Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 06:42 PM EDT

PDB ID	:	5V2A
Title	:	Crystal structure of Fab H7.167 in complex with influenza virus hemagglutinin from A/Shanghai/02/2013 (H7N9)
Authors	:	Zhang, H.; Zhu, X.; Wilson, I.A.
Deposited on	:	2017-03-03
Resolution	:	4.66 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

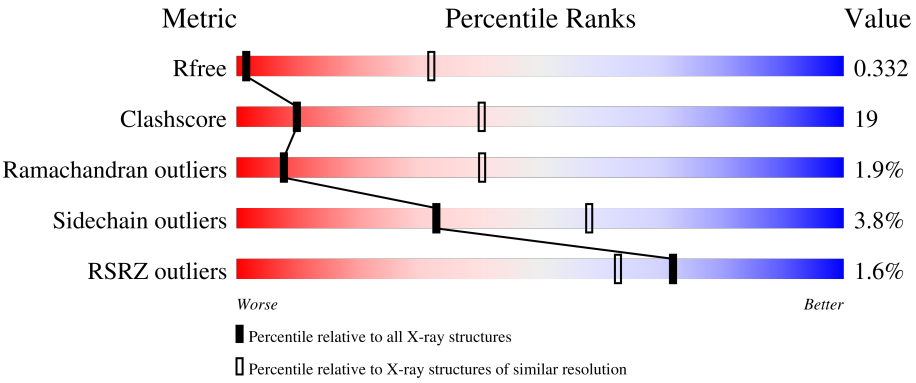
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.66 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	1083 (5.52-3.80)
Clashscore	141614	1156 (5.52-3.80)
Ramachandran outliers	138981	1092 (5.52-3.80)
Sidechain outliers	138945	1072 (5.50-3.80)
RSRZ outliers	127900	1114 (5.54-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	321	2% 51% 45%
2	B	183	% 57% 34% 7%
3	L	221	65% 29% 5%
4	H	220	4% 65% 24% 5%
5	C	3	67% 33%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7198 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2420	1504	437	464	15			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1384	854	242	281	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP A0A097PHH8
B	178	GLY	-	expression tag	UNP A0A097PHH8
B	179	ARG	-	expression tag	UNP A0A097PHH8
B	180	LEU	-	expression tag	UNP A0A097PHH8
B	181	VAL	-	expression tag	UNP A0A097PHH8
B	182	PRO	-	expression tag	UNP A0A097PHH8
B	183	ARG	-	expression tag	UNP A0A097PHH8

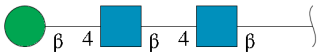
- Molecule 3 is a protein called Light chain (kappa) of H7.167 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	221	Total	C	N	O	S	0	0	0
			1702	1066	283	347	6			

- Molecule 4 is a protein called Heavy chain of H7.167 antibody.

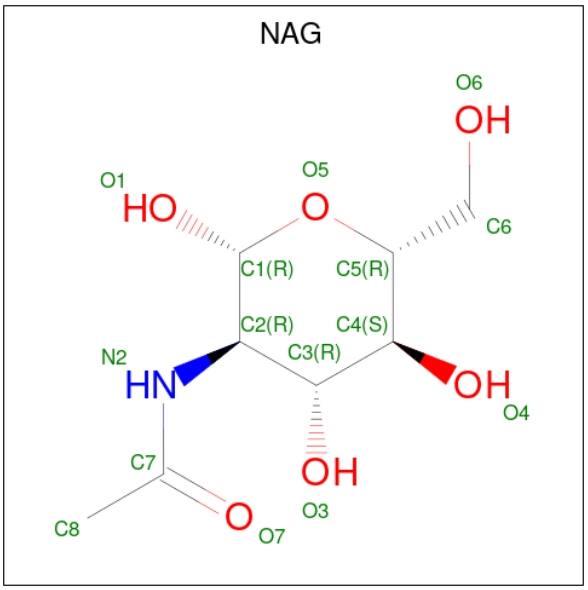
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	214	Total	C	N	O	S	0	0	0
			1625	1035	271	313	6			

- Molecule 5 is an oligosaccharide called 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
5	C	3	Total C N O 39 22 2 15	0	0	0

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



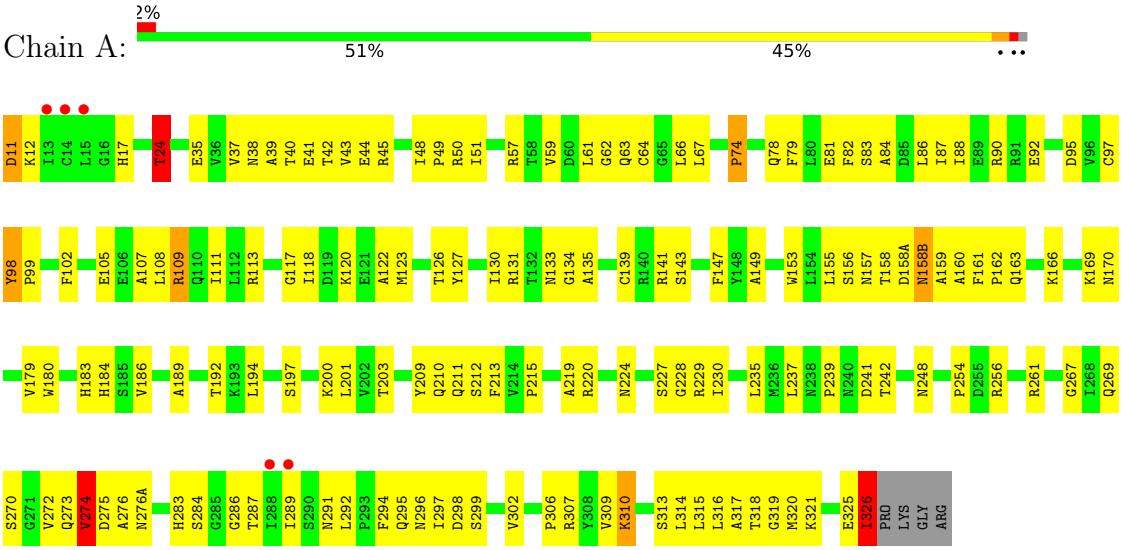
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0

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.

