Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:19 AM JST

PDB ID	:	7CJ2
Title	:	Crystal structure of the Fab antibody complexed with human YKL-40
Authors	:	Choi, S.; Na, J.H.; Lee, S.J.; Woo, J.R.; Kim, D.Y.; Hong, J.T.; Lee, W.K.
Deposited on	:	2020-07-09
Resolution	:	2.70 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:

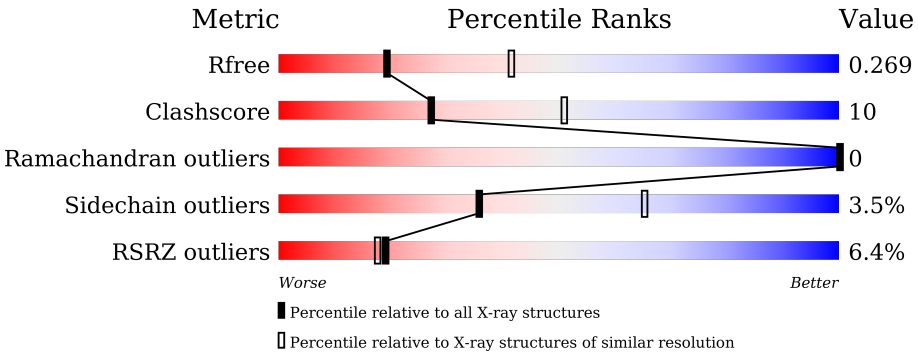
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	C	222	9% 67% 24% • 8%
1	K	222	8% 66% 18% 15%
2	D	215	12% 74% 21% • •
2	L	215	13% 71% 24% • •
3	A	362	% 82% 17% •
3	B	362	% 81% 19%

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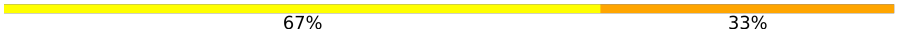
Mol	Chain	Length	Quality of chain
4	E	3	
5	F	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11717 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 Fab(Heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	204	Total	C	N	O	S	0	0	0
			1456	916	243	291	6			
1	K	188	Total	C	N	O	S	0	0	0
			1335	845	222	263	5			

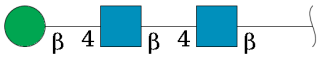
- Molecule 2 is a protein called Fab(Light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	211	Total	C	N	O	S	0	0	0
			1539	963	254	317	5			
2	L	208	Total	C	N	O	S	0	0	0
			1517	952	250	310	5			

- Molecule 3 is a protein called Chitinase 3-like 1 (Cartilage glycoprotein-39), isoform CRA_a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	361	Total	C	N	O	S	0	0	0
			2785	1781	472	521	11			
3	B	361	Total	C	N	O	S	0	0	0
			2809	1800	474	524	11			

- Molecule 4 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
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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

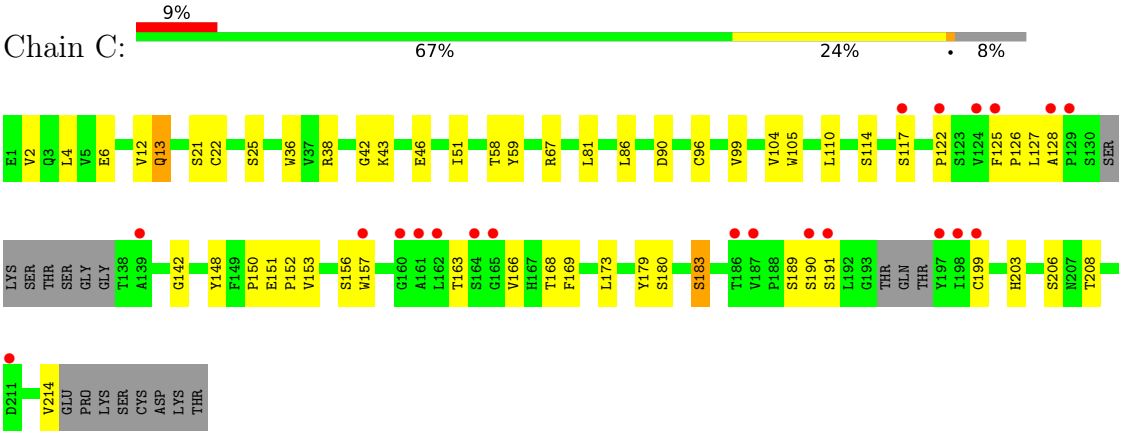
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	32	Total	O	0	0
			32	32		
6	D	24	Total	O	0	0
			24	24		
6	A	48	Total	O	0	0
			48	48		
6	B	46	Total	O	0	0
			46	46		
6	K	27	Total	O	0	0
			27	27		
6	L	32	Total	O	0	0
			32	32		

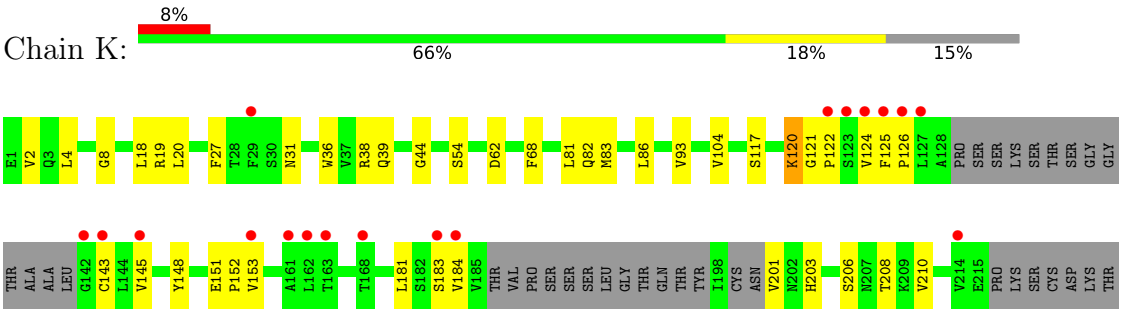
3 Residue-property plots (i)

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.

