Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:37 PM BST

PDB ID	:	4ZSO
Title	:	Crystal structure of a complex between B7-H6, a tumor cell ligand for natural cytotoxicity receptor NKp30, and an inhibitory antibody
Authors	:	Xu, X.; Li, Y.; Mariuzza, R.A.
Deposited on	:	2015-05-13
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

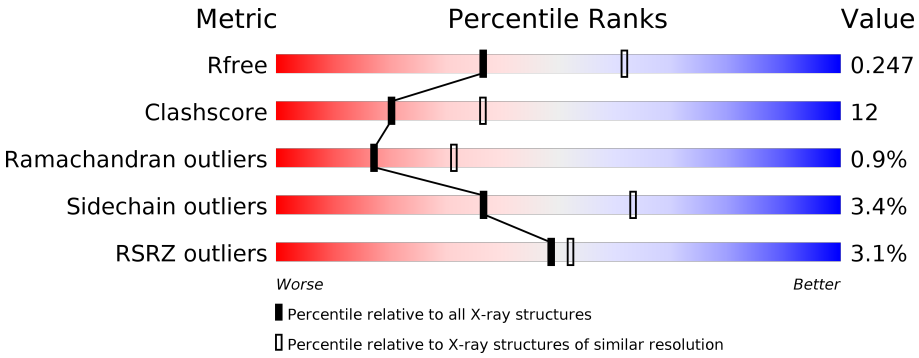
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	214	75% 24%
1	C	214	% 78% 21%
2	B	219	75% 21%
2	D	219	74% 24%
3	E	253	5% 60% 24% 14%
3	F	253	10% 60% 23% 15%

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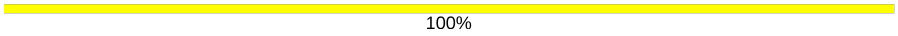
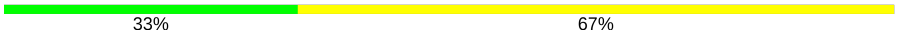
Mol	Chain	Length	Quality of chain
4	G	2	
5	H	2	
5	J	2	
6	I	3	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10273 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1646	1025	272	337	12			
1	C	214	Total	C	N	O	S	0	0	0
			1646	1025	272	337	12			

- Molecule 2 is a protein called Antibody Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1624	1025	264	327	8			
2	D	219	Total	C	N	O	S	0	0	0
			1628	1027	265	328	8			

- Molecule 3 is a protein called Natural cytotoxicity triggering receptor 3 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	217	Total	C	N	O	S	0	0	0
			1684	1074	277	322	11			
3	F	214	Total	C	N	O	S	0	0	0
			1658	1060	274	313	11			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	19	ALA	-	expression tag	UNP Q68D85
E	20	ASP	-	expression tag	UNP Q68D85
E	21	LEU	-	expression tag	UNP Q68D85
E	22	GLY	-	expression tag	UNP Q68D85
E	23	SER	-	expression tag	UNP Q68D85
E	24	MET	-	expression tag	UNP Q68D85
E	263	ALA	-	expression tag	UNP Q68D85
E	264	ALA	-	expression tag	UNP Q68D85

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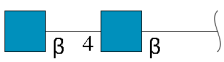
Chain	Residue	Modelled	Actual	Comment	Reference
E	265	ALA	-	expression tag	UNP Q68D85
E	266	HIS	-	expression tag	UNP Q68D85
E	267	HIS	-	expression tag	UNP Q68D85
E	268	HIS	-	expression tag	UNP Q68D85
E	269	HIS	-	expression tag	UNP Q68D85
E	270	HIS	-	expression tag	UNP Q68D85
E	271	HIS	-	expression tag	UNP Q68D85
F	19	ALA	-	expression tag	UNP Q68D85
F	20	ASP	-	expression tag	UNP Q68D85
F	21	LEU	-	expression tag	UNP Q68D85
F	22	GLY	-	expression tag	UNP Q68D85
F	23	SER	-	expression tag	UNP Q68D85
F	24	MET	-	expression tag	UNP Q68D85
F	263	ALA	-	expression tag	UNP Q68D85
F	264	ALA	-	expression tag	UNP Q68D85
F	265	ALA	-	expression tag	UNP Q68D85
F	266	HIS	-	expression tag	UNP Q68D85
F	267	HIS	-	expression tag	UNP Q68D85
F	268	HIS	-	expression tag	UNP Q68D85
F	269	HIS	-	expression tag	UNP Q68D85
F	270	HIS	-	expression tag	UNP Q68D85
F	271	HIS	-	expression tag	UNP Q68D85

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

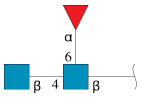
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



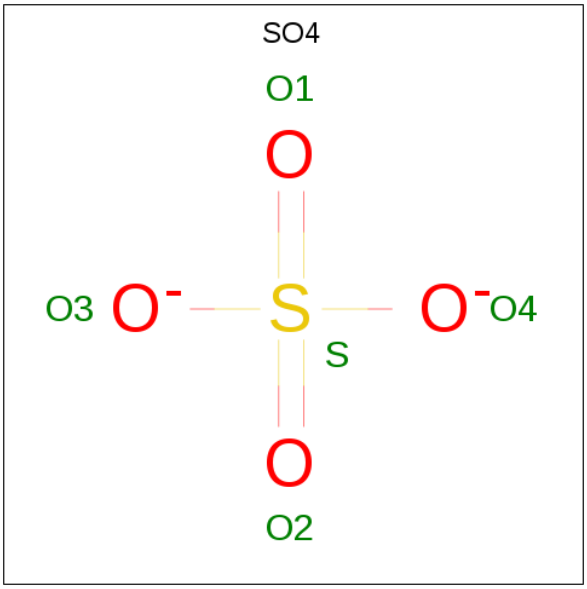
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



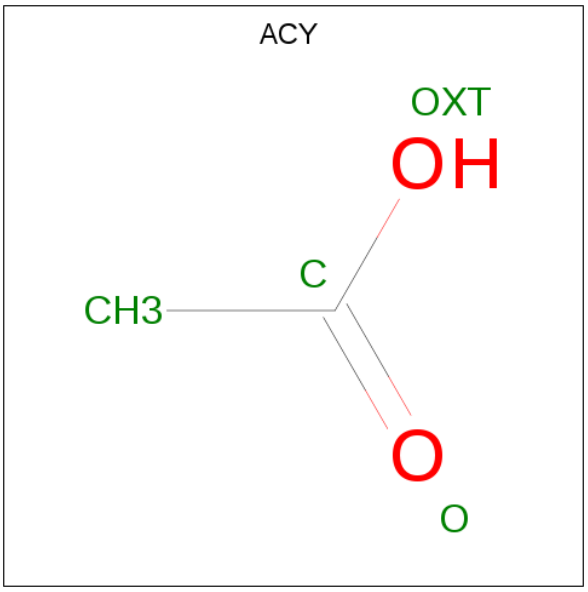
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0

- Molecule 9 is water.