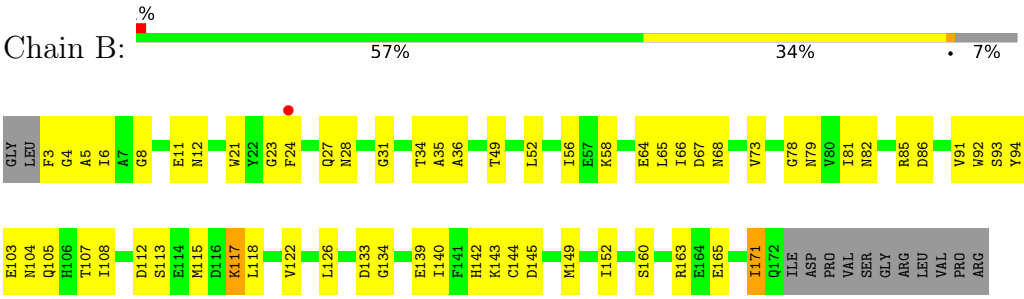
• Molecule 1: Hemagglutinin

Chain A:



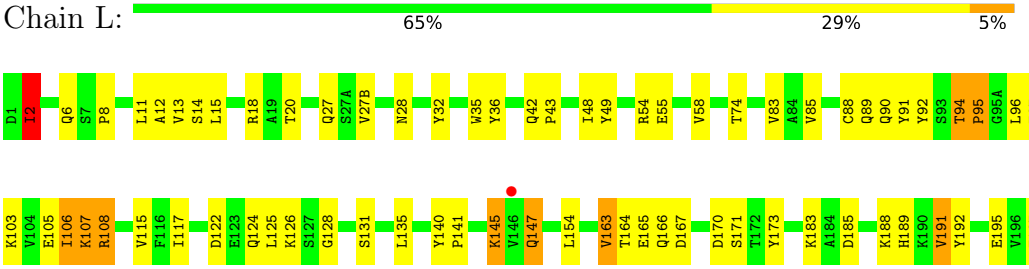
• Molecule 2: Hemagglutinin

Chain B:



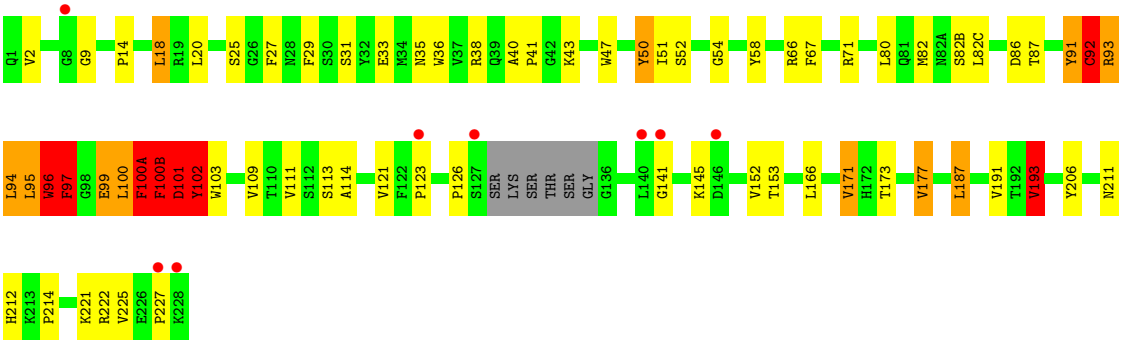
• Molecule 3: Light chain (kappa) of H7.167 antibody

Chain L:



• Molecule 4: Heavy chain of H7.167 antibody

Chain H:



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

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α, β, γ	207.28Å 207.28Å 207.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.35 – 4.66 46.35 – 4.66	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.35-4.66) 100.0 (46.35-4.66)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.258 , 0.334 0.262 , 0.332	Depositor DCC
R_{free} test set	409 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	230.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 202.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7198	wwPDB-VP
Average B, all atoms (Å^2)	303.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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

5.1 Standard geometry

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

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	0.79	0/2466	1.06	7/3333 (0.2%)
2	B	0.70	0/1408	0.86	3/1897 (0.2%)
3	L	0.69	0/1739	1.14	11/2363 (0.5%)
4	H	0.79	0/1666	1.16	10/2268 (0.4%)
All	All	0.75	0/7279	1.07	31/9861 (0.3%)

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
2	B	0	1
4	H	0	8
All	All	0	9

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	163	VAL	CG1-CB-CG2	-17.49	82.91	110.90
1	A	274	VAL	CG1-CB-CG2	-16.81	84.01	110.90
1	A	326	ILE	CG1-CB-CG2	-16.55	74.99	111.40
4	H	171	VAL	CG1-CB-CG2	-14.53	87.65	110.90
3	L	83	VAL	CG1-CB-CG2	-12.68	90.62	110.90
3	L	106	ILE	CG1-CB-CG2	-10.20	88.95	111.40
3	L	94	THR	C-N-CD	9.40	148.15	128.40
2	B	34	THR	OG1-CB-CG2	-8.78	89.82	110.00
3	L	205	VAL	CG1-CB-CG2	8.13	123.90	110.90
4	H	173	THR	OG1-CB-CG2	-8.04	91.51	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	2	ILE	CG1-CB-CG2	7.74	128.43	111.40
2	B	171	ILE	CG1-CB-CG2	7.44	127.78	111.40
4	H	193	VAL	CG1-CB-CG2	7.37	122.69	110.90
3	L	102	THR	OG1-CB-CG2	-7.14	93.57	110.00
3	L	207	LYS	CA-CB-CG	-6.88	98.27	113.40
3	L	191	VAL	CG1-CB-CG2	6.65	121.54	110.90
4	H	152	VAL	CB-CA-C	-6.55	98.95	111.40
4	H	177	VAL	CG1-CB-CG2	6.55	121.38	110.90
1	A	109	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	289	ILE	CG1-CB-CG2	6.34	125.36	111.40
4	H	193	VAL	CA-CB-CG2	6.22	120.22	110.90
3	L	117	ILE	CG1-CB-CG2	6.19	125.03	111.40
3	L	145	LYS	N-CA-CB	-5.75	100.25	110.60
1	A	310	LYS	CB-CA-C	-5.69	99.02	110.40
1	A	24	THR	OG1-CB-CG2	5.53	122.71	110.00
2	B	117	LYS	CB-CA-C	5.52	121.44	110.40
4	H	96	TRP	N-CA-C	-5.48	96.21	111.00
1	A	109	ARG	NE-CZ-NH1	5.40	123.00	120.30
4	H	97	PHE	N-CA-C	-5.23	96.87	111.00
4	H	187	LEU	CA-CB-CG	5.15	127.14	115.30
4	H	152	VAL	CA-CB-CG1	5.11	118.56	110.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	79	ASN	Sidechain
4	H	100	LEU	Peptide
4	H	100(A)	PHE	Peptide
4	H	100(B)	PHE	Peptide
4	H	101	ASP	Peptide
4	H	91	TYR	Peptide
4	H	94	LEU	Peptide
4	H	96	TRP	Peptide
4	H	99	GLU	Peptide