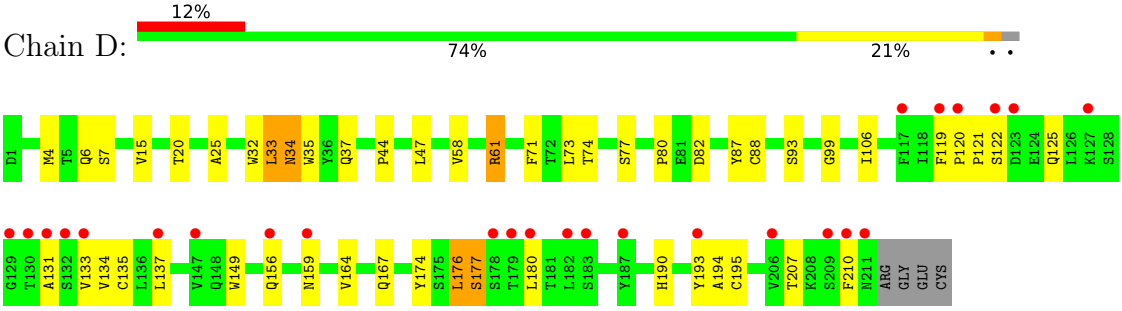
• Molecule 1: Fab(Heavy chain)



• Molecule 1: Fab(Heavy chain)

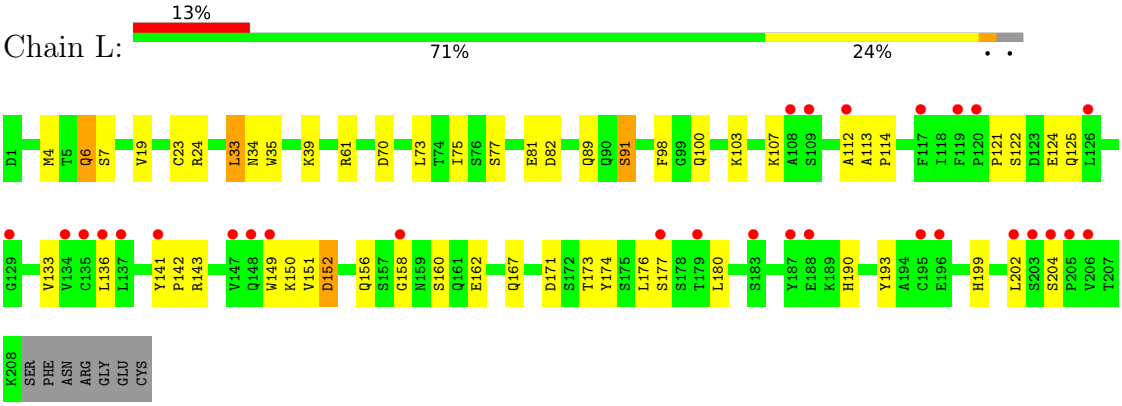


• Molecule 2: Fab(Light chain)



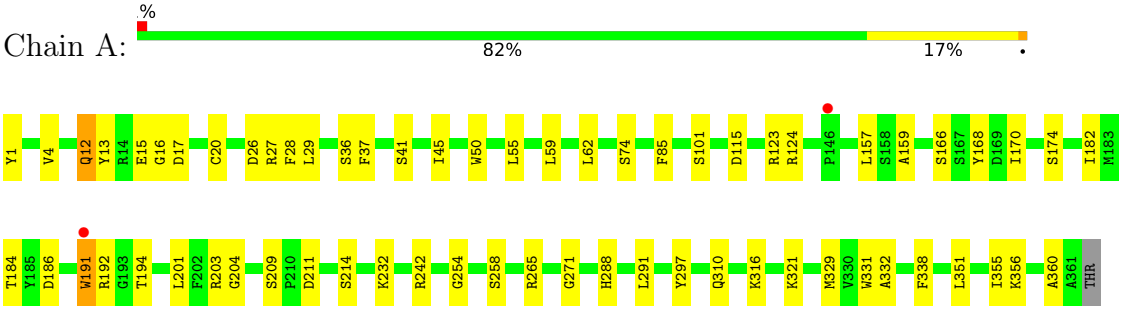
• Molecule 2: Fab(Light chain)

Chain L:



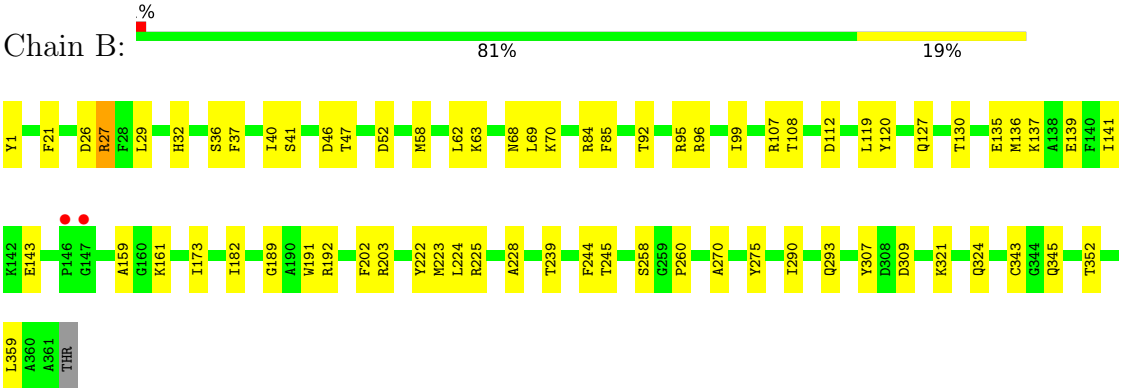
• Molecule 3: Chitinase 3-like 1 (Cartilage glycoprotein-39), isoform CRA_a

Chain A:



• Molecule 3: Chitinase 3-like 1 (Cartilage glycoprotein-39), isoform CRA_a

Chain B:



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

Chain E:

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

Chain F:


NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.58Å 132.53Å 160.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.83 – 2.70 45.83 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.83-2.70) 99.8 (45.83-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.212 , 0.269 0.212 , 0.269	Depositor DCC
R_{free} test set	2640 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11717	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	C	0.45	0/1488	0.62	1/2035 (0.0%)
1	K	0.48	0/1364	0.64	0/1860
2	D	0.42	0/1574	0.62	2/2156 (0.1%)
2	L	0.47	0/1551	0.68	1/2121 (0.0%)
3	A	0.47	0/2858	0.63	0/3881
3	B	0.47	0/2885	0.61	0/3918
All	All	0.46	0/11720	0.63	4/15971 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	33	LEU	CA-CB-CG	-5.86	101.82	115.30
2	D	33	LEU	CA-CB-CG	-5.73	102.12	115.30
1	C	96	CYS	CA-CB-SG	5.57	124.03	114.00
2	D	176	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1456	0	1366	32	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1335	0	1230	34	1
2	D	1539	0	1411	39	0
2	L	1517	0	1404	45	0
3	A	2785	0	2653	45	1
3	B	2809	0	2681	47	1
4	E	39	0	34	2	0
5	F	28	0	25	2	0
6	A	48	0	0	2	0
6	B	46	0	0	0	0
6	C	32	0	0	0	0
6	D	24	0	0	0	0
6	K	27	0	0	0	0
6	L	32	0	0	1	0
All	All	11717	0	10804	226	2

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 10.

