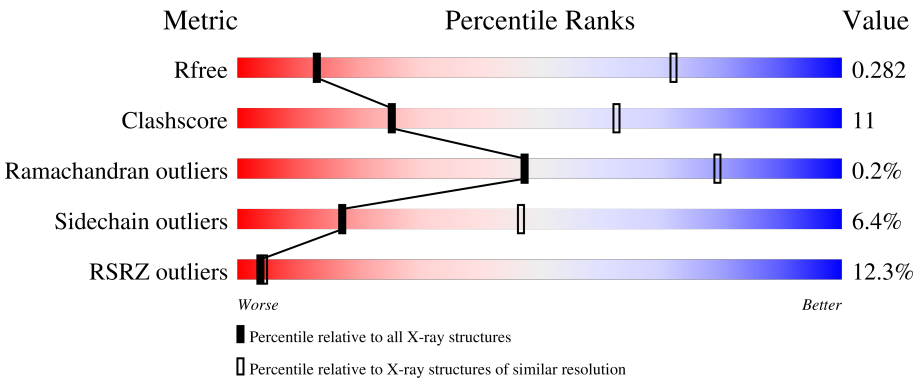
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	833	.% 62% 24% • 13%
2	B	138	2% 69% 25% • •
3	C	214	30% 76% 18% • •
4	D	283	28% 53% 19% • 27%
5	E	4	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9724 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 H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5601	3597	934	1045	25	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	796	GLY	-	expression tag	UNP Q775J3
A	797	SER	-	expression tag	UNP Q775J3
A	798	GLU	-	expression tag	UNP Q775J3
A	799	ASN	-	expression tag	UNP Q775J3
A	800	LEU	-	expression tag	UNP Q775J3
A	801	TYR	-	expression tag	UNP Q775J3
A	802	PHE	-	expression tag	UNP Q775J3
A	803	GLN	-	expression tag	UNP Q775J3
A	804	GLY	-	expression tag	UNP Q775J3
A	805	SER	-	expression tag	UNP Q775J3
A	806	TRP	-	expression tag	UNP Q775J3
A	807	SER	-	expression tag	UNP Q775J3
A	808	HIS	-	expression tag	UNP Q775J3
A	809	PRO	-	expression tag	UNP Q775J3
A	810	GLN	-	expression tag	UNP Q775J3
A	811	PHE	-	expression tag	UNP Q775J3
A	812	GLU	-	expression tag	UNP Q775J3
A	813	LYS	-	expression tag	UNP Q775J3
A	814	GLY	-	expression tag	UNP Q775J3
A	815	GLY	-	expression tag	UNP Q775J3
A	816	GLY	-	expression tag	UNP Q775J3
A	817	SER	-	expression tag	UNP Q775J3
A	818	GLY	-	expression tag	UNP Q775J3
A	819	GLY	-	expression tag	UNP Q775J3
A	820	GLY	-	expression tag	UNP Q775J3
A	821	SER	-	expression tag	UNP Q775J3
A	822	GLY	-	expression tag	UNP Q775J3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	823	GLY	-	expression tag	UNP Q775J3
A	824	GLY	-	expression tag	UNP Q775J3
A	825	SER	-	expression tag	UNP Q775J3
A	826	TRP	-	expression tag	UNP Q775J3
A	827	SER	-	expression tag	UNP Q775J3
A	828	HIS	-	expression tag	UNP Q775J3
A	829	PRO	-	expression tag	UNP Q775J3
A	830	GLN	-	expression tag	UNP Q775J3
A	831	PHE	-	expression tag	UNP Q775J3
A	832	GLU	-	expression tag	UNP Q775J3
A	833	LYS	-	expression tag	UNP Q775J3

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	132	1007	647	163	192	5	0	0	0

- Molecule 3 is a protein called Fab-94 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1525	956	255	309	5	0	0	0

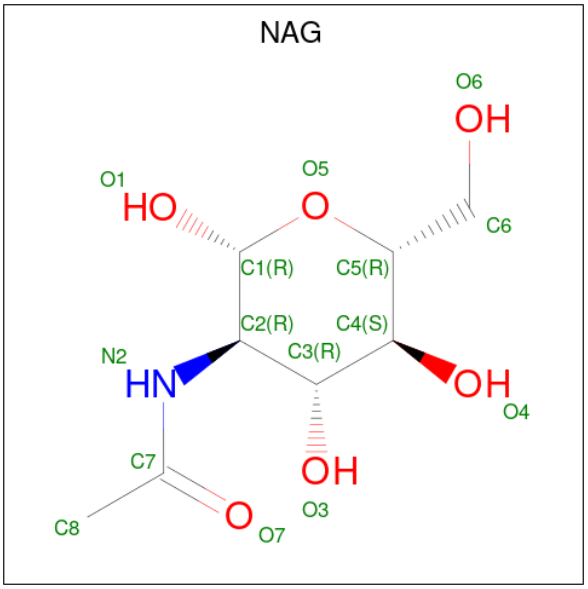
- Molecule 4 is a protein called Fab-94 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1499	951	248	293	7	0	0	0

- Molecule 5 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
			Total	C	N	O			
5	E	4	50	28	2	20	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