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	2420	0	2380	134	0
2	B	1384	0	1283	48	0
3	L	1702	0	1650	56	0
4	H	1625	0	1587	61	0
5	C	39	0	34	2	0
6	A	28	0	26	0	0
All	All	7198	0	6960	271	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 (271) 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)
2:B:3:PHE:HB2	2:B:112:ASP:HB3	1.42	0.98
1:A:37:VAL:HB	1:A:319:GLY:HA3	1.53	0.89
4:H:52:SER:O	4:H:71:ARG:NH1	2.05	0.88
3:L:6:GLN:NE2	3:L:101:GLY:H	1.74	0.85
3:L:105:GLU:OE1	3:L:173:TYR:OH	1.95	0.85
1:A:157:ASN:HB3	3:L:94:THR:HG21	1.59	0.83
4:H:87:THR:HG22	4:H:111:VAL:H	1.42	0.82
1:A:310:LYS:N	2:B:93:SER:OG	2.09	0.82
1:A:299:SER:HB2	2:B:85:ARG:HD3	1.60	0.81
3:L:91:TYR:HA	3:L:96:LEU:HD22	1.60	0.81
1:A:157:ASN:HB3	3:L:94:THR:CG2	2.12	0.79
1:A:62:GLY:HA2	1:A:90:ARG:HG3	1.65	0.78
2:B:5:ALA:HB1	2:B:115:MET:HG2	1.62	0.78
3:L:35:TRP:HD1	3:L:48:ILE:HB	1.49	0.78
2:B:95:ASN:O	2:B:99:LEU:N	2.17	0.77
1:A:310:LYS:H	2:B:93:SER:HG	1.32	0.76
1:A:272:VAL:HG22	1:A:273:GLN:H	1.50	0.76
3:L:164:THR:HG22	3:L:165:GLU:O	1.86	0.75
3:L:125:LEU:O	3:L:183:LYS:HD2	1.88	0.74
3:L:35:TRP:CD1	3:L:48:ILE:HB	2.22	0.73
1:A:12:LYS:HE2	2:B:139:GLU:HG2	1.71	0.73
1:A:99:PRO:HB2	1:A:229:ARG:HD3	1.72	0.72
3:L:147:GLN:HG2	3:L:154:LEU:HD11	1.72	0.72
1:A:184:HIS:HB2	1:A:220:ARG:HH12	1.53	0.71
4:H:14:PRO:HD2	4:H:113:SER:HB3	1.72	0.71
1:A:41:GLU:OE2	1:A:313:SER:OG	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:92:CYS:SG	4:H:93:ARG:N	2.62	0.70
1:A:109:ARG:O	1:A:113:ARG:N	2.22	0.70
1:A:78:GLN:N	1:A:78:GLN:OE1	2.25	0.69
4:H:35:ASN:OD1	4:H:47:TRP:NE1	2.22	0.68
1:A:141:ARG:NH2	1:A:147:PHE:O	2.28	0.67
2:B:142:HIS:HB2	2:B:165:GLU:CD	2.15	0.67
4:H:51:ILE:HD12	4:H:71:ARG:HG3	1.77	0.67
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.78	0.66
1:A:38:ASN:O	1:A:318:THR:N	2.29	0.65
1:A:123:MET:HG3	1:A:256:ARG:HA	1.79	0.65
1:A:126:THR:O	1:A:166:LYS:NZ	2.20	0.65
3:L:48:ILE:HD13	3:L:54:ARG:HA	1.79	0.65
3:L:18:ARG:HH21	3:L:20:THR:HG21	1.62	0.64
3:L:12:ALA:HA	3:L:105:GLU:O	1.98	0.64
1:A:314:LEU:HB3	2:B:100:VAL:HG11	1.80	0.64
4:H:212:HIS:CD2	4:H:214:PRO:HD2	2.33	0.63
3:L:6:GLN:HE21	3:L:100:GLY:H	1.47	0.63
4:H:95:LEU:HD23	4:H:100(B):PHE:HB2	1.80	0.63
4:H:31:SER:HB3	5:C:1:NAG:H83	1.79	0.62
1:A:57:ARG:HH21	1:A:83:SER:HB2	1.64	0.62
4:H:153:THR:OG1	4:H:211:ASN:HB3	1.99	0.62
1:A:131:ARG:HD2	1:A:133:ASN:OD1	1.99	0.61
1:A:127:TYR:HB3	1:A:130:ILE:HD11	1.81	0.61
4:H:14:PRO:HG3	4:H:111:VAL:HG12	1.81	0.61
4:H:100(B):PHE:CD1	4:H:101:ASP:HB2	2.35	0.61
1:A:79:PHE:HA	1:A:82:PHE:HB3	1.83	0.61
2:B:105:GLN:O	2:B:105:GLN:NE2	2.31	0.60
1:A:325:GLU:HA	2:B:12:ASN:HD22	1.67	0.60
1:A:153:TRP:HZ2	1:A:194:LEU:HD13	1.66	0.60
1:A:184:HIS:CB	1:A:220:ARG:HH12	2.13	0.60
4:H:51:ILE:HG22	4:H:54:GLY:HA2	1.84	0.60
4:H:95:LEU:CD2	4:H:100(B):PHE:HB2	2.32	0.60
4:H:51:ILE:CG2	4:H:54:GLY:HA2	2.32	0.60
2:B:82:ASN:O	2:B:86:ASP:HB2	2.02	0.60
4:H:66:ARG:NH1	4:H:82(B):SER:O	2.34	0.59
1:A:40:THR:N	1:A:316:LEU:O	2.32	0.59
1:A:102:PHE:HB2	1:A:105:GLU:HB3	1.82	0.59
4:H:18:LEU:O	4:H:82:MET:N	2.32	0.59
2:B:4:GLY:O	2:B:8:GLY:HA3	2.02	0.59
3:L:32:TYR:HD2	3:L:92:TYR:HA	1.67	0.59
1:A:186:VAL:CG2	1:A:227:SER:HB2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:GLU:O	2:B:107:THR:OG1	2.17	0.59
1:A:40:THR:HG22	1:A:316:LEU:O	2.02	0.59
2:B:126:LEU:HD21	2:B:152:ILE:HD13	1.84	0.58
4:H:166:LEU:HD21	4:H:191:VAL:HG21	1.85	0.58
1:A:316:LEU:HA	2:B:104:ASN:HD21	1.68	0.58
4:H:96:TRP:CE3	4:H:97:PHE:N	2.71	0.58
1:A:200:LYS:O	1:A:215:PRO:HD2	2.05	0.57
3:L:131:SER:OG	4:H:145:LYS:NZ	2.36	0.57
3:L:18:ARG:NH2	3:L:20:THR:HG21	2.19	0.57
3:L:107:LYS:HA	3:L:140:TYR:OH	2.05	0.57
1:A:74:PRO:HB3	1:A:141:ARG:HG3	1.87	0.57
1:A:59:VAL:HG13	1:A:84:ALA:HB2	1.87	0.56
1:A:97:CYS:O	1:A:224:ASN:ND2	2.38	0.56
1:A:201:LEU:HD11	1:A:212:SER:OG	2.04	0.56
1:A:272:VAL:HG22	1:A:273:GLN:N	2.19	0.56
2:B:23:GLY:HA2	2:B:36:ALA:HA	1.86	0.56
1:A:86:LEU:HD12	1:A:87:ILE:H	1.70	0.56
1:A:48:ILE:O	1:A:287:THR:N	2.37	0.56
1:A:81:GLU:HG2	1:A:120:LYS:H	1.69	0.56
1:A:24:THR:O	1:A:35:GLU:HG2	2.06	0.56
1:A:296:ASN:O	1:A:297:ILE:HD13	2.06	0.56