All (226) 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:L:150:LYS:HG2	2:L:151:VAL:H	1.41	0.85
2:L:149:TRP:CH2	2:L:180:LEU:HB3	2.12	0.85
3:A:203:ARG:HH21	3:B:203:ARG:NH2	1.73	0.85
1:C:126:PRO:HB3	1:C:214:VAL:HG22	1.58	0.83
3:B:21:PHE:HB3	3:B:58:MET:HE1	1.60	0.83
3:A:203:ARG:NH2	3:B:203:ARG:NH2	2.27	0.83
2:D:20:THR:HG22	2:D:74:THR:HG23	1.63	0.80
1:K:18:LEU:HD12	1:K:19:ARG:H	1.47	0.80
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.64	0.79
3:A:203:ARG:HH21	3:B:203:ARG:HH21	1.27	0.79
1:C:206:SER:OG	1:C:208:THR:OG1	2.02	0.77
3:B:99:ILE:HG12	3:B:136:MET:HE2	1.68	0.76
1:C:110:LEU:HD23	1:C:152:PRO:HD3	1.69	0.73
2:L:61:ARG:NH2	2:L:82:ASP:OD1	2.22	0.72
2:D:156:GLN:HB3	2:D:159:ASN:HD21	1.55	0.71
2:L:150:LYS:HD3	2:L:156:GLN:OE1	1.89	0.71
2:D:61:ARG:NH1	2:D:82:ASP:OD1	2.25	0.70
2:D:133:VAL:HG13	2:D:180:LEU:HB3	1.76	0.68
1:K:124:VAL:HG21	1:K:201:VAL:HG21	1.76	0.67
2:L:171:ASP:HB3	2:L:173:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:203:ARG:NH2	3:B:203:ARG:CZ	2.58	0.65
2:D:193:TYR:HB2	2:D:210:PHE:CE1	2.32	0.63
2:L:150:LYS:HD2	2:L:152:ASP:O	1.99	0.63
1:K:4:LEU:HD11	1:K:104:VAL:HG23	1.81	0.63
2:L:112:ALA:O	2:L:199:HIS:NE2	2.32	0.63
3:B:191:TRP:CD1	3:B:192:ARG:HD3	2.34	0.63
2:L:202:LEU:HD12	2:L:202:LEU:O	1.99	0.62
2:D:167:GLN:HG3	2:D:174:TYR:CE1	2.34	0.62
1:K:18:LEU:HD12	1:K:19:ARG:N	2.14	0.62
2:L:61:ARG:HH21	2:L:82:ASP:CG	2.02	0.61
1:K:203:HIS:ND1	1:K:206:SER:HB3	2.15	0.61
2:L:149:TRP:HH2	2:L:180:LEU:HB3	1.66	0.60
3:B:107:ARG:NH1	3:B:143:GLU:OE1	2.34	0.60
2:D:120:PRO:HB3	2:D:210:PHE:CE2	2.37	0.60
1:C:67:ARG:NH2	1:C:90:ASP:OD2	2.34	0.60
1:C:13:GLN:CD	1:C:13:GLN:H	2.06	0.60
3:A:41:SER:HB2	4:E:1:NAG:H61	1.84	0.59
2:D:106:ILE:H	2:D:167:GLN:HE22	1.48	0.59
2:D:193:TYR:HB2	2:D:210:PHE:HE1	1.67	0.58
3:A:310:GLN:HG3	6:A:423:HOH:O	2.04	0.58
3:A:186:ASP:OD1	3:A:242:ARG:NH1	2.31	0.58
2:L:39:LYS:HE2	2:L:81:GLU:O	2.04	0.58
2:L:141:TYR:CD1	2:L:142:PRO:HA	2.39	0.57
2:D:137:LEU:HB2	2:D:176:LEU:HB3	1.86	0.57
2:D:6:GLN:HE22	2:D:87:TYR:HA	1.68	0.57
2:D:164:VAL:HG22	2:D:176:LEU:HD23	1.87	0.57
1:C:203:HIS:ND1	1:C:206:SER:HB3	2.21	0.56
3:A:123:ARG:HG2	3:A:166:SER:HB3	1.88	0.56
2:D:164:VAL:HG22	2:D:176:LEU:CD2	2.35	0.56
1:K:120:LYS:HD3	1:K:121:GLY:O	2.06	0.55
2:L:89:GLN:HB2	2:L:98:PHE:CD1	2.41	0.55
1:K:122:PRO:HB3	1:K:148:TYR:HB3	1.89	0.55
3:A:27:ARG:NH1	6:A:401:HOH:O	2.35	0.55
3:A:36:SER:HB2	3:A:37:PHE:CD1	2.42	0.55
2:L:19:VAL:HG12	2:L:75:ILE:HB	1.88	0.55
1:C:2:VAL:HG11	1:C:104:VAL:HG11	1.89	0.55
2:D:195:CYS:O	2:D:207:THR:HA	2.06	0.55
3:B:239:THR:O	3:B:275:TYR:HB2	2.07	0.55
2:D:119:PHE:HB2	2:D:134:VAL:HG23	1.89	0.54
2:L:107:LYS:HA	2:L:141:TYR:OH	2.07	0.54
1:C:128:ALA:HB3	2:D:120:PRO:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:GLY:O	1:C:43:LYS:HD3	2.08	0.54
1:C:122:PRO:HB3	1:C:148:TYR:HB3	1.90	0.54
3:B:139:GLU:O	3:B:139:GLU:HG3	2.07	0.53
2:L:150:LYS:HG2	2:L:151:VAL:N	2.19	0.53
2:L:151:VAL:HG21	2:L:193:TYR:CD2	2.43	0.53
1:C:51:ILE:HG13	1:C:58:THR:HG22	1.89	0.53
2:L:81:GLU:OE1	2:L:81:GLU:N	2.30	0.53
5:F:1:NAG:H83	5:F:1:NAG:H3	1.90	0.53
1:C:36:TRP:CD1	1:C:81:LEU:HD13	2.43	0.53
2:L:113:ALA:HA	2:L:199:HIS:CD2	2.44	0.53
2:L:158:GLY:O	2:L:180:LEU:HD11	2.09	0.53
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.44	0.52
2:D:35:TRP:CE2	2:D:73:LEU:HB2	2.43	0.52
3:B:95:ARG:NH1	3:B:135:GLU:OE2	2.36	0.52
2:L:151:VAL:HG22	2:L:193:TYR:HA	1.91	0.52
3:A:41:SER:HB2	4:E:1:NAG:C6	2.40	0.51
3:B:159:ALA:HA	3:B:182:ILE:HD11	1.91	0.51
3:A:288:HIS:HB2	3:A:297:TYR:CE2	2.46	0.51
3:B:137:LYS:O	3:B:141:ILE:HG13	2.10	0.51
1:C:173:LEU:HD13	1:C:179:TYR:CE1	2.45	0.51
3:B:47:THR:HB	3:B:52:ASP:HB2	1.93	0.51
1:C:168:THR:HA	1:C:183:SER:HB2	1.92	0.51
1:K:124:VAL:HG22	1:K:145:VAL:HG13	1.92	0.51
1:K:125:PHE:CE2	2:L:125:GLN:HG3	2.46	0.50
1:K:2:VAL:HG13	1:K:27:PHE:CD1	2.47	0.50
2:L:124:GLU:H	2:L:124:GLU:CD	2.15	0.50
2:L:162:GLU:OE1	2:L:176:LEU:HD11	2.11	0.50
3:B:260:PRO:HB2	3:B:270:ALA:HB1	1.93	0.50
3:B:36:SER:HB2	3:B:37:PHE:CD2	2.47	0.50
1:K:2:VAL:HG13	1:K:27:PHE:HD1	1.77	0.50
2:D:106:ILE:N	2:D:167:GLN:HE22	2.10	0.49
3:A:1:TYR:CZ	3:A:321:LYS:HG2	2.47	0.49
2:L:6:GLN:O	2:L:100:GLN:NE2	2.45	0.49
2:L:114:PRO:HD3	2:L:199:HIS:CD2	2.46	0.49
3:A:15:GLU:OE2	3:A:265:ARG:NH1	2.45	0.49
3:A:28:PHE:O	3:A:356:LYS:NZ	2.44	0.49
2:L:142:PRO:HD2	2:L:199:HIS:CE1	2.47	0.49
2:L:151:VAL:CG2	2:L:193:TYR:HA	2.43	0.49
3:B:40:ILE:O	3:B:84:ARG:NH2	2.46	0.49
2:D:194:ALA:HB1	2:D:207:THR:CG2	2.42	0.49
3:A:211:ASP:OD2	3:A:214:SER:OG	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:VAL:CG2	1:C:203:HIS:HD2	2.25	0.48
2:L:190:HIS:HB3	6:L:301:HOH:O	2.12	0.48
3:B:32:HIS:HA	3:B:70:LYS:O	2.13	0.48
2:D:32:TRP:HE1	3:A:12:GLN:HG3	1.77	0.48
3:A:15:GLU:HG2	3:A:16:GLY:N	2.28	0.48
2:L:202:LEU:HB2	2:L:204:SER:O	2.13	0.48
3:A:174:SER:O	3:A:232:LYS:NZ	2.44	0.48
3:B:130:THR:HG22	3:B:173:ILE:HG23	1.96	0.48
3:A:203:ARG:CZ	3:B:203:ARG:NH2	2.77	0.48