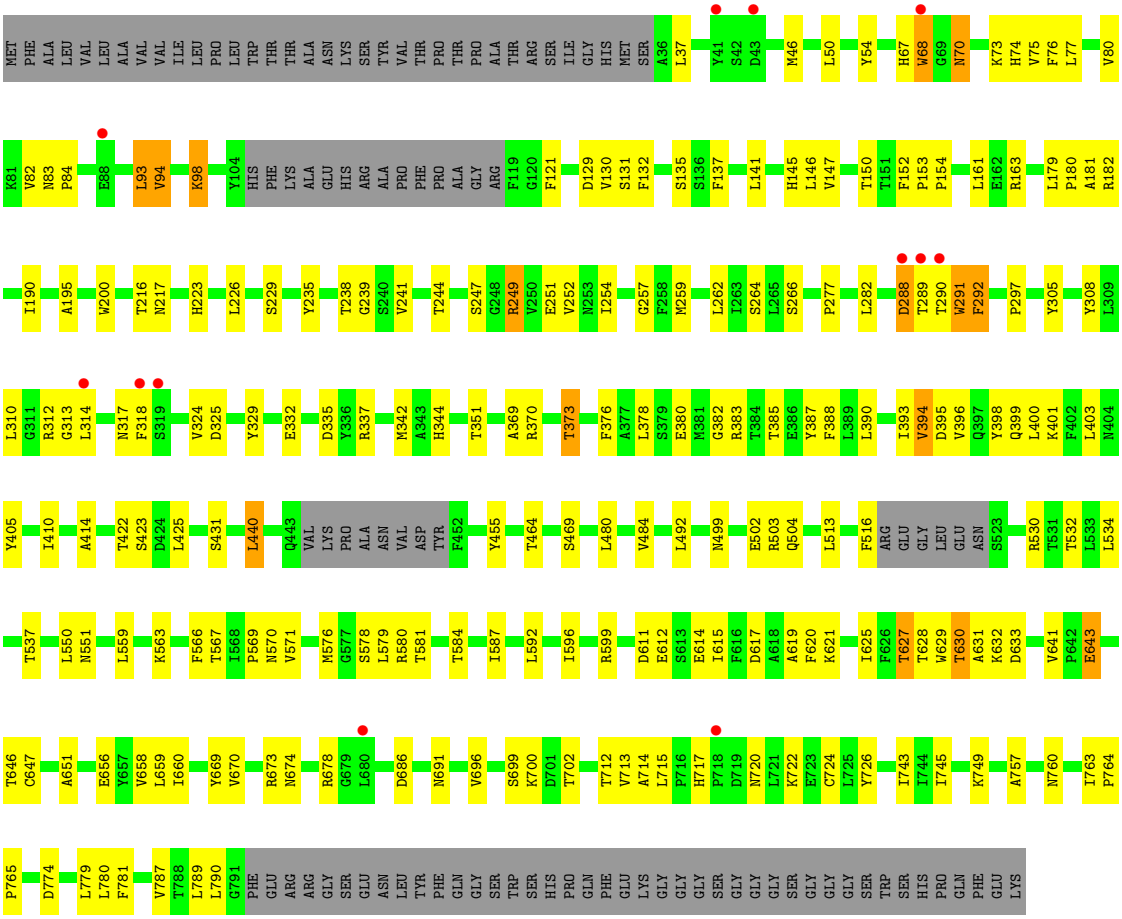
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0

3 Residue-property plots (i)

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.

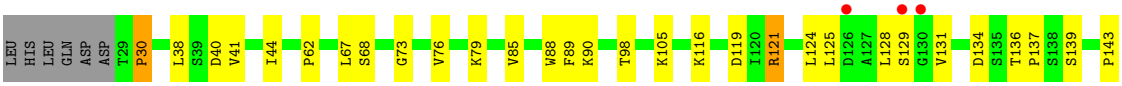
• Molecule 1: Envelope glycoprotein H

Chain A:



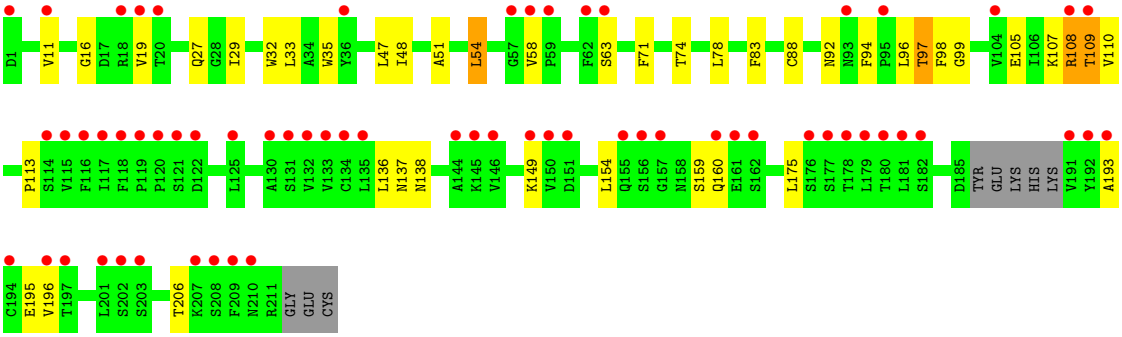
• Molecule 2: Envelope glycoprotein L

Chain B:



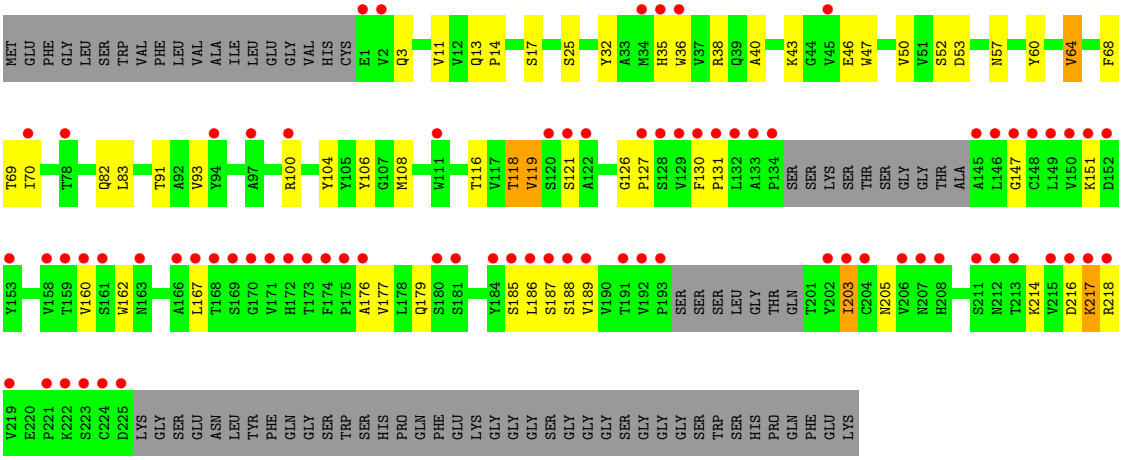
• Molecule 3: Fab-94 light chain

Chain C:



• Molecule 4: Fab-94 heavy chain

Chain D:



• Molecule 5: 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:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	102.00Å 280.55Å 175.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.32 – 3.90 43.83 – 3.89	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.32-3.90) 98.3 (43.83-3.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.245 , 0.276 0.247 , 0.282	Depositor DCC
R_{free} test set	1194 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	171.4	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9724	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	0.24	0/5740	0.45	0/7842
2	B	0.22	0/1034	0.47	1/1416 (0.1%)
3	C	0.24	0/1556	0.51	0/2119
4	D	0.24	0/1537	0.61	3/2107 (0.1%)
All	All	0.24	0/9867	0.49	4/13484 (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
4	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	119	VAL	O-C-N	-14.96	98.76	122.70
4	D	119	VAL	CA-C-N	8.05	134.91	117.20
2	B	30	PRO	N-CA-CB	5.99	110.49	103.30
4	D	119	VAL	C-N-CA	5.84	136.31	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	119	VAL	Mainchain

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	5601	0	5443	127	0
2	B	1007	0	972	26	0
3	C	1525	0	1459	31	0
4	D	1499	0	1391	40	0
5	E	50	0	43	2	0
6	A	42	0	39	0	0
All	All	9724	0	9347	203	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 11.

All (203) 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)
4:D:13:GLN:OE1	4:D:121:SER:OG	1.67	1.10
3:C:48:ILE:HG12	3:C:54:LEU:HB3	1.62	0.80
2:B:121:ARG:NH2	4:D:57:ASN:OD1	2.18	0.77
3:C:33:LEU:HD22	3:C:71:PHE:HB2	1.70	0.74
1:A:98:LYS:HD2	2:B:68:SER:HB3	1.68	0.74
1:A:70:ASN:HD22	2:B:88:TRP:HH2	1.37	0.71
3:C:160:GLN:NE2	4:D:185:SER:OG	2.24	0.69
4:D:69:THR:HB	4:D:82:GLN:HB3	1.75	0.68
2:B:144:GLU:O	2:B:157:ARG:NH2	2.27	0.68
1:A:247:SER:H	1:A:414:ALA:HB2	1.58	0.67
1:A:180:PRO:O	1:A:337:ARG:NH1	2.24	0.67
1:A:699:SER:HB2	1:A:702:THR:HB	1.75	0.66
1:A:717:HIS:HB3	1:A:720:ASN:HB2	1.76	0.66
1:A:121:PHE:HE2	1:A:383:ARG:HH22	1.44	0.66
1:A:628:THR:HA	1:A:632:LYS:HB2	1.77	0.65
1:A:405:TYR:OH	1:A:633:ASP:OD2	2.13	0.65
4:D:38:ARG:NH2	4:D:46:GLU:OE1	2.31	0.64
1:A:70:ASN:HB2	2:B:90:LYS:HD2	1.79	0.64
1:A:75:VAL:HG23	1:A:98:LYS:HZ1	1.63	0.64
1:A:195:ALA:HB1	1:A:390:LEU:HD13	1.80	0.64
3:C:94:PHE:HZ	4:D:50:VAL:HG21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:LYS:NZ	2:B:134:ASP:OD2	2.26	0.63
1:A:581:THR:HA	1:A:627:THR:HB	1.81	0.63
1:A:313:GLY:HA2	1:A:317:ASN:HB2	1.81	0.62
1:A:576:MET:O	1:A:630:THR:OG1	2.15	0.62
1:A:244:THR:HG22	1:A:249:ARG:HB2	1.82	0.61
1:A:297:PRO:HB3	1:A:314:LEU:HD11	1.80	0.61
4:D:162:TRP:HB3	4:D:167:LEU:HD12	1.83	0.61
1:A:129:ASP:OD2	1:A:135:SER:OG	2.19	0.60
1:A:332:GLU:OE2	1:A:370:ARG:NH2	2.35	0.60
1:A:724:CYS:HB2	1:A:749:LYS:HG3	1.84	0.60
1:A:241:VAL:HB	1:A:252:VAL:HB	1.84	0.60
1:A:342:MET:HB2	1:A:370:ARG:HD2	1.83	0.59
1:A:291:TRP:CD1	4:D:57:ASN:HB2	2.38	0.59
4:D:203:ILE:HG22	4:D:218:ARG:HA	1.85	0.58
1:A:266:SER:HA	2:B:146:GLY:HA2	1.85	0.58
4:D:91:THR:HG23	4:D:118:THR:HA	1.84	0.58
1:A:504:GLN:NE2	1:A:570:ASN:OD1	2.28	0.57
1:A:239:GLY:HA3	1:A:425:LEU:HD23	1.85	0.57
1:A:161:LEU:HB3	1:A:324:VAL:HG12	1.86	0.57
1:A:344:HIS:HD2	1:A:403:LEU:HD21	1.69	0.57
1:A:537:THR:HA	1:A:578:SER:HB2	1.88	0.56
1:A:592:LEU:HD23	1:A:619:ALA:HB1	1.86	0.56
3:C:96:LEU:HD13	4:D:47:TRP:HE3	1.71	0.56
4:D:36:TRP:HD1	4:D:70:ILE:HD11	1.71	0.56
4:D:176:ALA:HB2	4:D:186:LEU:HD23	1.87	0.56
1:A:146:LEU:HD23	1:A:150:THR:HG22	1.89	0.55
5:E:1:NAG:H61	5:E:2:NAG:N2	2.21	0.55
4:D:11:VAL:HG22	4:D:118:THR:HB	1.88	0.55
1:A:351:THR:HG21	1:A:629:TRP:HZ3	1.72	0.55