1:A:37:VAL:HB	1:A:319:GLY:CA	2.33	0.56
1:A:131:ARG:HB3	1:A:133:ASN:OD1	2.04	0.55
1:A:326:ILE:H	2:B:12:ASN:HD22	1.54	0.55
3:L:167:ASP:HB3	3:L:170:ASP:OD1	2.06	0.55
3:L:191:VAL:HG22	3:L:210:ASN:OD1	2.07	0.55
1:A:237:LEU:HD11	1:A:241:ASP:HB3	1.89	0.55
1:A:321:LYS:HB2	2:B:108:ILE:HG23	1.88	0.55
1:A:315:LEU:O	2:B:104:ASN:ND2	2.38	0.55
4:H:102:TYR:C	4:H:103:TRP:CD1	2.81	0.55
1:A:158:THR:HG22	4:H:50:TYR:CZ	2.42	0.54
1:A:201:LEU:HD12	1:A:213:PHE:O	2.08	0.54
1:A:291:ASN:HA	2:B:58:LYS:HE3	1.90	0.54
1:A:156:SER:HA	1:A:161:PHE:HD2	1.72	0.54
2:B:49:THR:HA	2:B:52:LEU:HB2	1.90	0.54
3:L:167:ASP:O	3:L:171:SER:N	2.34	0.53
1:A:37:VAL:HG21	1:A:320:MET:HG2	1.90	0.53
3:L:128:GLY:C	3:L:183:LYS:HB2	2.29	0.53
4:H:222:ARG:CZ	4:H:222:ARG:HB3	2.37	0.53
4:H:141:GLY:O	4:H:225:VAL:HG21	2.09	0.53
3:L:115:VAL:HA	3:L:135:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:82(C):LEU:HB3	4:H:111:VAL:HG11	1.90	0.53
1:A:40:THR:O	1:A:316:LEU:N	2.31	0.52
2:B:24:PHE:HB2	2:B:35:ALA:HB3	1.91	0.52
3:L:124:GLN:HE22	3:L:131:SER:N	2.06	0.52
3:L:140:TYR:CG	3:L:141:PRO:HA	2.45	0.52
4:H:33:GLU:OE1	4:H:33:GLU:N	2.43	0.52
1:A:189:ALA:O	1:A:192:THR:N	2.42	0.52
1:A:163:GLN:OE1	1:A:248:ASN:HB3	2.08	0.52
1:A:87:ILE:HB	1:A:267:GLY:HA2	1.92	0.52
2:B:118:LEU:O	2:B:122:VAL:HG23	2.10	0.52
3:L:91:TYR:HA	3:L:96:LEU:CD2	2.37	0.51
1:A:63:GLN:HA	1:A:92:GLU:HG2	1.92	0.51
1:A:170:ASN:HD22	1:A:239:PRO:HA	1.76	0.51
1:A:270:SER:HA	1:A:284:SER:HA	1.92	0.51
3:L:14:SER:OG	3:L:107:LYS:HB2	2.11	0.51
3:L:101:GLY:O	3:L:102:THR:HG23	2.10	0.51
1:A:170:ASN:ND2	1:A:239:PRO:HA	2.25	0.51
1:A:159:ALA:HA	4:H:96:TRP:HH2	1.75	0.51
1:A:307:ARG:HG3	2:B:92:TRP:CE3	2.46	0.51
3:L:15:LEU:HD13	3:L:106:ILE:HD13	1.92	0.50
4:H:2:VAL:HG13	4:H:27:PHE:CE1	2.45	0.50
1:A:158:THR:OG1	1:A:158(A):ASP:N	2.44	0.50
3:L:124:GLN:HE22	3:L:131:SER:H	1.60	0.50
1:A:179:VAL:O	1:A:254:PRO:HB3	2.12	0.50
1:A:153:TRP:CZ2	1:A:194:LEU:HD13	2.45	0.50
1:A:39:ALA:HA	1:A:317:ALA:HA	1.92	0.49
2:B:91:VAL:O	2:B:94:TYR:HB3	2.11	0.49
3:L:90:GLN:OE1	3:L:92:TYR:N	2.44	0.49
1:A:61:LEU:HB3	1:A:64:CYS:HB3	1.95	0.49
3:L:27(B):VAL:HG12	3:L:92:TYR:HB2	1.93	0.49
1:A:17:HIS:CE1	2:B:6:ILE:HG23	2.48	0.49
4:H:102:TYR:C	4:H:103:TRP:HD1	2.16	0.49
2:B:143:LYS:HD3	2:B:144:CYS:N	2.27	0.49
4:H:95:LEU:HB2	4:H:100(B):PHE:HB2	1.95	0.49
1:A:49:PRO:O	1:A:272:VAL:HG21	2.13	0.49
1:A:159:ALA:HA	4:H:96:TRP:CH2	2.47	0.49
4:H:31:SER:CB	5:C:1:NAG:H83	2.42	0.49
4:H:96:TRP:HE3	4:H:97:PHE:N	2.11	0.49
4:H:100(A):PHE:CD2	4:H:100(B):PHE:CE1	3.00	0.49
4:H:9:GLY:HA2	4:H:109:VAL:HG22	1.94	0.48
1:A:78:GLN:H	1:A:78:GLN:CD	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:CG2	1:A:273:GLN:H	2.24	0.48
4:H:102:TYR:O	4:H:103:TRP:CD1	2.66	0.48
1:A:320:MET:CE	2:B:21:TRP:HB3	2.44	0.48
4:H:100(B):PHE:HD1	4:H:101:ASP:HB2	1.76	0.48
1:A:88:ILE:HG21	1:A:90:ARG:NH2	2.29	0.48
1:A:197:SER:OG	3:L:28:ASN:ND2	2.45	0.48
1:A:316:LEU:HD12	2:B:104:ASN:OD1	2.14	0.48
1:A:186:VAL:HG23	1:A:227:SER:HB2	1.95	0.48
3:L:107:LYS:HA	3:L:140:TYR:CZ	2.49	0.48
4:H:20:LEU:HB2	4:H:80:LEU:HB3	1.95	0.48
1:A:107:ALA:O	1:A:111:ILE:HG13	2.13	0.48
3:L:14:SER:OG	3:L:107:LYS:HD2	2.14	0.48
4:H:35:ASN:HB3	4:H:92:CYS:SG	2.54	0.47
1:A:95:ASP:OD2	1:A:109:ARG:NH2	2.47	0.47
1:A:120:LYS:HA	1:A:120:LYS:HD3	1.56	0.47
2:B:160:SER:HA	2:B:163:ARG:HB2	1.95	0.47
1:A:211:GLN:HG3	1:A:212:SER:H	1.79	0.47
2:B:27:GLN:HA	2:B:31:GLY:O	2.15	0.47
4:H:126:PRO:HG2	4:H:227:PRO:HB3	1.97	0.47
3:L:6:GLN:CD	3:L:101:GLY:H	2.18	0.46
1:A:66:LEU:HD23	1:A:109:ARG:HA	1.97	0.46
2:B:145:ASP:O	2:B:149:MET:HG2	2.15	0.46
3:L:2:ILE:HG23	3:L:27:GLN:HB2	1.96	0.46
1:A:122:ALA:HA	1:A:256:ARG:HG2	1.96	0.46
4:H:123:PRO:HD3	4:H:221:LYS:NZ	2.31	0.46
3:L:94:THR:HG23	3:L:95:PRO:N	2.30	0.46
4:H:40:ALA:HB3	4:H:43:LYS:HB2	1.97	0.46
1:A:141:ARG:HH22	1:A:149:ALA:N	2.14	0.46
2:B:142:HIS:HB2	2:B:165:GLU:OE1	2.14	0.46
4:H:193:VAL:HG11	4:H:206:TYR:CZ	2.51	0.46
1:A:51:ILE:HD13	1:A:286:GLY:HA2	1.97	0.46
1:A:283:HIS:ND1	1:A:286:GLY:O	2.49	0.46
4:H:67:PHE:CZ	4:H:82:MET:HE3	2.51	0.46
3:L:189:HIS:HB2	3:L:192:TYR:OH	2.16	0.46