1:K:39:GLN:HG3	1:K:44:GLY:O	2.14	0.48
1:K:153:VAL:CG2	1:K:181:LEU:HD21	2.44	0.48
2:L:33:LEU:HG	2:L:34:ASN:N	2.28	0.48
2:D:133:VAL:CG1	2:D:180:LEU:HB3	2.43	0.47
3:B:36:SER:HA	3:B:37:PHE:HA	1.65	0.47
2:L:114:PRO:HD3	2:L:199:HIS:CG	2.50	0.47
2:L:149:TRP:O	2:L:156:GLN:NE2	2.48	0.47
2:D:6:GLN:HE21	2:D:99:GLY:HA3	1.79	0.47
3:A:26:ASP:HB3	3:A:29:LEU:HB2	1.96	0.47
3:A:74:SER:HA	3:A:115:ASP:O	2.15	0.47
3:B:36:SER:HB2	3:B:37:PHE:CG	2.49	0.47
1:K:83:MET:HE2	1:K:86:LEU:HD21	1.96	0.47
3:B:84:ARG:NH2	5:F:1:NAG:H62	2.30	0.47
1:K:153:VAL:HG23	1:K:181:LEU:HD21	1.96	0.47
3:A:20:CYS:HB2	3:A:338:PHE:CZ	2.49	0.47
3:A:182:ILE:HG13	3:A:184:THR:HG23	1.96	0.47
3:B:29:LEU:HD21	3:B:352:THR:HB	1.96	0.47
3:B:224:LEU:HD23	3:B:228:ALA:O	2.15	0.47
2:L:4:MET:HE2	2:L:23:CYS:SG	2.55	0.47
2:D:6:GLN:NE2	2:D:88:CYS:H	2.12	0.47
1:K:8:GLY:O	1:K:18:LEU:HD11	2.15	0.47
2:L:24:ARG:HG3	2:L:70:ASP:OD1	2.15	0.47
1:K:68:PHE:CE2	1:K:83:MET:HG2	2.50	0.47
3:A:45:ILE:HG22	3:A:101:SER:OG	2.16	0.46
3:B:92:THR:O	3:B:96:ARG:HG3	2.14	0.46
3:B:95:ARG:O	3:B:99:ILE:HG13	2.14	0.46
1:K:83:MET:HB3	1:K:86:LEU:HD21	1.98	0.46
3:A:1:TYR:OH	3:A:321:LYS:HG2	2.15	0.46
3:B:27:ARG:HB3	3:B:62:LEU:HB3	1.97	0.46
1:C:142:GLY:HA2	1:C:157:TRP:CH2	2.50	0.46
1:C:157:TRP:CZ3	1:C:199:CYS:HB3	2.51	0.45
3:A:157:LEU:HB3	3:A:168:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:PHE:HB2	2:D:134:VAL:CG2	2.47	0.45
3:B:202:PHE:O	3:B:293:GLN:HG2	2.17	0.45
3:A:203:ARG:NH1	3:A:204:GLY:O	2.40	0.45
3:B:26:ASP:OD2	3:B:29:LEU:HB2	2.17	0.45
1:K:20:LEU:N	1:K:81:LEU:O	2.46	0.45
1:K:36:TRP:CE2	1:K:81:LEU:HB2	2.52	0.45
2:L:160:SER:OG	2:L:180:LEU:HD13	2.17	0.45
1:C:153:VAL:HG22	1:C:203:HIS:HD2	1.82	0.45
2:L:167:GLN:HG3	2:L:174:TYR:CZ	2.51	0.45
3:B:108:THR:OG1	1:K:31:ASN:OD1	2.29	0.45
1:K:203:HIS:O	1:K:206:SER:OG	2.31	0.45
3:A:159:ALA:HA	3:A:182:ILE:HD11	1.99	0.44
3:A:59:LEU:HD12	3:A:62:LEU:HD12	1.98	0.44
3:B:119:LEU:HA	3:B:120:TYR:CD1	2.53	0.44
1:C:169:PHE:CZ	2:D:177:SER:HB3	2.53	0.44
3:A:194:THR:HG23	3:A:254:GLY:HA2	1.99	0.44
1:K:203:HIS:HB3	1:K:206:SER:OG	2.17	0.44
3:B:343:CYS:O	3:B:345:GLN:NE2	2.50	0.44
1:C:4:LEU:HD22	1:C:22:CYS:SG	2.58	0.43
3:A:36:SER:HA	3:A:37:PHE:HA	1.59	0.43
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.99	0.43
3:A:36:SER:HB2	3:A:37:PHE:CE1	2.52	0.43
1:K:208:THR:HG22	1:K:210:VAL:HG23	1.99	0.43
2:L:124:GLU:OE2	2:L:124:GLU:N	2.46	0.43
2:L:149:TRP:O	2:L:150:LYS:HB2	2.19	0.43
2:D:4:MET:HE1	2:D:25:ALA:HB2	2.00	0.43
2:D:121:PRO:HG2	2:D:131:ALA:HB1	2.01	0.43
2:D:149:TRP:CD2	2:D:180:LEU:HD22	2.54	0.43
2:D:32:TRP:CE3	2:D:32:TRP:HA	2.53	0.43
1:K:143:CYS:N	1:K:183:SER:O	2.51	0.43
1:C:36:TRP:CE2	1:C:81:LEU:HB2	2.54	0.43
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.84	0.42
2:D:135:CYS:HB2	2:D:149:TRP:CH2	2.53	0.42
3:B:189:GLY:C	3:B:244:PHE:HE1	2.22	0.42
1:K:152:PRO:O	1:K:203:HIS:HD2	2.02	0.42
1:C:12:VAL:HG11	1:C:86:LEU:HD13	2.00	0.42
3:A:12:GLN:HG2	3:A:13:TYR:CD2	2.55	0.42
3:B:46:ASP:OD2	1:K:54:SER:OG	2.34	0.42
2:L:121:PRO:HG3	2:L:133:VAL:HG23	2.01	0.42
1:C:163:THR:O	1:C:166:VAL:HG23	2.19	0.42
1:K:83:MET:HE2	1:K:86:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:19:VAL:CG1	2:L:75:ILE:HB	2.50	0.42
1:C:127:LEU:N	1:C:142:GLY:O	2.53	0.42
2:D:15:VAL:HG22	2:D:80:PRO:HD3	2.02	0.42
1:C:150:PRO:C	1:C:152:PRO:HD2	2.40	0.42
1:C:6:GLU:HA	1:C:21:SER:O	2.20	0.42
2:D:167:GLN:HG3	2:D:174:TYR:CZ	2.55	0.42
3:A:170:ILE:HD13	3:A:170:ILE:HA	1.86	0.42
1:K:184:VAL:HG21	2:L:136:LEU:HD22	2.02	0.41
2:D:33:LEU:HG	2:D:34:ASN:N	2.33	0.41
3:B:290:ILE:HG21	3:B:293:GLN:OE1	2.20	0.41
1:K:126:PRO:HD2	2:L:122:SER:OG	2.20	0.41
3:A:191:TRP:CE3	3:A:192:ARG:HG2	2.55	0.41
3:A:201:LEU:HD13	3:A:316:LYS:HG2	2.02	0.41
1:K:81:LEU:HD12	1:K:81:LEU:HA	1.90	0.41
3:B:69:LEU:HD12	3:B:70:LYS:N	2.34	0.41
1:K:19:ARG:HG2	1:K:82:GLN:HG3	2.02	0.41
3:A:203:ARG:NH2	3:B:203:ARG:NE	2.68	0.41
3:B:127:GLN:HA	3:B:130:THR:OG1	2.20	0.41
3:B:307:TYR:HE2	3:B:309:ASP:HB3	1.85	0.41
1:K:122:PRO:HB2	1:K:145:VAL:HG12	2.01	0.41
3:A:4:VAL:O	3:A:329:MET:HA	2.20	0.41
3:A:331:TRP:HA	3:A:332:ALA:HA	1.86	0.41
3:A:351:LEU:O	3:A:355:ILE:HG13	2.21	0.41
3:B:182:ILE:HD13	3:B:223:MET:SD	2.61	0.41
3:B:245:THR:O	3:B:258:SER:N	2.52	0.41
1:C:125:PHE:CG	2:D:125:GLN:HB2	2.56	0.41
2:D:4:MET:CE	2:D:25:ALA:HB2	2.51	0.41
3:A:12:GLN:NE2	3:A:55:LEU:HD22	2.36	0.41
3:B:130:THR:HG22	3:B:173:ILE:CG2	2.51	0.41
3:B:359:LEU:HD23	3:B:359:LEU:HA	1.92	0.41
3:B:63:LYS:NZ	3:B:112:ASP:OD2	2.48	0.41
1:C:105:TRP:CE3	2:D:44:PRO:HD2	2.57	0.40
2:D:33:LEU:HD22	2:D:71:PHE:CB	2.51	0.40
3:B:1:TYR:CZ	3:B:321:LYS:HG2	2.55	0.40
3:B:161:LYS:HE2	3:B:222:TYR:CZ	2.56	0.40
1:K:38:ARG:HA	1:K:93:VAL:O	2.21	0.40
1:C:38:ARG:HG2	1:C:46:GLU:HB2	2.03	0.40
1:C:99:VAL:HG23	3:A:50:TRP:NE1	2.36	0.40
3:A:242:ARG:HA	3:A:271:GLY:O	2.21	0.40
1:C:151:GLU:N	1:C:152:PRO:HD2	2.37	0.40
3:A:291:LEU:HD12	3:A:291:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:34:ASN:HD21	2:L:91:SER:HB3	1.86	0.40