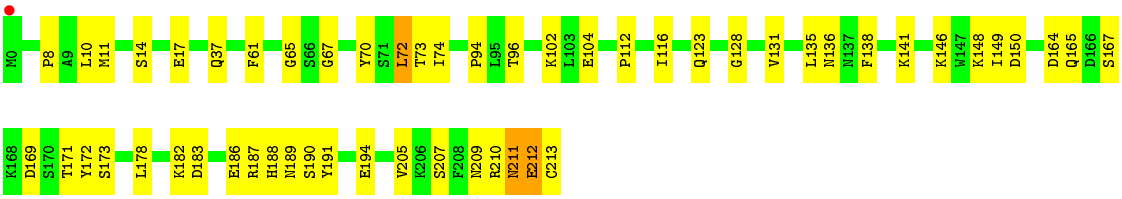
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	57	Total O 57 57	0	0
9	B	49	Total O 49 49	0	0
9	C	53	Total O 53 53	0	0
9	D	52	Total O 52 52	0	0
9	E	22	Total O 22 22	0	0
9	F	18	Total O 18 18	0	0

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.

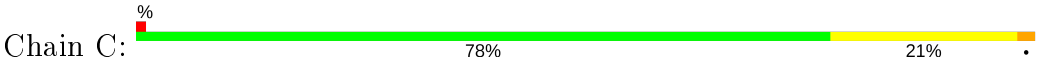
- Molecule 1: Antibody Light Chain

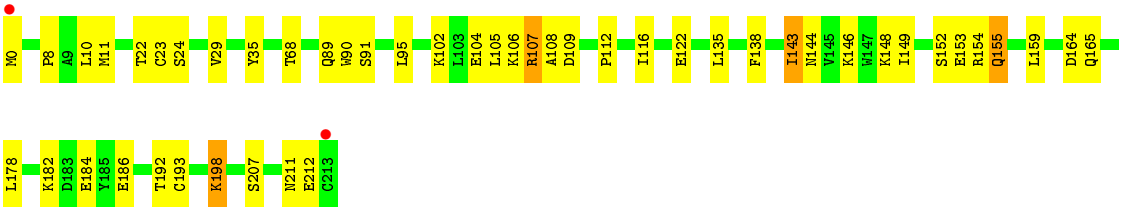
Chain A:



- Molecule 1: Antibody Light Chain

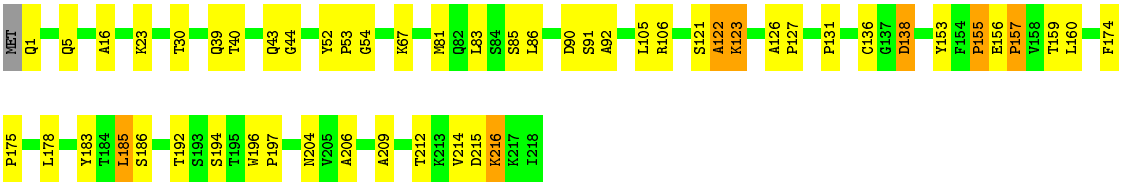
Chain C:





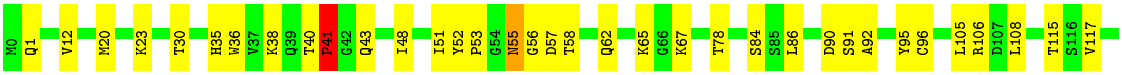
- Molecule 2: Antibody Heavy Chain

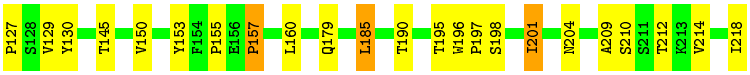
Chain B:



- Molecule 2: Antibody Heavy Chain

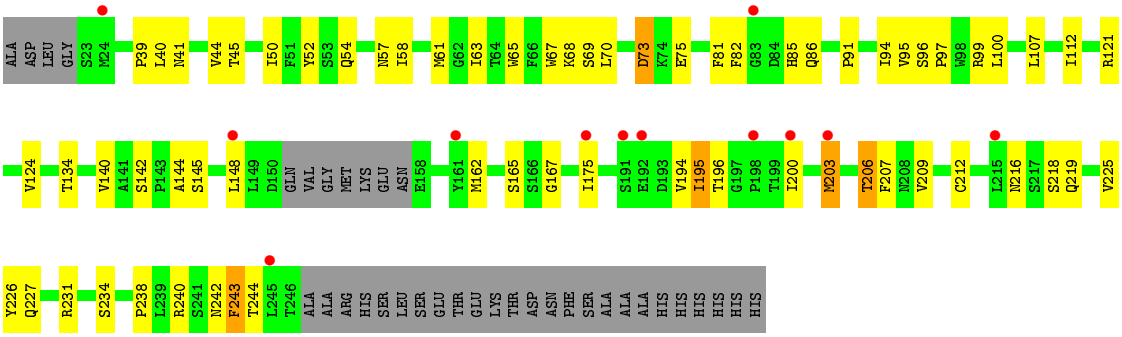
Chain D:





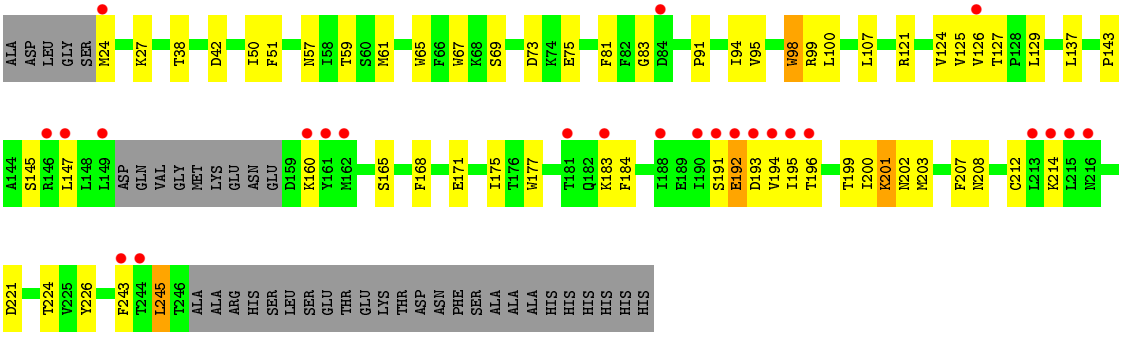
• Molecule 3: Natural cytotoxicity triggering receptor 3 ligand 1

Chain E:



• Molecule 3: Natural cytotoxicity triggering receptor 3 ligand 1

Chain F:



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

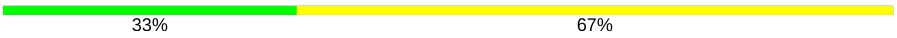
Chain H:

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

Chain J:

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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.63Å 138.03Å 171.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.50) 99.7 (48.19-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.257 0.216 , 0.247	Depositor DCC
R_{free} test set	4002 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10273	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5296e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FUC, ACY, SO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/1686	0.64	0/2291
1	C	0.37	0/1686	0.64	0/2291
2	B	0.38	0/1664	0.70	0/2271
2	D	0.37	0/1668	0.68	0/2276
3	E	0.35	0/1724	0.61	0/2347
3	F	0.35	0/1698	0.60	0/2307
All	All	0.37	0/10126	0.64	0/13783

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1646	0	1573	35	0
1	C	1646	0	1573	33	0
2	B	1624	0	1588	33	0
2	D	1628	0	1589	45	0
3	E	1684	0	1616	51	0
3	F	1658	0	1601	48	0
4	G	24	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	28	0	25	6	0
5	J	28	0	25	4	0
6	I	38	0	34	2	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
8	E	4	0	3	0	0
8	F	4	0	3	0	0
9	A	57	0	0	1	0
9	B	49	0	0	2	0
9	C	53	0	0	0	0
9	D	52	0	0	0	0
9	E	22	0	0	0	0
9	F	18	0	0	0	0
All	All	10273	0	9652	243	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 12.