4:H:212:HIS:CE1	4:H:214:PRO:HB2	2.50	0.46
1:A:135:ALA:O	1:A:153:TRP:HZ3	1.98	0.45
1:A:275:ASP:OD1	1:A:276:ALA:N	2.49	0.45
1:A:67:LEU:HD13	1:A:108:LEU:HD23	1.98	0.45
1:A:98:TYR:N	1:A:139:CYS:SG	2.89	0.45
3:L:107:LYS:O	3:L:108:ARG:HG2	2.17	0.45
1:A:40:THR:HG23	1:A:316:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:166:LEU:CD2	4:H:191:VAL:HG21	2.46	0.45
1:A:180:TRP:CH2	1:A:235:LEU:HD23	2.51	0.45
3:L:18:ARG:HG2	3:L:74:THR:HG23	1.98	0.45
3:L:36:TYR:HE1	3:L:89:GLN:OE1	2.00	0.45
3:L:195:GLU:HB2	3:L:206:THR:HG22	1.99	0.45
4:H:50:TYR:HE1	4:H:58:TYR:HD2	1.64	0.45
1:A:200:LYS:HB2	1:A:215:PRO:HG3	1.99	0.45
1:A:273:GLN:HG3	1:A:274:VAL:N	2.31	0.45
1:A:57:ARG:NH2	1:A:83:SER:HB2	2.28	0.44
4:H:66:ARG:C	4:H:67:PHE:HD1	2.20	0.44
1:A:118:ILE:HD12	1:A:120:LYS:HE3	1.99	0.44
2:B:64:GLU:O	2:B:66:ILE:HG23	2.17	0.44
3:L:13:VAL:O	3:L:106:ILE:HA	2.17	0.44
1:A:12:LYS:HE3	1:A:12:LYS:HB2	1.75	0.44
1:A:42:THR:C	1:A:292:LEU:HD13	2.38	0.44
1:A:160:ALA:O	1:A:162:PRO:HD3	2.17	0.44
1:A:302:VAL:HG11	2:B:65:LEU:HA	1.99	0.44
1:A:326:ILE:HD13	1:A:326:ILE:HG21	1.56	0.44
3:L:49:TYR:HE1	3:L:55:GLU:HA	1.83	0.44
4:H:2:VAL:HA	4:H:25:SER:O	2.18	0.44
1:A:219:ALA:C	1:A:220:ARG:HG3	2.38	0.43
2:B:113:SER:O	2:B:117:LYS:HB2	2.17	0.43
4:H:29:PHE:O	4:H:31:SER:N	2.51	0.43
4:H:36:TRP:CE3	4:H:91:TYR:O	2.71	0.43
2:B:66:ILE:HD12	2:B:81:ILE:HD13	2.00	0.43
1:A:219:ALA:O	1:A:220:ARG:HG3	2.18	0.43
4:H:20:LEU:HD12	4:H:80:LEU:HD23	2.01	0.43
1:A:316:LEU:HA	2:B:104:ASN:ND2	2.31	0.43
2:B:56:ILE:O	2:B:58:LYS:HG3	2.19	0.43
1:A:209:TYR:C	1:A:210:GLN:HG3	2.39	0.43
1:A:98:TYR:HE1	1:A:228:GLY:O	2.02	0.43
3:L:42:GLN:HG2	3:L:43:PRO:HD2	1.99	0.43
3:L:8:PRO:O	3:L:102:THR:HG22	2.19	0.43
2:B:28:ASN:ND2	2:B:145:ASP:HA	2.34	0.42
1:A:158(B):ASN:ND2	4:H:97:PHE:C	2.73	0.42
1:A:283:HIS:HB2	1:A:298:ASP:OD2	2.19	0.42
1:A:320:MET:HE3	2:B:21:TRP:HB3	2.00	0.42
2:B:52:LEU:HD23	2:B:52:LEU:HA	1.89	0.42
1:A:42:THR:O	1:A:292:LEU:HB3	2.19	0.42
3:L:2:ILE:HG23	3:L:27:GLN:H	1.83	0.42
3:L:85:VAL:HG22	3:L:103:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:HG3	1:A:141:ARG:HE	1.84	0.42
1:A:86:LEU:HD12	1:A:87:ILE:N	2.33	0.42
1:A:269:GLN:HE22	2:B:68:ASN:CG	2.22	0.42
1:A:45:ARG:HA	1:A:297:ILE:HD11	2.01	0.42
1:A:295:GLN:HG2	1:A:306:PRO:HG2	2.00	0.42
1:A:117:GLY:O	1:A:261:ARG:HG3	2.20	0.42
1:A:158(B):ASN:HB3	4:H:96:TRP:CH2	2.55	0.42
3:L:8:PRO:HD2	3:L:11:LEU:HD23	2.01	0.42
4:H:38:ARG:NH1	4:H:86:ASP:HA	2.35	0.42
4:H:82(C):LEU:HA	4:H:82(C):LEU:HD23	1.49	0.42
1:A:98:TYR:CD1	1:A:99:PRO:HD2	2.55	0.42
1:A:130:ILE:HD12	1:A:131:ARG:O	2.20	0.42
3:L:6:GLN:HE21	3:L:100:GLY:N	2.15	0.42
3:L:90:GLN:HG2	3:L:97:THR:OG1	2.19	0.42
4:H:121:VAL:O	4:H:221:LYS:HE3	2.19	0.42
1:A:186:VAL:HG21	1:A:227:SER:HB2	2.00	0.42
1:A:320:MET:HG3	1:A:321:LYS:O	2.20	0.41
2:B:78:GLY:O	2:B:82:ASN:HB2	2.20	0.41
3:L:54:ARG:HD3	3:L:58:VAL:HG12	2.02	0.41
1:A:131:ARG:CZ	1:A:155:LEU:HD12	2.50	0.41
1:A:11:ASP:OD1	1:A:11:ASP:N	2.53	0.41
1:A:131:ARG:NH1	1:A:155:LEU:HD12	2.35	0.41
1:A:153:TRP:HZ2	1:A:194:LEU:CD1	2.32	0.41
2:B:140:ILE:HG22	2:B:142:HIS:H	1.85	0.41
4:H:95:LEU:HB2	4:H:100(B):PHE:CB	2.49	0.41
3:L:185:ASP:HA	3:L:188:LYS:HD3	2.02	0.41
4:H:51:ILE:HB	4:H:71:ARG:HD2	2.02	0.41
1:A:43:VAL:HG22	1:A:309:VAL:HG21	2.02	0.41
1:A:183:HIS:HD2	1:A:230:ILE:HG12	1.86	0.41
1:A:50:ARG:HD3	1:A:273:GLN:HE21	1.86	0.41
4:H:35:ASN:HD22	4:H:94:LEU:HD11	1.86	0.41
1:A:24:THR:HG21	1:A:39:ALA:HB3	2.02	0.41
1:A:169:LYS:HG2	1:A:242:THR:HG22	2.01	0.40
3:L:122:ASP:O	3:L:126:LYS:HG2	2.22	0.40
4:H:193:VAL:HG21	4:H:206:TYR:CE2	2.56	0.40
3:L:145:LYS:HB2	3:L:197:THR:HB	2.02	0.40
1:A:43:VAL:HG22	1:A:294:PHE:HB2	2.02	0.40
1:A:44:GLU:H	1:A:295:GLN:HA	1.85	0.40
2:B:133:ASP:OD1	2:B:133:ASP:N	2.53	0.40
2:B:67:ASP:HB3	2:B:68:ASN:H	1.77	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	315/321 (98%)	285 (90%)	27 (9%)	3 (1%)	15 54
2	B	168/183 (92%)	152 (90%)	14 (8%)	2 (1%)	13 50
3	L	219/221 (99%)	197 (90%)	19 (9%)	3 (1%)	11 47
4	H	210/220 (96%)	186 (89%)	15 (7%)	9 (4%)	2 25
All	All	912/945 (96%)	820 (90%)	75 (8%)	17 (2%)	8 40