1:A:763:ILE:HG22	1:A:765:PRO:HD2	1.89	0.55
1:A:335:ASP:OD2	1:A:337:ARG:NH2	2.29	0.54
1:A:670:VAL:HG12	1:A:696:VAL:HB	1.90	0.54
1:A:660:ILE:HG12	1:A:670:VAL:HG23	1.90	0.54
2:B:67:LEU:HD12	2:B:67:LEU:H	1.73	0.54
1:A:147:VAL:O	2:B:139:SER:OG	2.20	0.54
1:A:351:THR:HG22	1:A:410:ILE:HD13	1.90	0.53
1:A:530:ARG:NH2	1:A:643:GLU:OE2	2.42	0.53
2:B:38:LEU:HD13	2:B:44:ILE:HG12	1.90	0.53
1:A:137:PHE:CG	2:B:67:LEU:HD11	2.44	0.53
1:A:76:PHE:CE1	2:B:73:GLY:HA3	2.44	0.53
1:A:291:TRP:HE3	1:A:291:TRP:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:NH1	1:A:251:GLU:OE2	2.41	0.53
1:A:394:VAL:HG11	1:A:464:THR:HG22	1.90	0.53
1:A:179:LEU:O	1:A:181:ALA:N	2.42	0.52
1:A:312:ARG:HD2	2:B:143:PRO:HD2	1.91	0.52
3:C:107:LYS:HG2	3:C:108:ARG:N	2.23	0.52
1:A:673:ARG:NE	1:A:691:ASN:OD1	2.39	0.52
1:A:651:ALA:HA	1:A:656:GLU:HB2	1.92	0.52
3:C:160:GLN:OE1	4:D:179:GLN:NE2	2.43	0.52
1:A:625:ILE:HA	1:A:628:THR:HG22	1.92	0.51
4:D:60:TYR:OH	4:D:70:ILE:N	2.43	0.51
1:A:534:LEU:HB3	1:A:745:ILE:HD11	1.93	0.51
3:C:16:GLY:H	3:C:78:LEU:HB3	1.76	0.51
1:A:551:ASN:OD1	1:A:599:ARG:NH2	2.43	0.51
1:A:686:ASP:OD1	1:A:686:ASP:N	2.41	0.51
3:C:47:LEU:HD22	3:C:58:VAL:HG21	1.93	0.51
4:D:100:ARG:HB3	4:D:106:TYR:HB2	1.92	0.51
1:A:153:PRO:HG3	1:A:314:LEU:HD12	1.92	0.50
4:D:93:VAL:HG22	4:D:116:THR:HG22	1.94	0.50
1:A:646:THR:HG21	1:A:700:LYS:HG3	1.93	0.50
4:D:47:TRP:HZ2	4:D:50:VAL:HG23	1.76	0.50
1:A:669:TYR:CE1	1:A:780:LEU:HB3	2.47	0.50
4:D:47:TRP:CZ2	4:D:50:VAL:HG23	2.46	0.50
1:A:226:LEU:HD13	1:A:262:LEU:HD11	1.94	0.50
1:A:141:LEU:HD13	2:B:98:THR:HG21	1.94	0.50
1:A:291:TRP:HE1	4:D:52:SER:HB3	1.77	0.50
1:A:369:ALA:O	1:A:373:THR:OG1	2.24	0.50
1:A:579:LEU:HA	1:A:631:ALA:HB2	1.94	0.49
1:A:179:LEU:HD13	1:A:563:LYS:HD2	1.94	0.49
3:C:136:LEU:HD21	3:C:196:VAL:HG21	1.93	0.49
1:A:216:THR:OG1	1:A:217:ASN:N	2.45	0.49
2:B:125:LEU:O	2:B:129:SER:N	2.45	0.49
1:A:67:HIS:CE1	1:A:70:ASN:HD21	2.31	0.49
4:D:40:ALA:HB3	4:D:43:LYS:HD2	1.94	0.48
1:A:503:ARG:HD2	1:A:570:ASN:O	2.14	0.48
2:B:116:LYS:HB3	2:B:121:ARG:NE	2.29	0.48
1:A:559:LEU:HD13	1:A:566:PHE:HB2	1.95	0.47
3:C:83:PHE:HE1	3:C:105:GLU:HG2	1.79	0.47
1:A:305:TYR:OH	1:A:380:GLU:HG2	2.14	0.47
4:D:131:PRO:HG3	4:D:217:LYS:HD3	1.97	0.47
3:C:11:VAL:HG11	3:C:19:VAL:HG13	1.97	0.47
3:C:48:ILE:HG21	3:C:51:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:VAL:O	1:A:400:LEU:HB2	2.15	0.47
1:A:714:ALA:O	1:A:726:TYR:OH	2.33	0.47
3:C:88:CYS:O	3:C:99:GLY:N	2.47	0.47
3:C:137:ASN:ND2	3:C:138:ASN:OD1	2.48	0.47
3:C:113:PRO:HB2	3:C:136:LEU:HD22	1.98	0.46
1:A:223:HIS:HB2	1:A:235:TYR:HE1	1.80	0.46
1:A:382:GLY:HA3	1:A:388:PHE:CE1	2.51	0.46
1:A:73:LYS:O	1:A:98:LYS:HB2	2.15	0.46
1:A:313:GLY:O	1:A:318:PHE:HB2	2.15	0.46
1:A:757:ALA:HB1	1:A:760:ASN:HB2	1.97	0.46
2:B:128:LEU:HA	2:B:131:VAL:HG23	1.98	0.46
3:C:29:ILE:HB	3:C:92:ASN:HB2	1.96	0.46
1:A:50:LEU:H	1:A:50:LEU:HD12	1.81	0.46
1:A:401:LYS:NZ	1:A:469:SER:OG	2.48	0.46
2:B:128:LEU:HD23	2:B:131:VAL:HG21	1.97	0.46
1:A:131:SER:OG	1:A:132:PHE:N	2.48	0.46
1:A:513:LEU:HD13	1:A:532:THR:HG21	1.98	0.46
1:A:154:PRO:HD3	1:A:312:ARG:NH2	2.31	0.45
4:D:160:VAL:HA	4:D:205:ASN:O	2.17	0.45
1:A:329:TYR:CE2	1:A:370:ARG:HG2	2.52	0.45
4:D:3:GLN:HB2	4:D:25:SER:HB2	1.97	0.45
3:C:109:THR:HB	3:C:110:VAL:H	1.66	0.45
4:D:17:SER:HA	4:D:83:LEU:O	2.16	0.45
1:A:182:ARG:NH2	1:A:387:TYR:O	2.49	0.45
3:C:195:GLU:HA	3:C:206:THR:HG22	1.96	0.45
3:C:35:TRP:CZ3	3:C:88:CYS:HB3	2.52	0.45
1:A:646:THR:HG21	1:A:700:LYS:HA	1.99	0.44
3:C:160:GLN:HG3	4:D:177:VAL:HG11	1.99	0.44
1:A:179:LEU:HB2	1:A:563:LYS:O	2.17	0.44
3:C:96:LEU:HD12	3:C:97:THR:H	1.81	0.44
1:A:93:LEU:HG	1:A:94:VAL:N	2.33	0.44