All (243) 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:1:GLN:HB2	3:E:203:MET:HG2	1.27	1.14
3:F:201:LYS:H	3:F:201:LYS:HE3	1.23	1.00
1:C:89:GLN:HE21	1:C:91:SER:H	1.05	0.98
3:E:200:ILE:HD12	5:H:1:NAG:H82	1.41	0.97
6:I:1:NAG:H62	6:I:2:NAG:HN2	1.30	0.97
2:D:1:GLN:HB3	3:F:203:MET:HG2	1.49	0.94
1:C:89:GLN:NE2	1:C:91:SER:H	1.67	0.91
3:F:201:LYS:HE3	3:F:201:LYS:N	1.91	0.86
2:D:127:PRO:HB3	2:D:153:TYR:HB3	1.57	0.85
3:F:245:LEU:H	3:F:245:LEU:HD12	1.43	0.83
1:C:143:ILE:HD13	1:C:144:ASN:H	1.45	0.81
2:B:1:GLN:CB	3:E:203:MET:HG2	2.10	0.81
3:F:143:PRO:HB3	3:F:168:PHE:HB3	1.63	0.81
2:D:145:THR:HG22	2:D:190:THR:OG1	1.80	0.81
6:I:1:NAG:H62	6:I:2:NAG:N2	1.95	0.80
3:F:50:ILE:HD12	3:F:124:VAL:HG21	1.62	0.80
1:C:143:ILE:HD13	1:C:144:ASN:N	1.97	0.79
3:E:200:ILE:CD1	5:H:1:NAG:H82	2.11	0.78
3:F:202:ASN:OD1	5:J:1:NAG:H83	1.84	0.78
2:D:12:VAL:HG11	2:D:86:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:THR:O	2:D:43:GLN:HB2	1.86	0.75
2:D:20:MET:HE2	2:D:115:THR:HB	1.69	0.74
3:E:227:GLN:OE1	3:E:240:ARG:HD3	1.87	0.74
3:F:226:TYR:HE2	3:F:245:LEU:HD11	1.54	0.73
3:E:216:ASN:HD22	3:E:219:GLN:HG3	1.53	0.72
2:B:40:THR:HG22	9:B:624:HOH:O	1.90	0.71
3:F:61:MET:HE1	3:F:100:LEU:HG	1.72	0.71
1:C:107:ARG:HD3	1:C:108:ALA:O	1.91	0.70
2:D:62:GLN:OE1	2:D:65:LYS:HD2	1.91	0.70
3:E:50:ILE:HD12	3:E:124:VAL:HG21	1.72	0.70
3:E:195:ILE:HD13	3:E:195:ILE:H	1.55	0.70
2:B:105:LEU:HG	2:B:106:ARG:HG3	1.72	0.70
3:F:27:LYS:HG3	3:F:51:PHE:HB2	1.73	0.69
2:D:105:LEU:HG	2:D:106:ARG:HG3	1.78	0.66
1:A:8:PRO:HG2	1:A:11:MET:HG3	1.78	0.65
2:D:38:LYS:HB2	2:D:48:ILE:HD11	1.77	0.65
2:B:155:PRO:HD2	2:B:209:ALA:CB	2.27	0.65
3:E:68:LYS:HE2	3:E:73:ASP:OD2	1.96	0.65
3:E:216:ASN:HD21	3:E:218:SER:HB3	1.61	0.65
2:B:44:GLY:HA2	9:B:641:HOH:O	1.97	0.64
1:C:89:GLN:NE2	1:C:91:SER:N	2.45	0.64
3:F:57:ASN:OD1	3:F:59:THR:HG22	1.98	0.64
5:H:1:NAG:H61	5:H:2:NAG:O7	1.98	0.63
3:F:200:ILE:HG13	3:F:208:ASN:HB2	1.79	0.63
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.81	0.63
2:B:123:LYS:HE2	2:B:123:LYS:HA	1.81	0.62
3:F:201:LYS:HG3	3:F:207:PHE:CE1	2.34	0.62
5:J:1:NAG:O3	5:J:2:NAG:H82	1.99	0.62
3:E:195:ILE:HD13	3:E:195:ILE:N	2.13	0.62
1:A:37:GLN:HE22	2:B:39:GLN:HE22	1.46	0.61
2:D:210:SER:O	2:D:212:THR:HG23	2.01	0.61
3:E:148:LEU:HD11	3:E:162:MET:HB2	1.83	0.60
3:F:50:ILE:CD1	3:F:124:VAL:HG21	2.30	0.60
2:B:136:CYS:HB2	2:B:138:ASP:OD1	2.03	0.59
1:C:29:VAL:HG11	1:C:89:GLN:HG3	1.84	0.59
3:E:94:ILE:HG12	3:E:95:VAL:N	2.18	0.59
3:E:63:ILE:CD1	3:E:124:VAL:HG22	2.33	0.58
1:C:146:LYS:HE3	1:C:153:GLU:OE1	2.03	0.58
3:E:63:ILE:HD12	3:E:124:VAL:HG22	1.86	0.58
2:B:54:GLY:O	4:G:2:FUC:H63	2.04	0.58
1:C:112:PRO:HB3	1:C:138:PHE:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ALA:O	2:B:86:LEU:HD12	2.05	0.57
2:D:20:MET:CE	2:D:115:THR:HB	2.34	0.57
3:E:216:ASN:ND2	3:E:218:SER:HB3	2.20	0.57
3:E:40:LEU:O	3:E:41:ASN:HB2	2.04	0.57
3:E:50:ILE:CD1	3:E:124:VAL:HG21	2.35	0.57
3:F:194:VAL:HA	3:F:212:CYS:O	2.05	0.57
1:A:112:PRO:HB3	1:A:138:PHE:HB3	1.87	0.57
3:F:75:GLU:CD	3:F:121:ARG:HH11	2.08	0.56
2:D:150:VAL:HB	2:D:185:LEU:CD2	2.35	0.56
2:B:67:LYS:HE2	2:B:90:ASP:OD1	2.06	0.56
3:E:175:ILE:HD11	3:E:209:VAL:HG11	1.87	0.56
1:A:194:GLU:HG2	1:A:205:VAL:HG22	1.86	0.55
3:F:195:ILE:HD12	3:F:195:ILE:O	2.06	0.55
1:C:116:ILE:HD13	1:C:193:CYS:HB2	1.87	0.55
1:A:149:ILE:HD12	1:A:191:TYR:CE2	2.42	0.55
3:E:242:ASN:O	3:E:243:PHE:HB3	2.06	0.55
1:C:24:SER:HA	1:C:68:THR:O	2.07	0.54
3:F:193:ASP:OD1	3:F:214:LYS:HE2	2.07	0.54
2:D:1:GLN:HB3	3:F:203:MET:CG	2.32	0.54
3:E:75:GLU:CD	3:E:121:ARG:HH11	2.11	0.54
1:A:116:ILE:HD11	1:A:131:VAL:HG12	1.90	0.53
1:C:90:TRP:CE2	2:D:106:ARG:NH2	2.76	0.53
2:D:55:ASN:HD22	2:D:55:ASN:C	2.11	0.53
2:D:67:LYS:HE3	2:D:90:ASP:OD1	2.09	0.52
1:A:213:CYS:O	1:A:213:CYS:SG	2.67	0.52
5:H:2:NAG:H3	5:H:2:NAG:H82	1.91	0.52