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158(B)	ASN
3	L	107	LYS
3	L	108	ARG
4	H	92	CYS
4	H	93	ARG
4	H	100(A)	PHE
4	H	101	ASP
4	H	114	ALA
4	H	97	PHE
4	H	102	TYR
4	H	99	GLU
1	A	143	SER
3	L	95	PRO
1	A	74	PRO
2	B	73	VAL
2	B	134	GLY
4	H	41	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	266/269 (99%)	259 (97%)	7 (3%)	46	67
2	B	146/157 (93%)	144 (99%)	2 (1%)	67	81
3	L	194/194 (100%)	188 (97%)	6 (3%)	40	63
4	H	181/186 (97%)	166 (92%)	15 (8%)	11	36
All	All	787/806 (98%)	757 (96%)	30 (4%)	33	58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	24	THR
1	A	98	TYR
1	A	203	THR
1	A	274	VAL
1	A	276(A)	ASN
1	A	326	ILE
2	B	11	GLU
2	B	171	ILE
3	L	2	ILE
3	L	88	CYS
3	L	147	GLN
3	L	163	VAL
3	L	166	GLN
3	L	205	VAL
4	H	18	LEU
4	H	50	TYR
4	H	92	CYS
4	H	95	LEU
4	H	96	TRP
4	H	97	PHE
4	H	100	LEU
4	H	100(A)	PHE
4	H	100(B)	PHE
4	H	101	ASP
4	H	102	TYR
4	H	171	VAL
4	H	177	VAL