3:C:96:LEU:HD12	3:C:97:THR:N	2.32	0.44
1:A:480:LEU:O	1:A:484:VAL:HG23	2.16	0.44
2:B:146:GLY:O	2:B:157:ARG:NH1	2.51	0.44
4:D:131:PRO:HG3	4:D:217:LYS:HB3	2.00	0.44
1:A:779:LEU:HD22	1:A:789:LEU:HD21	1.99	0.44
1:A:400:LEU:HD23	1:A:423:SER:HB3	2.00	0.44
1:A:611:ASP:HB3	1:A:614:GLU:HG3	2.00	0.44
2:B:76:VAL:HG22	2:B:85:VAL:HG22	2.00	0.44
1:A:73:LYS:O	1:A:98:LYS:NZ	2.41	0.44
1:A:68:TRP:HA	1:A:68:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:HIS:ND1	4:D:50:VAL:HG22	2.33	0.43
1:A:200:TRP:CE2	1:A:440:LEU:HD22	2.52	0.43
1:A:77:LEU:HB3	1:A:94:VAL:HG13	1.99	0.43
1:A:584:THR:HB	1:A:620:PHE:HE1	1.83	0.43
1:A:152:PHE:CZ	1:A:229:SER:HB3	2.53	0.43
1:A:223:HIS:HB2	1:A:235:TYR:CE1	2.53	0.43
1:A:288:ASP:O	2:B:105:LYS:HD3	2.19	0.43
2:B:62:PRO:HG3	2:B:89:PHE:CZ	2.54	0.43
1:A:75:VAL:HG23	1:A:98:LYS:NZ	2.32	0.43
1:A:259:MET:HB2	1:A:376:PHE:CD1	2.54	0.43
1:A:550:LEU:HD12	1:A:550:LEU:HA	1.85	0.43
1:A:611:ASP:O	1:A:615:ILE:HG13	2.19	0.43
1:A:292:PHE:HD2	4:D:104:TYR:HD2	1.67	0.42
1:A:291:TRP:NE1	4:D:52:SER:HB3	2.33	0.42
1:A:292:PHE:CD2	4:D:104:TYR:HD2	2.37	0.42
3:C:63:SER:HG	3:C:74:THR:HG1	1.68	0.42
4:D:176:ALA:HA	4:D:186:LEU:HB3	2.01	0.42
3:C:108:ARG:HB3	3:C:109:THR:H	1.65	0.42
1:A:611:ASP:OD1	1:A:612:GLU:N	2.52	0.42
3:C:107:LYS:CG	3:C:108:ARG:N	2.82	0.42
1:A:264:SER:HB2	2:B:147:CYS:HA	2.00	0.42
1:A:567:THR:OG1	1:A:569:PRO:HD2	2.20	0.42
1:A:713:VAL:HG22	1:A:787:VAL:HG11	2.01	0.42
1:A:399:GLN:O	1:A:403:LEU:HB2	2.19	0.42
1:A:257:GLY:O	1:A:277:PRO:HD3	2.19	0.42
1:A:292:PHE:HD1	1:A:292:PHE:HA	1.78	0.41
1:A:282:LEU:HD12	1:A:308:TYR:CD2	2.55	0.41
3:C:154:LEU:HD23	3:C:159:SER:HB3	2.02	0.41
1:A:592:LEU:O	1:A:596:ILE:HG13	2.21	0.41
1:A:145:HIS:CE1	1:A:146:LEU:HG	2.54	0.41
1:A:154:PRO:HD3	1:A:312:ARG:HH22	1.85	0.41
1:A:179:LEU:HA	1:A:179:LEU:HD12	1.86	0.41
1:A:763:ILE:HA	1:A:764:PRO:HD2	1.88	0.41
3:C:149:LYS:HG2	3:C:193:ALA:HB3	2.02	0.41
4:D:35:HIS:CE1	4:D:50:VAL:HG22	2.55	0.41
4:D:130:PHE:HE2	4:D:151:LYS:HE2	1.85	0.41
1:A:587:ILE:HD12	1:A:587:ILE:H	1.86	0.41
2:B:156:GLN:HG2	2:B:158:VAL:H	1.86	0.41
2:B:136:THR:HA	2:B:137:PRO:HD3	1.87	0.41
4:D:187:SER:OG	4:D:188:SER:N	2.53	0.41
3:C:29:ILE:HB	3:C:92:ASN:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:GLN:CD	4:D:14:PRO:HD2	2.41	0.41
4:D:126:GLY:HA2	4:D:127:PRO:HD3	1.76	0.41
1:A:80:VAL:HG12	1:A:82:VAL:HG22	2.02	0.41
1:A:83:ASN:HA	1:A:84:PRO:HD3	1.90	0.41
2:B:125:LEU:HA	2:B:128:LEU:HB2	2.02	0.41
4:D:64:VAL:HG11	4:D:68:PHE:CZ	2.56	0.41
4:D:147:GLY:HA2	4:D:189:VAL:HA	2.02	0.41
1:A:238:THR:OG1	1:A:254:ILE:HG22	2.21	0.40
1:A:580:ARG:HG2	1:A:659:LEU:HD12	2.02	0.40
1:A:455:TYR:CE2	1:A:502:GLU:HG2	2.56	0.40
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.89	0.40
1:A:499:ASN:O	1:A:503:ARG:HG3	2.21	0.40
1:A:669:TYR:OH	1:A:781:PHE:O	2.27	0.40
1:A:712:THR:HB	1:A:790:LEU:HD21	2.04	0.40
3:C:27:GLN:HB2	3:C:29:ILE:HG23	2.04	0.40
1:A:98:LYS:CG	5:E:1:NAG:H62	2.52	0.40
1:A:247:SER:O	1:A:266:SER:N	2.33	0.40
3:C:29:ILE:HD12	3:C:92:ASN:HD22	1.85	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	A	720/833 (86%)	681 (95%)	39 (5%)	0	100	100
2	B	130/138 (94%)	122 (94%)	7 (5%)	1 (1%)	19	57
3	C	202/214 (94%)	183 (91%)	17 (8%)	2 (1%)	15	52
4	D	202/283 (71%)	186 (92%)	16 (8%)	0	100	100
All	All	1254/1468 (85%)	1172 (94%)	79 (6%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	109	THR
3	C	108	ARG
2	B	30	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/717 (84%)	557 (92%)	46 (8%)	13	42
2	B	111/121 (92%)	104 (94%)	7 (6%)	18	47
3	C	168/185 (91%)	163 (97%)	5 (3%)	41	64
4	D	157/231 (68%)	148 (94%)	9 (6%)	20	50
All	All	1039/1254 (83%)	972 (94%)	67 (6%)	17	47