2:D:52:TYR:CD1	3:F:91:PRO:HB2	2.44	0.52
3:F:125:VAL:O	3:F:125:VAL:HG23	2.09	0.52
2:D:55:ASN:ND2	2:D:57:ASP:H	2.07	0.52
3:E:86:GLN:HE22	3:E:94:ILE:HG13	1.74	0.52
3:F:160:LYS:HA	3:F:214:LYS:HA	1.91	0.52
1:C:146:LYS:HE3	1:C:153:GLU:CD	2.30	0.51
3:E:52:TYR:CE2	3:E:54:GLN:HB2	2.44	0.51
1:A:182:LYS:O	1:A:186:GLU:HG3	2.10	0.51
3:E:162:MET:HG2	3:E:212:CYS:SG	2.51	0.51
2:D:67:LYS:NZ	2:D:84:SER:O	2.44	0.51
1:A:167:SER:HB3	9:A:324:HOH:O	2.10	0.50
1:C:122:GLU:HG2	2:D:130:TYR:CE1	2.46	0.50
1:A:135:LEU:N	1:A:135:LEU:HD12	2.26	0.50
3:F:201:LYS:HG3	3:F:207:PHE:HE1	1.75	0.50
5:H:2:NAG:H3	5:H:2:NAG:C8	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:OD1	1:A:209:ASN:HB3	2.12	0.50
2:D:55:ASN:HD22	2:D:56:GLY:N	2.08	0.50
1:C:122:GLU:HG2	2:D:130:TYR:HE1	1.76	0.50
1:C:109:ASP:OD2	1:C:198:LYS:HD2	2.11	0.50
3:E:61:MET:HE1	3:E:100:LEU:HG	1.93	0.50
1:C:104:GLU:HG2	1:C:105:LEU:N	2.27	0.50
3:F:38:THR:HG22	3:F:137:LEU:HD11	1.94	0.50
2:B:160:LEU:HA	2:B:204:ASN:O	2.12	0.49
3:E:81:PHE:HD1	3:E:86:GLN:HG2	1.78	0.49
2:D:201:ILE:H	2:D:201:ILE:HD13	1.77	0.49
3:F:192:GLU:O	3:F:193:ASP:HB2	2.11	0.49
4:G:1:NAG:C8	4:G:1:NAG:H3	2.43	0.49
1:C:89:GLN:HE21	1:C:91:SER:N	1.89	0.49
3:F:147:LEU:HD21	3:F:243:PHE:CD2	2.48	0.49
3:E:142:SER:HA	3:E:234:SER:OG	2.13	0.49
1:A:141:LYS:HD2	1:A:172:TYR:CE2	2.48	0.48
3:F:183:LYS:HG3	3:F:184:PHE:CE1	2.48	0.48
3:F:171:GLU:HG3	3:F:199:THR:HG21	1.95	0.48
2:D:150:VAL:HB	2:D:185:LEU:HD22	1.95	0.48
3:F:245:LEU:HD12	3:F:245:LEU:N	2.22	0.48
1:A:10:LEU:HD12	1:A:102:LYS:O	2.13	0.48
1:A:8:PRO:HG2	1:A:11:MET:CG	2.43	0.48
5:J:1:NAG:O3	5:J:1:NAG:O7	2.30	0.48
2:B:178:LEU:HD13	2:B:183:TYR:CE1	2.48	0.48
1:A:211:ASN:C	1:A:213:CYS:H	2.17	0.48
1:A:72:LEU:HD23	1:A:73:THR:N	2.29	0.48
3:E:121:ARG:HB2	3:E:134:THR:HG22	1.95	0.48
2:D:195:THR:O	2:D:198:SER:HB3	2.14	0.48
3:E:145:SER:HA	3:E:165:SER:HA	1.95	0.47
3:F:175:ILE:O	3:F:175:ILE:HG23	2.13	0.47
2:B:52:TYR:CD1	3:E:91:PRO:HB2	2.49	0.47
3:F:194:VAL:HG13	3:F:194:VAL:O	2.14	0.47
3:E:206:THR:HG23	3:E:207:PHE:N	2.29	0.47
3:F:67:TRP:CH2	3:F:69:SER:HB2	2.48	0.47
1:A:10:LEU:HD11	1:A:104:GLU:HG2	1.96	0.47
2:D:52:TYR:HD2	2:D:55:ASN:ND2	2.12	0.47
3:E:39:PRO:HA	3:E:140:VAL:O	2.14	0.47
1:A:14:SER:HB2	1:A:17:GLU:HG3	1.95	0.47
2:D:30:THR:HA	2:D:53:PRO:HB2	1.97	0.47
3:E:148:LEU:CD1	3:E:162:MET:HB2	2.44	0.47
2:B:185:LEU:HD23	2:B:185:LEU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:HD2	1:A:148:LYS:HE3	1.97	0.46
2:D:35:HIS:O	2:D:96:CYS:HA	2.15	0.46
2:B:192:THR:OG1	2:B:194:SER:HB3	2.14	0.46
3:F:191:SER:O	3:F:192:GLU:HB2	2.15	0.46
3:E:144:ALA:O	3:E:165:SER:HA	2.15	0.46
2:B:30:THR:HA	2:B:53:PRO:O	2.14	0.46
3:E:226:TYR:HB2	3:E:243:PHE:CZ	2.51	0.46
2:D:55:ASN:ND2	2:D:55:ASN:C	2.69	0.46
2:B:54:GLY:O	4:G:2:FUC:C6	2.63	0.46
1:A:65:GLY:HA3	1:A:70:TYR:CD2	2.51	0.46
3:F:196:THR:HG23	3:F:196:THR:O	2.16	0.46
1:C:35:TYR:HE2	2:D:108:LEU:O	1.99	0.46
3:E:196:THR:HG23	3:E:196:THR:O	2.16	0.46
3:F:129:LEU:HD12	3:F:129:LEU:H	1.81	0.46
5:H:1:NAG:H61	5:H:2:NAG:C7	2.46	0.46
2:B:156:GLU:HG3	2:B:183:TYR:CE2	2.50	0.45
1:C:95:LEU:HD23	1:C:95:LEU:C	2.36	0.45
3:F:67:TRP:O	3:F:75:GLU:HA	2.16	0.45
3:E:94:ILE:CG1	3:E:95:VAL:N	2.79	0.45
1:C:10:LEU:HD23	1:C:102:LYS:HB3	1.99	0.45
2:B:159:THR:OG1	2:B:206:ALA:HB3	2.17	0.45
3:E:231:ARG:HG2	3:E:238:PRO:HG3	1.99	0.45
3:F:129:LEU:HD12	3:F:129:LEU:N	2.32	0.45
2:D:129:VAL:HG21	2:D:214:VAL:CG2	2.47	0.45
3:E:44:VAL:HG22	3:E:45:THR:N	2.33	0.44
1:C:159:LEU:CD1	2:D:179:GLN:HB2	2.47	0.44
2:D:91:SER:O	2:D:92:ALA:HB2	2.17	0.44
3:F:143:PRO:CB	3:F:168:PHE:HB3	2.40	0.44
2:B:196:TRP:CG	2:B:197:PRO:HA	2.53	0.44
1:A:191:TYR:O	1:A:207:SER:HB2	2.17	0.44
1:C:149:ILE:HD11	1:C:178:LEU:HD21	1.99	0.44
3:E:82:PHE:CD2	3:E:85:HIS:CE1	3.06	0.44
1:C:8:PRO:HG3	1:C:11:MET:HB3	2.00	0.44
2:D:36:TRP:HA	2:D:95:TYR:O	2.18	0.44