All (2) 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)
1:C:190:SER:OG	3:A:360:ALA:O[3_655]	1.85	0.35
3:B:192:ARG:NH2	1:K:117:SER:O[3_755]	2.11	0.09

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	C	198/222 (89%)	193 (98%)	5 (2%)	0	100	100
1	K	181/222 (82%)	173 (96%)	8 (4%)	0	100	100
2	D	209/215 (97%)	201 (96%)	8 (4%)	0	100	100
2	L	206/215 (96%)	194 (94%)	12 (6%)	0	100	100
3	A	359/362 (99%)	351 (98%)	8 (2%)	0	100	100
3	B	359/362 (99%)	349 (97%)	10 (3%)	0	100	100
All	All	1512/1598 (95%)	1461 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	154/182 (85%)	144 (94%)	10 (6%)	17 38
1	K	134/182 (74%)	131 (98%)	3 (2%)	52 79
2	D	165/189 (87%)	157 (95%)	8 (5%)	25 53
2	L	161/189 (85%)	153 (95%)	8 (5%)	24 51
3	A	284/302 (94%)	277 (98%)	7 (2%)	47 76
3	B	289/302 (96%)	283 (98%)	6 (2%)	53 80
All	All	1187/1346 (88%)	1145 (96%)	42 (4%)	36 65

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	13	GLN
1	C	25	SER
1	C	59	TYR
1	C	114	SER
1	C	117	SER
1	C	156	SER
1	C	180	SER
1	C	183	SER
1	C	189	SER
1	C	191	SER
2	D	7	SER
2	D	34	ASN
2	D	61	ARG
2	D	77	SER
2	D	93	SER
2	D	122	SER
2	D	177	SER
2	D	190	HIS
3	A	12	GLN
3	A	17	ASP
3	A	85	PHE
3	A	124	ARG
3	A	191	TRP
3	A	209	SER
3	A	258	SER
3	B	27	ARG
3	B	41	SER
3	B	68	ASN

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Mol	Chain	Res	Type
3	B	85	PHE
3	B	225	ARG
3	B	324	GLN
1	K	62	ASP
1	K	120	LYS
1	K	151	GLU
2	L	6	GLN
2	L	7	SER
2	L	77	SER
2	L	91	SER
2	L	103	LYS
2	L	143	ARG
2	L	152	ASP
2	L	177	SER