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	46	MET
1	A	54	TYR
1	A	68	TRP
1	A	70	ASN
1	A	74	HIS
1	A	93	LEU
1	A	94	VAL
1	A	98	LYS
1	A	130	VAL
1	A	163	ARG
1	A	190	ILE
1	A	249	ARG
1	A	288	ASP
1	A	289	THR
1	A	290	THR
1	A	291	TRP
1	A	292	PHE
1	A	310	LEU

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Mol	Chain	Res	Type
1	A	325	ASP
1	A	373	THR
1	A	378	LEU
1	A	385	THR
1	A	393	ILE
1	A	394	VAL
1	A	395	ASP
1	A	398	TYR
1	A	422	THR
1	A	431	SER
1	A	440	LEU
1	A	516	PHE
1	A	571	VAL
1	A	617	ASP
1	A	621	LYS
1	A	627	THR
1	A	630	THR
1	A	641	VAL
1	A	643	GLU
1	A	647	CYS
1	A	658	VAL
1	A	674	ASN
1	A	678	ARG
1	A	715	LEU
1	A	722	LYS
1	A	743	ILE
1	A	774	ASP
2	B	40	ASP
2	B	41	VAL
2	B	119	ASP
2	B	121	ARG
2	B	124	LEU
2	B	153	ARG
2	B	157	ARG
3	C	32	TRP
3	C	54	LEU
3	C	97	THR
3	C	98	PHE
3	C	175	LEU
4	D	32	TYR
4	D	53	ASP
4	D	64	VAL

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Mol	Chain	Res	Type
4	D	108	MET
4	D	118	THR
4	D	203	ILE
4	D	214	LYS
4	D	216	ASP
4	D	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
3	C	160	GLN
4	D	103	HIS
4	D	179	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

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	E	1	5,2	14,14,15	0.71	0	17,19,21	1.26	1 (5%)
5	NAG	E	2	5	14,14,15	0.50	0	17,19,21	1.09	1 (5%)
5	BMA	E	3	5	11,11,12	0.83	0	15,15,17	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MAN	E	4	5	11,11,12	0.63	0	15,15,17	0.61	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
5	NAG	E	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1	NAG	O5-C1-C2	-4.41	104.33	111.29
5	E	2	NAG	C1-O5-C5	2.93	116.16	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6