2:D:51:ILE:HG13	2:D:58:THR:HG22	2.00	0.44
3:E:167:GLY:HA2	3:E:206:THR:CG2	2.48	0.44
1:C:22:THR:HG22	1:C:23:CYS:N	2.33	0.44
2:B:174:PHE:HA	2:B:175:PRO:HD3	1.85	0.44
3:F:38:THR:CG2	3:F:137:LEU:HD11	2.47	0.44
1:A:123:GLN:HG2	1:A:128:GLY:O	2.18	0.43
1:A:94:PRO:O	1:A:96:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLN:HA	2:B:1:GLN:OE1	2.18	0.43
2:D:127:PRO:CB	2:D:153:TYR:HB3	2.39	0.43
1:C:192:THR:HA	1:C:207:SER:HB3	1.99	0.43
3:F:221:ASP:O	3:F:224:THR:HG22	2.18	0.43
3:F:94:ILE:HG12	3:F:95:VAL:N	2.32	0.43
1:C:135:LEU:HD12	1:C:135:LEU:N	2.32	0.43
2:D:185:LEU:C	2:D:185:LEU:HD23	2.38	0.43
3:F:65:TRP:CE2	3:F:107:LEU:HB2	2.52	0.43
3:E:216:ASN:ND2	3:E:219:GLN:HG3	2.29	0.43
2:B:126:ALA:HB1	2:B:212:THR:HG21	2.00	0.43
2:D:40:THR:HG23	2:D:41:PRO:HD2	2.00	0.43
3:E:67:TRP:CH2	3:E:69:SER:HB2	2.54	0.43
1:A:150:ASP:HA	1:A:190:SER:OG	2.19	0.43
1:A:73:THR:HG22	1:A:74:ILE:N	2.34	0.43
1:C:164:ASP:O	1:C:165:GLN:C	2.57	0.43
3:F:226:TYR:CE2	3:F:245:LEU:HD11	2.43	0.43
3:F:98:TRP:CZ2	3:F:99:ARG:HD3	2.54	0.43
1:A:136:ASN:HD22	1:A:173:SER:CB	2.32	0.43
1:C:154:ARG:HG3	1:C:155:GLN:N	2.33	0.42
2:D:160:LEU:HD23	2:D:160:LEU:C	2.40	0.42
3:E:96:SER:HA	3:E:97:PRO:HD3	1.92	0.42
1:A:188:HIS:O	1:A:210:ARG:HD3	2.19	0.42
2:B:23:LYS:HE3	2:B:23:LYS:HB3	1.83	0.42
3:E:194:VAL:HG13	3:E:194:VAL:O	2.20	0.42
2:B:131:PRO:HD3	2:B:216:LYS:HE2	2.01	0.42
1:C:148:LYS:HA	1:C:152:SER:O	2.20	0.42
2:D:201:ILE:HD11	2:D:218:ILE:HB	2.02	0.42
1:A:149:ILE:HD11	1:A:178:LEU:HD21	2.02	0.41
2:D:196:TRP:CG	2:D:197:PRO:HA	2.55	0.41
2:D:91:SER:HA	2:D:117:VAL:O	2.20	0.41
2:B:185:LEU:HD23	2:B:186:SER:N	2.36	0.41
1:C:182:LYS:O	1:C:186:GLU:HG3	2.20	0.41
3:E:65:TRP:CE2	3:E:107:LEU:HB2	2.55	0.41
3:E:175:ILE:N	3:E:175:ILE:HD12	2.35	0.41
2:D:160:LEU:HA	2:D:204:ASN:O	2.20	0.41
3:F:81:PHE:CE2	3:F:83:GLY:HA2	2.56	0.41
5:J:1:NAG:H4	5:J:2:NAG:H2	1.74	0.41
1:C:149:ILE:HD13	1:C:154:ARG:HB2	2.03	0.41
1:A:150:ASP:OD2	1:A:188:HIS:HB3	2.20	0.41
2:B:81:MET:CE	2:B:83:LEU:HD21	2.51	0.41
2:B:91:SER:O	2:B:92:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:148:LEU:HD12	3:E:148:LEU:O	2.20	0.41
3:F:126:VAL:O	3:F:127:THR:C	2.60	0.41
1:A:164:ASP:O	1:A:165:GLN:C	2.59	0.41
1:A:212:GLU:O	1:A:213:CYS:HB3	2.21	0.41
3:F:201:LYS:N	3:F:201:LYS:CE	2.73	0.41
1:A:169:ASP:CG	1:A:171:THR:HG23	2.42	0.40
3:E:226:TYR:HB2	3:E:243:PHE:CE1	2.56	0.40
3:E:82:PHE:HD2	3:E:85:HIS:CE1	2.40	0.40
3:F:177:TRP:CD1	3:F:194:VAL:HG21	2.56	0.40
1:A:8:PRO:CG	1:A:11:MET:CG	3.00	0.40
1:A:183:ASP:O	1:A:187:ARG:HG3	2.21	0.40
2:B:214:VAL:HG12	2:B:215:ASP:N	2.37	0.40
1:C:106:LYS:HG2	1:C:107:ARG:N	2.36	0.40
2:D:23:LYS:HG3	2:D:78:THR:OG1	2.21	0.40
3:E:225:VAL:HA	3:E:244:THR:HG22	2.03	0.40
1:A:61:PHE:HD1	1:A:72:LEU:HD21	1.86	0.40
2:B:121:SER:O	2:B:122:ALA:C	2.60	0.40
2:D:155:PRO:HD2	2:D:209:ALA:CB	2.52	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	212/214 (99%)	205 (97%)	5 (2%)	2 (1%)	17	31
1	C	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	29	48
2	B	216/219 (99%)	206 (95%)	7 (3%)	3 (1%)	11	20
2	D	217/219 (99%)	205 (94%)	10 (5%)	2 (1%)	17	31
3	E	213/253 (84%)	198 (93%)	13 (6%)	2 (1%)	17	31
3	F	210/253 (83%)	194 (92%)	15 (7%)	1 (0%)	29	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1280/1372 (93%)	1212 (95%)	57 (4%)	11 (1%)	17 31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
2	B	122	ALA
3	E	243	PHE
3	F	192	GLU
1	A	67	GLY
2	B	85	SER
2	D	41	PRO
1	C	211	ASN
3	E	58	ILE
2	B	157	PRO
2	D	157	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	189/189 (100%)	187 (99%)	2 (1%)	73 89
1	C	189/189 (100%)	182 (96%)	7 (4%)	34 60
2	B	183/184 (100%)	175 (96%)	8 (4%)	28 52
2	D	183/184 (100%)	178 (97%)	5 (3%)	44 71
3	E	186/222 (84%)	178 (96%)	8 (4%)	29 53
3	F	182/222 (82%)	174 (96%)	8 (4%)	28 52
All	All	1112/1190 (93%)	1074 (97%)	38 (3%)	37 63