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

Mol	Chain	Res	Type
2	D	6	GLN
2	D	148	GLN
2	D	167	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)

5 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	$\#\|Z\| > 2$
4	NAG	E	1	4,3	14,14,15	0.59	0	17,19,21	1.22	3 (17%)
4	NAG	E	2	4	14,14,15	0.77	1 (7%)	17,19,21	1.58	2 (11%)
4	BMA	E	3	4	11,11,12	0.46	0	15,15,17	1.28	1 (6%)
5	NAG	F	1	5,3	14,14,15	0.32	0	17,19,21	1.52	2 (11%)
5	NAG	F	2	5	14,14,15	1.35	1 (7%)	17,19,21	0.81	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
4	NAG	E	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,3	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2	NAG	O5-C1	-4.70	1.36	1.43
4	E	2	NAG	O4-C4	-2.20	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2	NAG	O4-C4-C5	5.69	123.43	109.30
5	F	1	NAG	C2-N2-C7	4.41	129.18	122.90
5	F	1	NAG	C1-C2-N2	3.04	115.68	110.49
4	E	1	NAG	C1-O5-C5	3.03	116.30	112.19
4	E	3	BMA	C1-O5-C5	2.57	115.67	112.19
5	F	2	NAG	C1-O5-C5	2.15	115.11	112.19
4	E	2	NAG	C1-O5-C5	2.12	115.07	112.19
4	E	1	NAG	O3-C3-C2	-2.05	105.23	109.47
4	E	1	NAG	C3-C4-C5	2.00	113.81	110.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
5	F	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
5	F	1	NAG	C3-C2-N2-C7
5	F	2	NAG	C3-C2-N2-C7

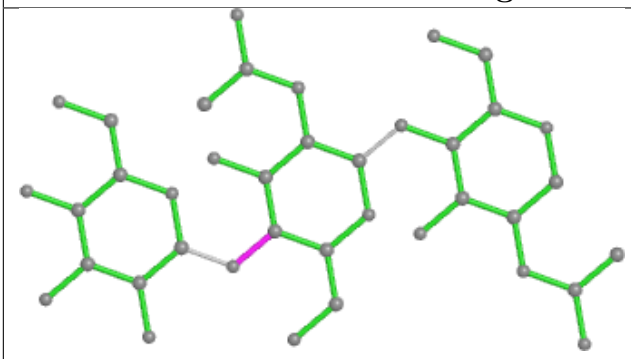
There are no ring outliers.

2 monomers are involved in 4 short contacts:

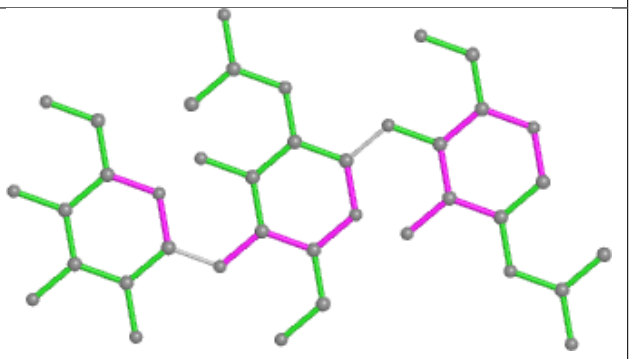
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	2	0
4	E	1	NAG	2	0