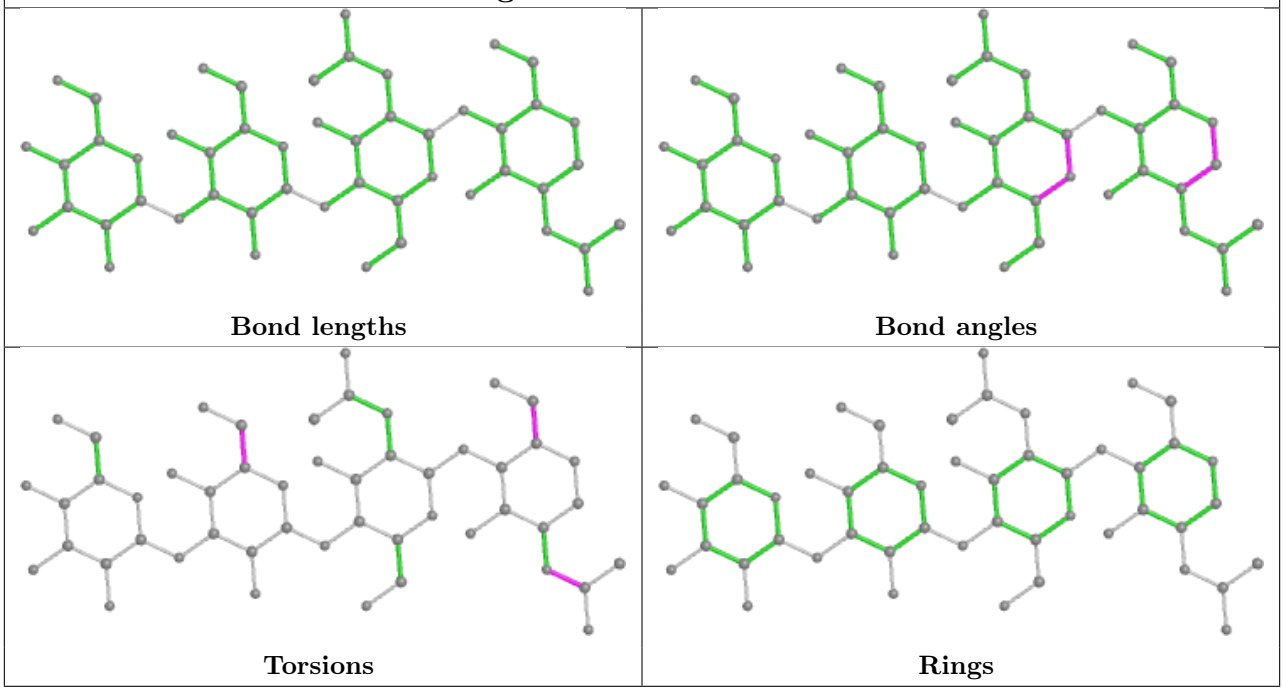
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
6	NAG	A	902	1	14,14,15	0.49	0	17,19,21	0.87	1 (5%)
6	NAG	A	901	1	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
6	NAG	A	903	1	14,14,15	0.51	0	17,19,21	0.84	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	902	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	901	1	-	4/6/23/26	0/1/1/1
6	NAG	A	903	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	902	NAG	C1-O5-C5	2.54	115.64	112.19
6	A	903	NAG	C1-O5-C5	2.52	115.61	112.19
6	A	901	NAG	C1-O5-C5	2.42	115.47	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	903	NAG	O5-C5-C6-O6
6	A	901	NAG	C8-C7-N2-C2
6	A	901	NAG	O7-C7-N2-C2
6	A	901	NAG	O5-C5-C6-O6
6	A	903	NAG	C4-C5-C6-O6
6	A	902	NAG	C8-C7-N2-C2
6	A	902	NAG	O7-C7-N2-C2
6	A	901	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	728/833 (87%)	0.07	12 (1%) 72 62	26, 69, 120, 174	0
2	B	132/138 (95%)	-0.02	3 (2%) 60 50	44, 78, 118, 131	0
3	C	206/214 (96%)	1.81	64 (31%) 0 0	96, 180, 277, 304	0
4	D	208/283 (73%)	2.37	78 (37%) 0 0	85, 169, 278, 314	0
All	All	1274/1468 (86%)	0.72	157 (12%) 4 4	26, 88, 264, 314	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	150	VAL	25.2
4	D	134	PRO	18.9
4	D	186	LEU	18.6
3	C	180	THR	17.8
3	C	119	PRO	13.8
4	D	149	LEU	13.2
3	C	178	THR	12.9
3	C	115	VAL	12.8
3	C	134	CYS	12.5
4	D	187	SER	11.6
4	D	160	VAL	10.9
3	C	177	SER	10.5
3	C	208	SER	10.2
3	C	144	ALA	9.9
4	D	193	PRO	9.7
3	C	133	VAL	9.2
4	D	128	SER	9.0
4	D	133	ALA	8.7
4	D	203	ILE	8.5
4	D	151	LYS	8.2
4	D	145	ALA	8.2