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU

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Mol	Chain	Res	Type
1	A	212	GLU
2	B	5	GLN
2	B	43	GLN
2	B	123	LYS
2	B	138	ASP
2	B	155	PRO
2	B	157	PRO
2	B	185	LEU
2	B	216	LYS
1	C	0	MET
1	C	107	ARG
1	C	143	ILE
1	C	155	GLN
1	C	184	GLU
1	C	198	LYS
1	C	212	GLU
2	D	41	PRO
2	D	55	ASN
2	D	157	PRO
2	D	185	LEU
2	D	201	ILE
3	E	57	ASN
3	E	70	LEU
3	E	73	ASP
3	E	99	ARG
3	E	112	ILE
3	E	195	ILE
3	E	203	MET
3	E	206	THR
3	F	24	MET
3	F	42	ASP
3	F	73	ASP
3	F	98	TRP
3	F	145	SER
3	F	165	SER
3	F	201	LYS
3	F	245	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN

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Mol	Chain	Res	Type
1	A	136	ASN
1	A	209	ASN
1	A	211	ASN
2	B	43	GLN
2	B	62	GLN
1	C	89	GLN
1	C	155	GLN
1	C	189	ASN
1	C	209	ASN
2	D	1	GLN
2	D	55	ASN
3	E	57	ASN
3	E	85	HIS
3	E	86	GLN
3	E	180	GLN
3	E	216	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	1	3,4	14,14,15	0.71	0	17,19,21	1.24	3 (17%)
4	FUC	G	2	4	10,10,11	0.69	0	14,14,16	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	H	1	3,5	14,14,15	0.70	0	17,19,21	0.86	0
5	NAG	H	2	5	14,14,15	0.62	0	17,19,21	0.70	0
6	NAG	I	1	3,6	14,14,15	0.52	0	17,19,21	0.65	0
6	NAG	I	2	6	14,14,15	0.47	0	17,19,21	0.73	0
6	FUC	I	3	6	10,10,11	0.67	0	14,14,16	0.55	0
5	NAG	J	1	3,5	14,14,15	0.61	0	17,19,21	1.17	1 (5%)
5	NAG	J	2	5	14,14,15	0.61	0	17,19,21	0.83	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	G	1	3,4	-	5/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
5	NAG	H	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	5/6/23/26	0/1/1/1
6	NAG	I	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
6	FUC	I	3	6	-	-	0/1/1/1
5	NAG	J	1	3,5	-	5/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	1	NAG	C1-O5-C5	2.94	116.17	112.19
5	J	2	NAG	C2-N2-C7	-2.38	119.52	122.90
4	G	1	NAG	C1-C2-N2	2.14	114.15	110.49
4	G	1	NAG	C4-C3-C2	-2.09	107.96	111.02
4	G	1	NAG	C6-C5-C4	-2.03	108.25	113.00

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	H	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C3-C2-N2-C7
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
6	I	2	NAG	C3-C2-N2-C7
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
5	H	2	NAG	O5-C5-C6-O6
5	H	1	NAG	C8-C7-N2-C2
6	I	1	NAG	C8-C7-N2-C2
6	I	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	H	2	NAG	C1-C2-N2-C7
5	H	2	NAG	C4-C5-C6-O6
5	H	1	NAG	O7-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
5	H	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C1-C2-N2-C7
6	I	2	NAG	C1-C2-N2-C7
5	H	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6

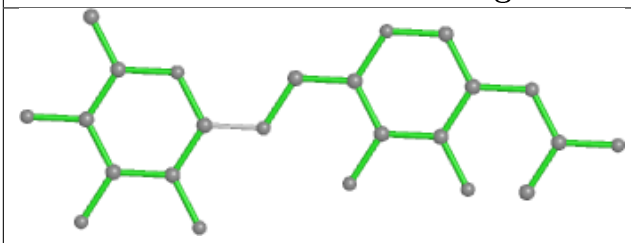
There are no ring outliers.

8 monomers are involved in 15 short contacts:

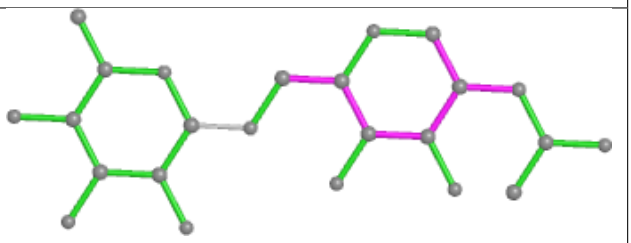
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	4	0
5	J	2	NAG	2	0
5	H	1	NAG	4	0
4	G	1	NAG	1	0
5	J	1	NAG	4	0
6	I	1	NAG	2	0
6	I	2	NAG	2	0
4	G	2	FUC	2	0