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

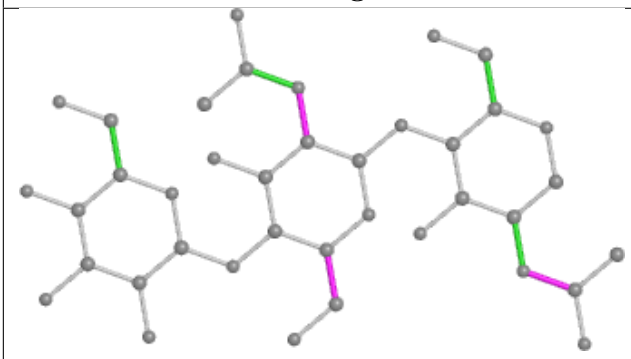
Oligosaccharide Chain E



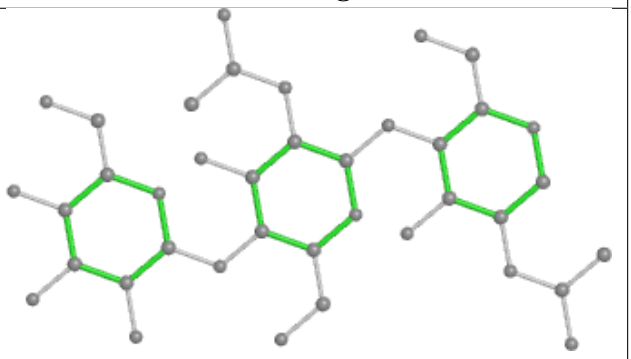
Bond lengths



Bond angles

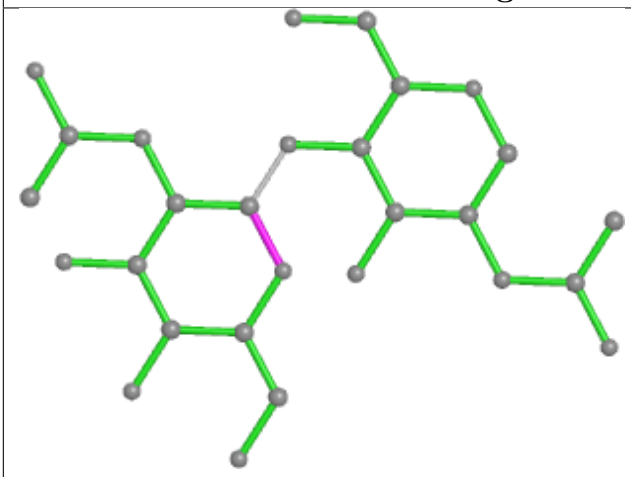


Torsions

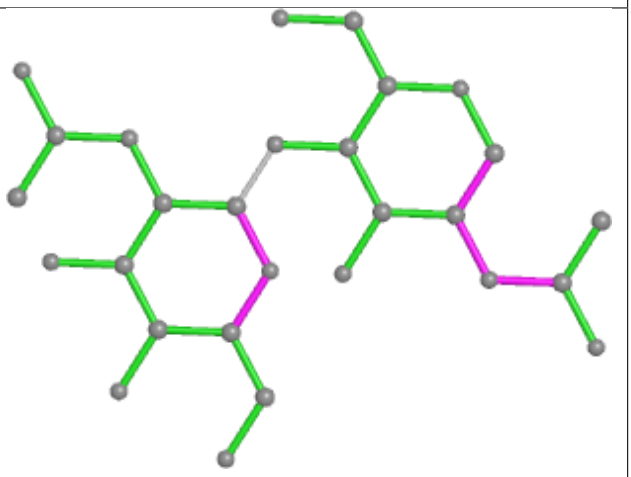


Rings

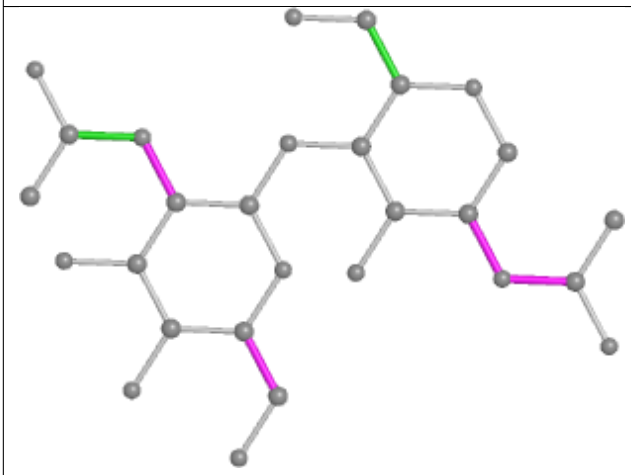
Oligosaccharide Chain F



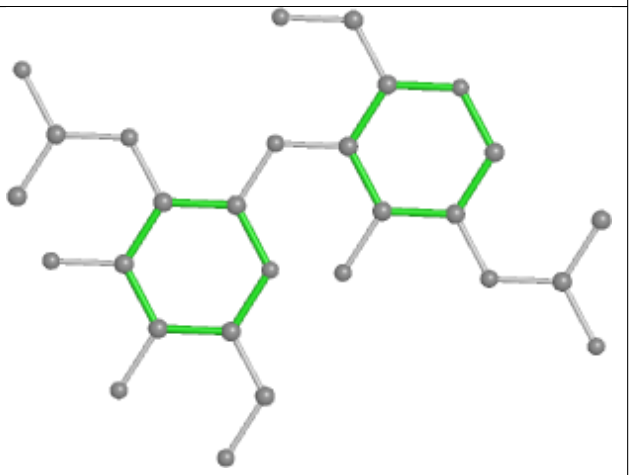
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	204/222 (91%)	0.27	21 (10%) 6 5	44, 63, 119, 163	0
1	K	188/222 (84%)	0.23	18 (9%) 8 6	43, 61, 109, 144	0
2	D	211/215 (98%)	0.31	26 (12%) 4 3	43, 61, 115, 125	0
2	L	208/215 (96%)	0.54	29 (13%) 2 2	42, 71, 123, 143	0
3	A	361/362 (99%)	-0.22	2 (0%) 89 91	37, 52, 76, 109	0
3	B	361/362 (99%)	-0.18	2 (0%) 89 91	41, 56, 79, 161	0
All	All	1533/1598 (95%)	0.09	98 (6%) 19 18	37, 57, 114, 163	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	ALA	6.9
2	L	195	CYS	6.7
2	L	136	LEU	6.3
2	L	141	TYR	5.7
2	D	133	VAL	5.0
1	C	161	ALA	5.0
2	L	108	ALA	4.7
3	B	146	PRO	4.7
1	C	124	VAL	4.7
3	A	191	TRP	4.6
1	K	126	PRO	4.6
2	L	158	GLY	4.6
2	L	134	VAL	4.6
1	C	165	GLY	4.3
2	L	187	TYR	4.2
2	D	131	ALA	4.2
2	L	149	TRP	4.1
3	B	147	GLY	4.0
2	L	135	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	L	204	SER	3.8
2	L	109	SER	3.7
2	L	137	LEU	3.7
1	C	160	GLY	3.7
3	A	146	PRO	3.6
2	L	148	GLN	3.6
2	D	130	THR	3.6
2	D	122	SER	3.5
1	C	157	TRP	3.5
1	K	162	LEU	3.5
1	K	125	PHE	3.4
2	L	177	SER	3.4
2	D	210	PHE	3.4
1	K	168	THR	3.4
2	D	117	PHE	3.3
1	C	162	LEU	3.3
2	L	206	VAL	3.3
1	K	143	CYS	3.3
2	D	209	SER	3.2
1	C	139	ALA	3.2
1	K	183	SER	3.2
2	L	147	VAL	3.2
1	K	123	SER	3.2
1	K	124	VAL	3.1
2	D	183	SER	3.1
2	D	206	VAL	3.0
2	L	119	PHE	3.0
2	D	187	TYR	2.9
1	C	117	SER	2.9
2	L	129	GLY	2.9
1	K	161	ALA	2.9
1	K	214	VAL	2.9
1	K	142	GLY	2.8
1	C	125	PHE	2.8
1	K	184	VAL	2.8
1	K	122	PRO	2.8
2	D	132	SER	2.8
2	L	183	SER	2.7
1	C	187	VAL	2.7
1	C	190	SER	2.7
2	D	156	GLN	2.6
2	D	182	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	127	LEU	2.5
2	L	117	PHE	2.5
2	L	196	GLU	2.5
2	D	193	TYR	2.5
2	D	180	LEU	2.5
2	L	112	ALA	2.4
2	L	203	SER	2.4
2	L	179	THR	2.4
1	C	191	SER	2.4
2	D	137	LEU	2.4
2	L	202	LEU	2.4
1	C	211	ASP	2.4
2	D	123	ASP	2.4
2	D	127	LYS	2.3
2	L	188	GLU	2.3
1	C	186	THR	2.3
2	L	126	LEU	2.3
2	D	119	PHE	2.3
1	K	153	VAL	2.3
1	C	122	PRO	2.2
1	C	164	SER	2.2
2	D	211	ASN	2.2
2	L	120	PRO	2.2
2	L	205	PRO	2.2
1	C	198	ILE	2.2
1	C	199	CYS	2.2
1	K	29	PHE	2.1
2	D	178	SER	2.1
1	C	197	TYR	2.1
2	D	120	PRO	2.1
1	K	163	THR	2.1
2	D	147	VAL	2.1
1	C	129	PRO	2.1
2	D	159	ASN	2.1
2	D	179	THR	2.1
2	D	129	GLY	2.0
1	K	145	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)