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Mol	Chain	Res	Type	RSRZ
3	C	176	SER	8.0
4	D	169	SER	7.6
4	D	192	VAL	7.6
4	D	170	GLY	7.3
3	C	179	LEU	7.1
4	D	148	CYS	7.0
3	C	116	PHE	7.0
3	C	120	PRO	6.8
4	D	176	ALA	6.7
3	C	150	VAL	6.7
4	D	132	LEU	6.6
3	C	145	LYS	6.4
4	D	127	PRO	6.2
4	D	204	CYS	6.1
4	D	146	LEU	6.1
3	C	117	ILE	5.9
4	D	202	TYR	5.9
4	D	147	GLY	5.7
3	C	196	VAL	5.6
4	D	185	SER	5.5
4	D	181	SER	5.5
3	C	132	VAL	5.4
4	D	161	SER	5.3
3	C	202	SER	5.3
4	D	1	GLU	5.1
3	C	118	PHE	5.1
4	D	171	VAL	5.1
4	D	131	PRO	5.0
3	C	151	ASP	5.0
4	D	130	PHE	4.9
3	C	121	SER	4.9
4	D	120	SER	4.9
4	D	223	SER	4.7
4	D	175	PRO	4.6
4	D	224	CYS	4.6
3	C	114	SER	4.6
3	C	193	ALA	4.6
4	D	168	THR	4.5
4	D	212	ASN	4.5
4	D	174	PHE	4.5
4	D	173	THR	4.4
4	D	94	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	146	VAL	4.3
3	C	122	ASP	4.3
3	C	181	LEU	4.3
1	A	314	LEU	4.2
3	C	149	LYS	4.2
3	C	1	ASP	4.1
4	D	2	VAL	4.1
3	C	131	SER	4.1
3	C	192	TYR	4.1
4	D	121	SER	4.1
3	C	19	VAL	4.0
4	D	213	THR	4.0
2	B	129	SER	4.0
3	C	130	ALA	3.9
4	D	111	TRP	3.8
4	D	166	ALA	3.7
4	D	180	SER	3.7
4	D	34	MET	3.7
3	C	156	SER	3.7
4	D	167	LEU	3.6
3	C	58	VAL	3.6
3	C	125	LEU	3.6
4	D	153	TYR	3.6
3	C	197	THR	3.6
2	B	130	GLY	3.6
4	D	152	ASP	3.5
4	D	163	ASN	3.5
1	A	43	ASP	3.5
3	C	155	GLN	3.5
4	D	159	THR	3.4
3	C	135	LEU	3.3
4	D	221	PRO	3.3
4	D	225	ASP	3.3
4	D	206	VAL	3.3
3	C	160	GLN	3.2
4	D	189	VAL	3.2
4	D	217	LYS	3.1
3	C	162	SER	3.1
1	A	290	THR	3.1
4	D	219	VAL	3.1
3	C	36	TYR	3.1
3	C	20	THR	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	62	PHE	3.0
3	C	59	PRO	3.0
4	D	122	ALA	3.0
3	C	207	LYS	3.0
4	D	35	HIS	2.9
4	D	100	ARG	2.9
4	D	208	HIS	2.9
4	D	191	THR	2.8
3	C	191	VAL	2.8
4	D	78	THR	2.7
3	C	161	GLU	2.7
1	A	319	SER	2.7
3	C	109	THR	2.7
1	A	288	ASP	2.7
3	C	201	LEU	2.6
1	A	289	THR	2.6
3	C	209	PHE	2.6
3	C	182	SER	2.6
3	C	93	ASN	2.6
4	D	207	ASN	2.6
4	D	70	ILE	2.6
1	A	680	LEU	2.6
3	C	194	CYS	2.5
3	C	210	ASN	2.5
4	D	222	LYS	2.5
4	D	97	ALA	2.5
4	D	184	TYR	2.4
4	D	129	VAL	2.4
4	D	218	ARG	2.4
4	D	36	TRP	2.4
1	A	88	GLU	2.4
3	C	95	PRO	2.4
3	C	63	SER	2.4
1	A	718	PRO	2.3
4	D	158	VAL	2.3
2	B	126	ASP	2.3
4	D	188	SER	2.2
3	C	203	SER	2.2
4	D	172	HIS	2.2
3	C	104	VAL	2.1
1	A	68	TRP	2.1
3	C	157	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	108	ARG	2.1
1	A	41	TYR	2.1
3	C	18	ARG	2.1
4	D	215	VAL	2.1
3	C	11	VAL	2.0
4	D	216	ASP	2.0
3	C	57	GLY	2.0
1	A	318	PHE	2.0
4	D	211	SER	2.0
4	D	45	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)

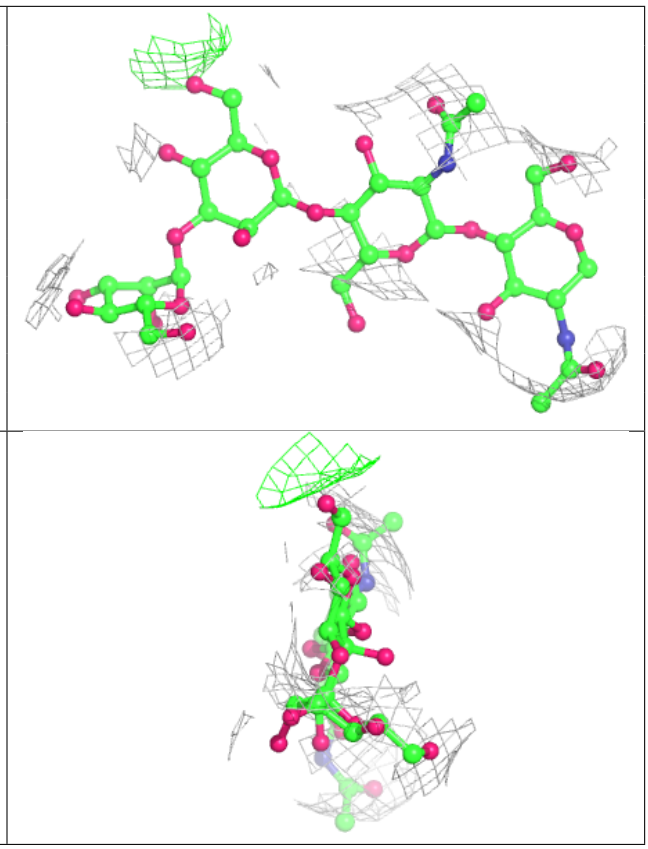
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	E	3	11/12	0.67	0.27	105,113,126,131	0
5	MAN	E	4	11/12	0.90	0.25	123,128,136,137	0
5	NAG	E	2	14/15	0.93	0.40	78,91,104,106	0
5	NAG	E	1	14/15	0.94	0.19	67,78,87,91	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(Å^2)	Q<0.9
6	NAG	A	902	14/15	0.81	0.22	76,85,93,95	0
6	NAG	A	901	14/15	0.86	0.25	35,46,60,64	0
6	NAG	A	903	14/15	0.90	0.15	88,99,110,111	0

6.5 Other polymers (i)

There are no such residues in this entry.