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

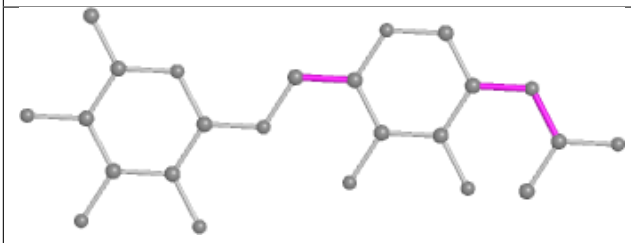
Oligosaccharide Chain G



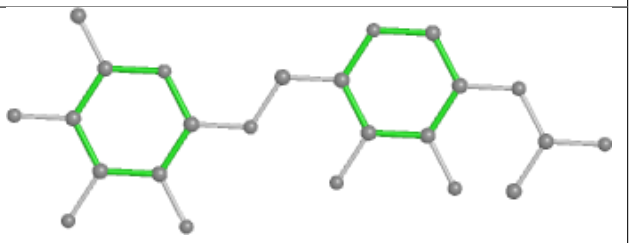
Bond lengths



Bond angles

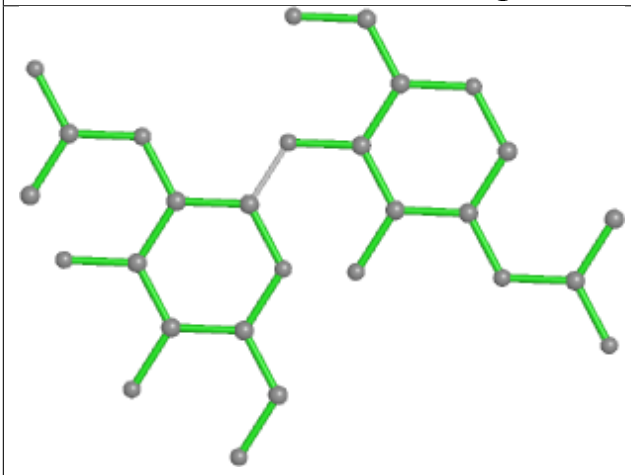


Torsions

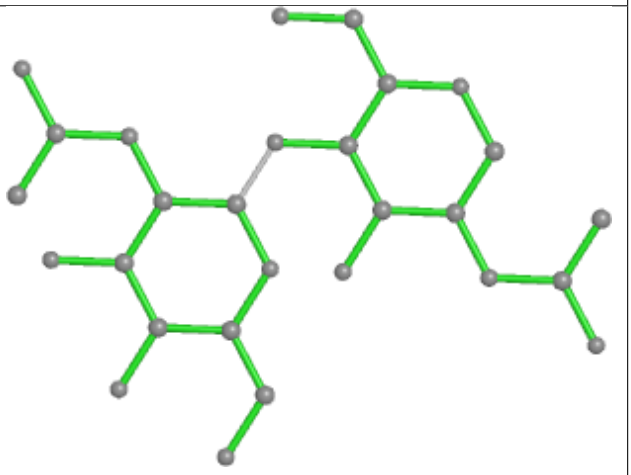


Rings

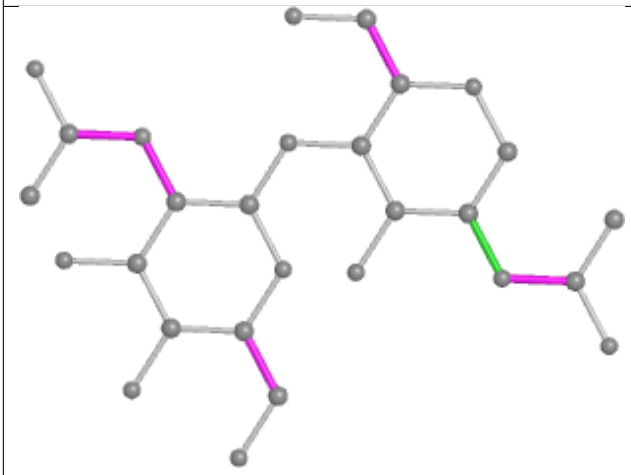
Oligosaccharide Chain H



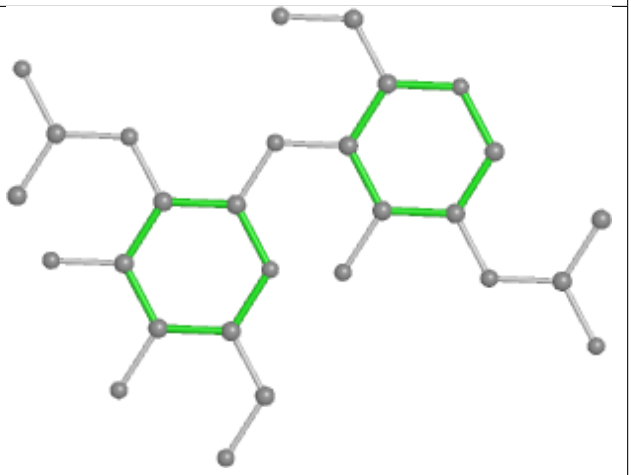
Bond lengths



Bond angles

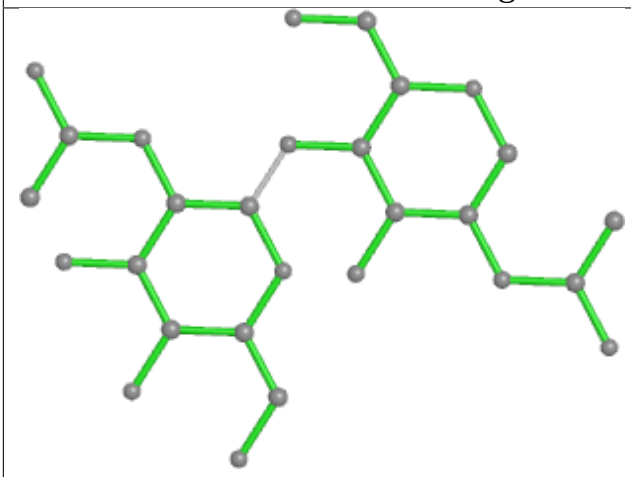


Torsions

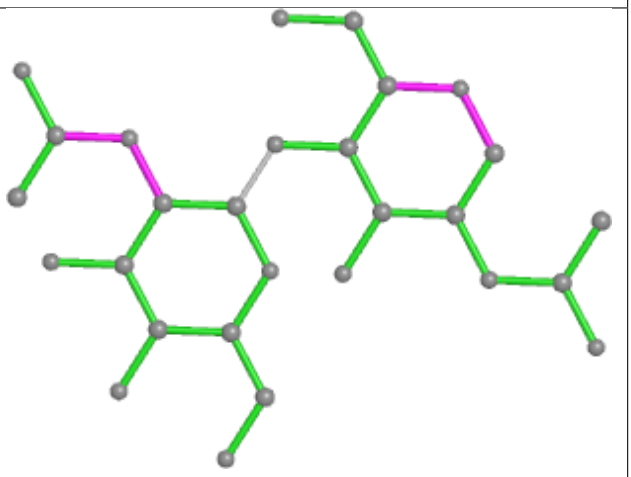


Rings

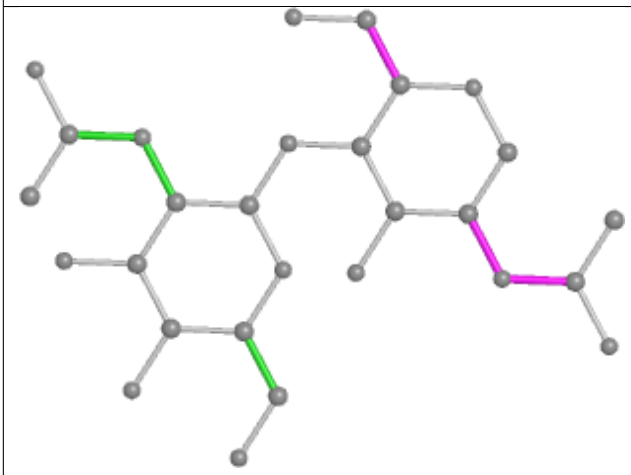
Oligosaccharide Chain J



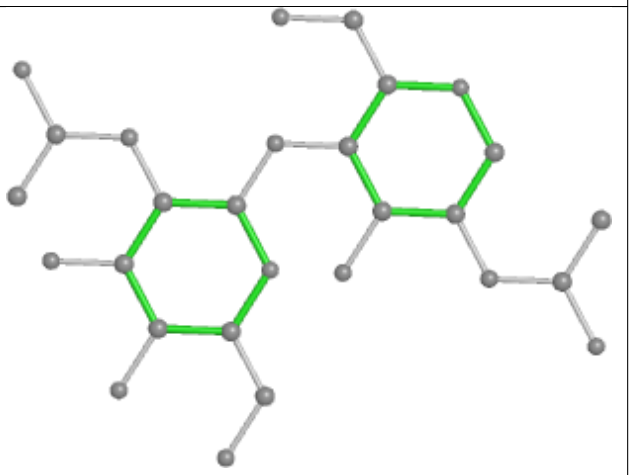
Bond lengths



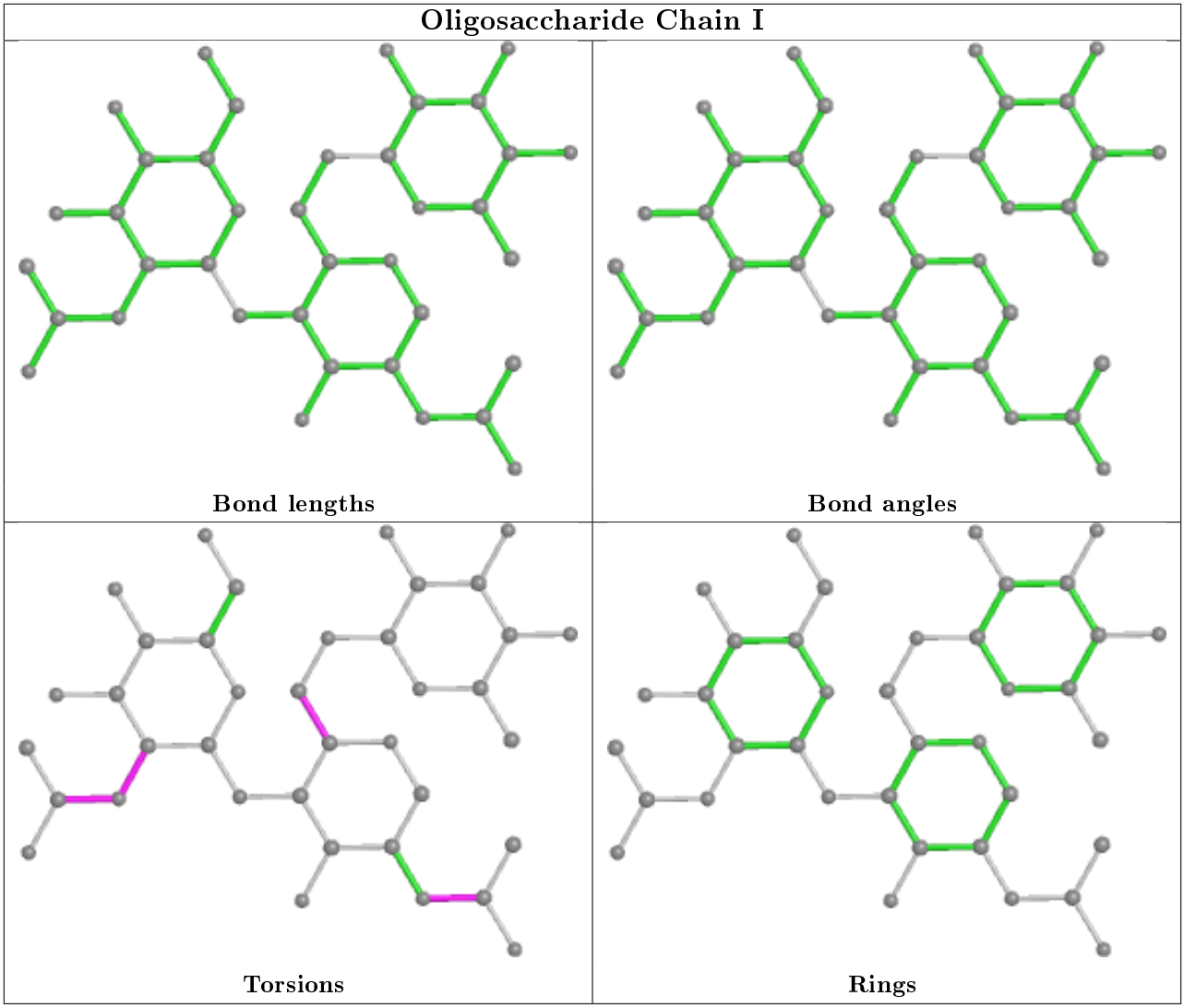
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SO4	B	501	-	4,4,4	0.26	0	6,6,6	0.08	0
7	SO4	D	601	-	4,4,4	0.26	0	6,6,6	0.06	0