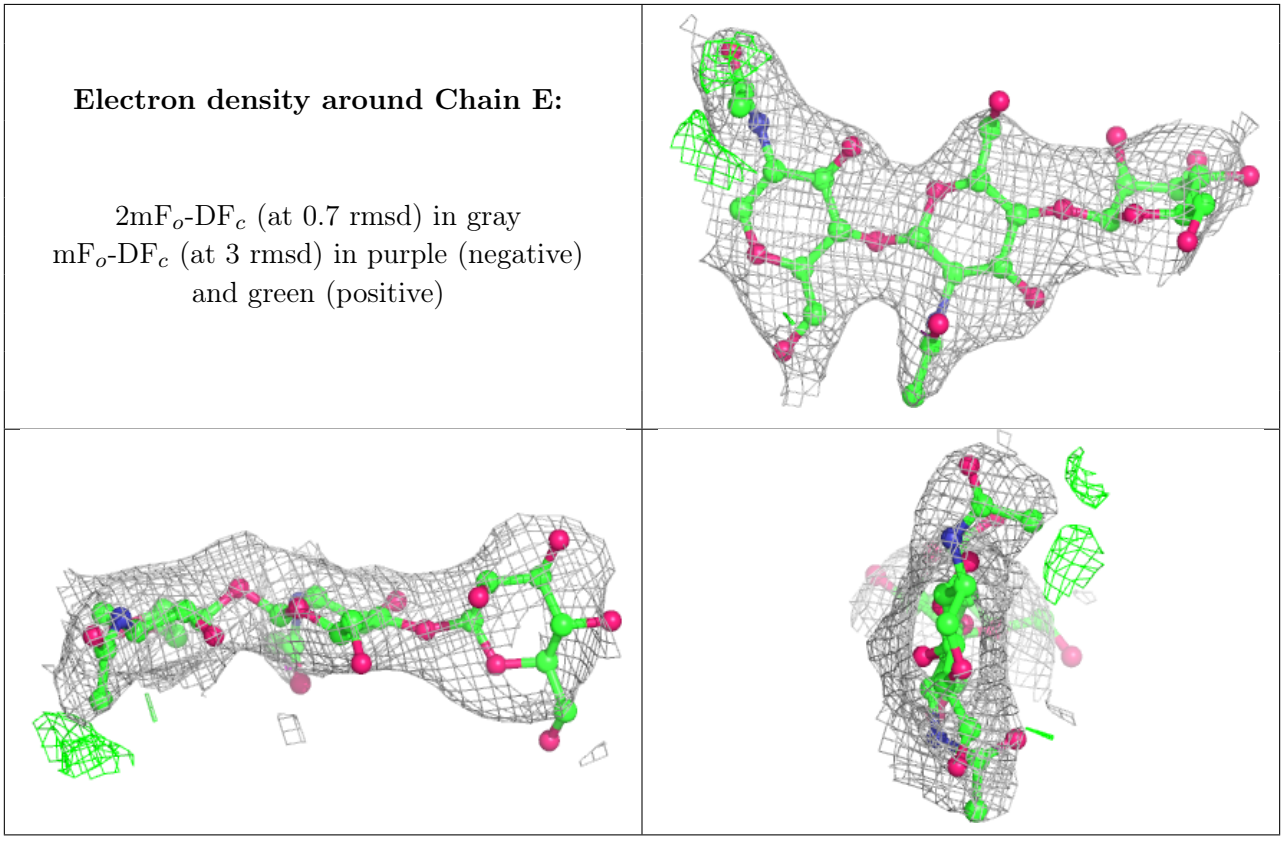
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	BMA	E	3	11/12	0.89	0.20	91,101,109,114	0
5	NAG	F	2	14/15	0.89	0.14	68,77,84,84	0
5	NAG	F	1	14/15	0.91	0.18	56,64,69,69	0
4	NAG	E	2	14/15	0.91	0.14	67,82,85,88	0
4	NAG	E	1	14/15	0.95	0.17	51,57,64,65	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.

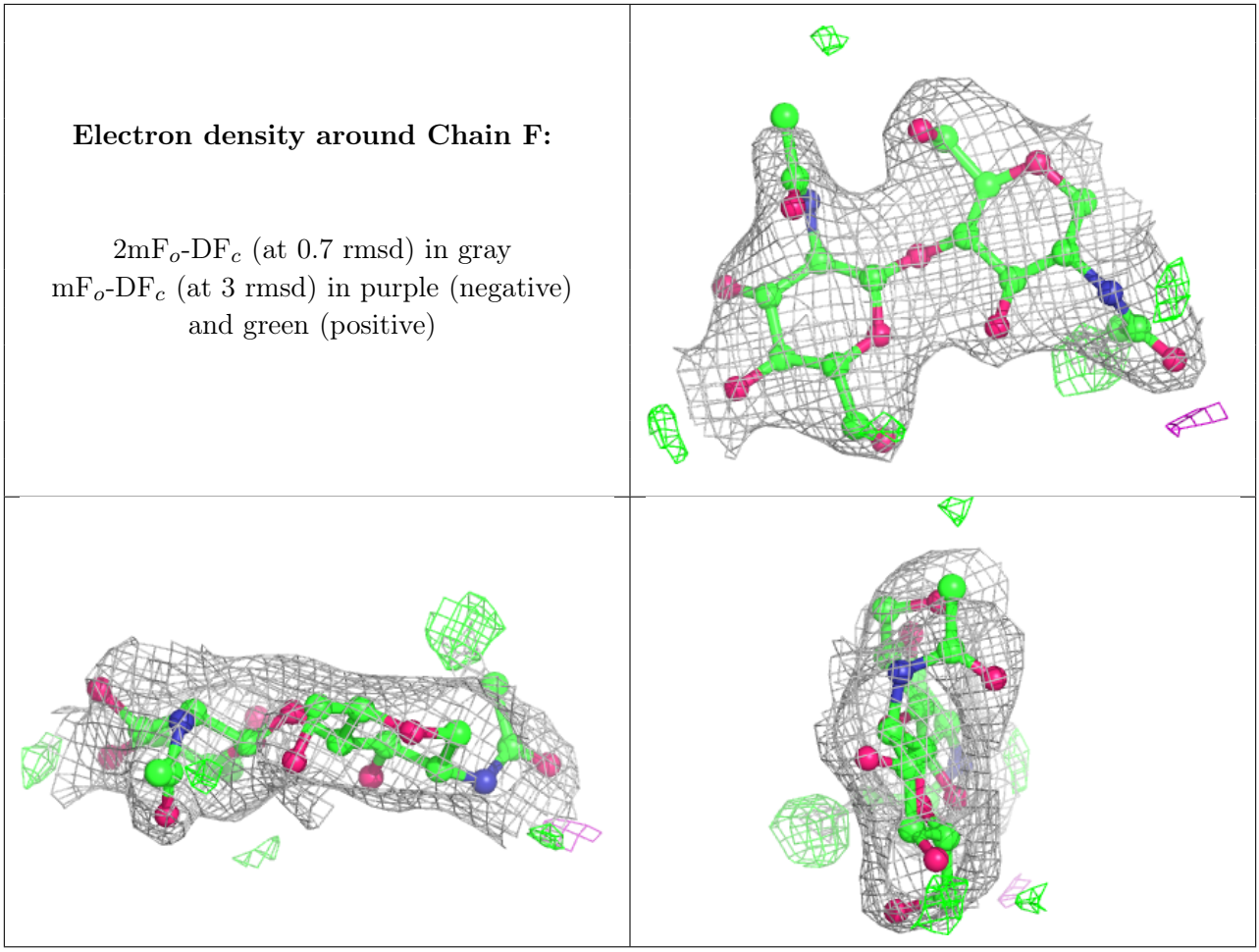
Electron density around Chain E:

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



Electron density around Chain F:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.