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Mol	Chain	Res	Type
4	H	187	LEU
4	H	193	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	273	GLN
2	B	12	ASN
3	L	6	GLN
3	L	124	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)

3 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	C	1	5,4	14,14,15	0.98	1 (7%)	17,19,21	0.99	0
5	NAG	C	2	5	14,14,15	0.99	1 (7%)	17,19,21	0.95	2 (11%)
5	BMA	C	3	5	11,11,12	3.37	6 (54%)	15,15,17	1.37	3 (20%)

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	C	1	5,4	-	4/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3	BMA	C4-C3	6.47	1.68	1.52
5	C	3	BMA	O5-C1	5.69	1.52	1.43
5	C	3	BMA	C4-C5	4.45	1.62	1.53
5	C	3	BMA	C1-C2	3.12	1.59	1.52
5	C	1	NAG	O5-C1	-2.87	1.39	1.43
5	C	2	NAG	C1-C2	2.59	1.56	1.52
5	C	3	BMA	O2-C2	2.35	1.48	1.43
5	C	3	BMA	C2-C3	2.24	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	3	BMA	O3-C3-C4	2.39	115.87	110.35
5	C	2	NAG	C3-C4-C5	2.32	114.38	110.24
5	C	2	NAG	C1-O5-C5	2.18	115.15	112.19
5	C	3	BMA	O2-C2-C1	2.02	113.28	109.15
5	C	3	BMA	C6-C5-C4	2.01	117.70	113.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

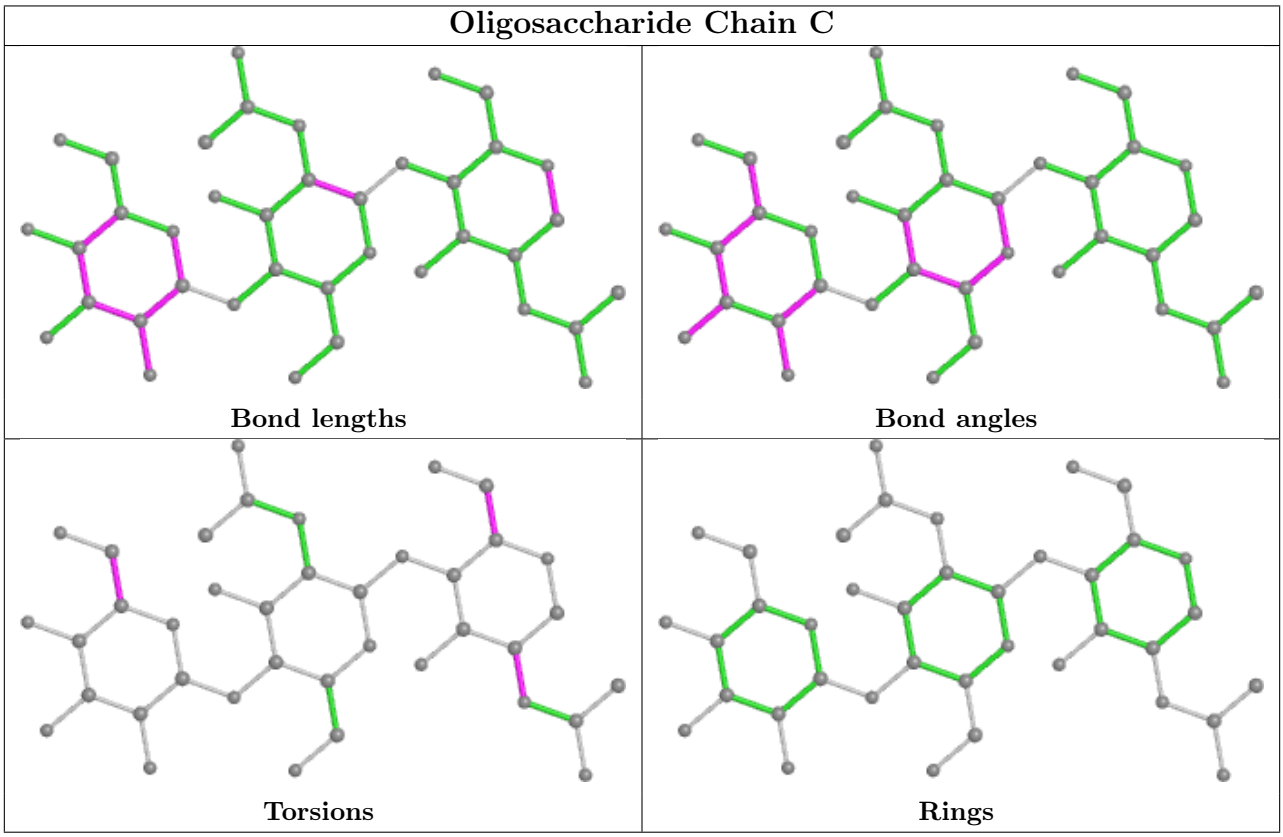
Mol	Chain	Res	Type	Atoms
5	C	1	NAG	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
5	C	3	BMA	C4-C5-C6-O6
5	C	1	NAG	C3-C2-N2-C7
5	C	3	BMA	O5-C5-C6-O6
5	C	1	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	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.



5.6 Ligand geometry

2 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	402	1	14,14,15	0.31	0	17,19,21	0.58	0
6	NAG	A	401	1	14,14,15	0.41	0	17,19,21	0.40	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	A	402	1	-	4/6/23/26	0/1/1/1
6	NAG	A	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	402	NAG	O5-C5-C6-O6
6	A	402	NAG	C4-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	A	401	NAG	O5-C5-C6-O6
6	A	402	NAG	C3-C2-N2-C7
6	A	402	NAG	C1-C2-N2-C7

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	317/321 (98%)	-0.44	5 (1%)	72	63	225, 266, 306, 354	0
2	B	170/183 (92%)	-0.27	1 (0%)	89	84	229, 310, 349, 380	0
3	L	221/221 (100%)	-0.31	1 (0%)	91	85	256, 327, 437, 476	0
4	H	214/220 (97%)	-0.24	8 (3%)	41	33	223, 286, 412, 431	0
All	All	922/945 (97%)	-0.33	15 (1%)	72	63	223, 285, 417, 476	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	140	LEU	4.9
1	A	14	CYS	4.2
4	H	228	LYS	3.5
1	A	288	ILE	3.2
4	H	123	PRO	2.9
1	A	15	LEU	2.8
2	B	24	PHE	2.6
4	H	127	SER	2.5
4	H	141	GLY	2.4
1	A	13	ILE	2.3
4	H	8	GLY	2.3
4	H	146	ASP	2.2
3	L	146	VAL	2.1
4	H	227	PRO	2.0
1	A	289	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

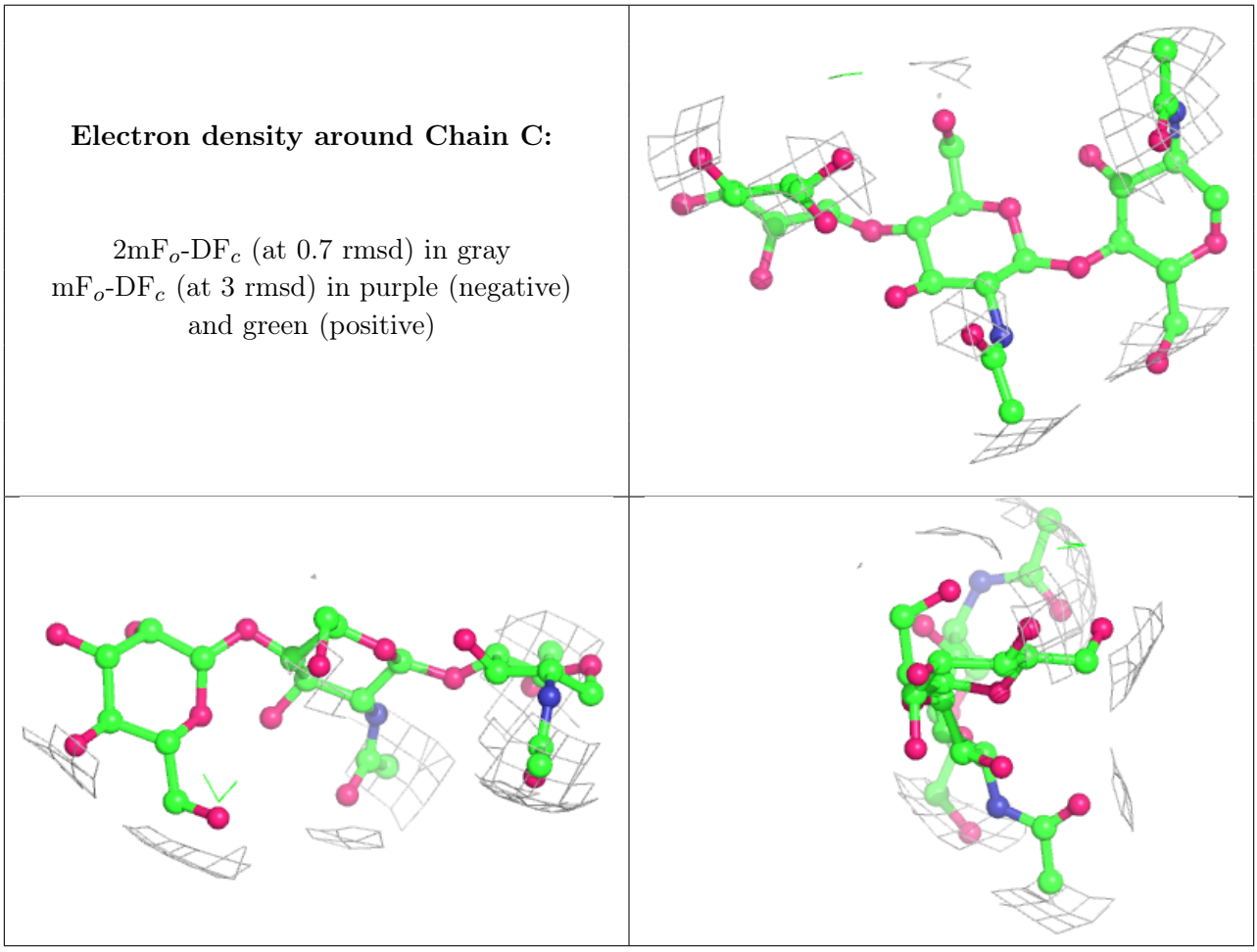
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	C	3	11/12	0.80	0.18	242,242,242,242	0
5	NAG	C	2	14/15	0.93	0.13	242,242,242,242	0
5	NAG	C	1	14/15	0.95	0.11	242,242,242,242	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.



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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	401	14/15	0.73	0.34	242,242,242,242	0
6	NAG	A	402	14/15	0.75	0.20	242,242,242,242	0

6.5 Other polymers (i)

There are no such residues in this entry.