8	ACY	F	306	-	1,3,3	2.34	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	ACY	E	305	-	1,3,3	2.02	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	306	ACY	CH3-C	2.34	1.51	1.48
8	E	305	ACY	CH3-C	2.02	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	214/214 (100%)	-0.31	1 (0%) 91 91	20, 33, 51, 70	0
1	C	214/214 (100%)	-0.24	2 (0%) 84 86	25, 36, 54, 74	0
2	B	218/219 (99%)	-0.26	0 100 100	22, 37, 53, 60	0
2	D	219/219 (100%)	-0.25	0 100 100	23, 39, 56, 70	0
3	E	217/253 (85%)	0.24	12 (5%) 25 26	25, 49, 80, 92	0
3	F	214/253 (84%)	0.60	25 (11%) 4 4	28, 55, 93, 106	0
All	All	1296/1372 (94%)	-0.04	40 (3%) 49 52	20, 39, 76, 106	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	161	TYR	4.8
3	F	191	SER	4.6
3	F	195	ILE	4.4
3	F	149	LEU	4.0
3	F	215	LEU	4.0
3	F	193	ASP	3.8
1	A	0	MET	3.5
3	F	160	LYS	3.5
3	F	194	VAL	3.4
3	E	83	GLY	3.3
3	F	147	LEU	3.3
3	F	213	LEU	3.2
3	F	190	ILE	3.0
3	E	245	LEU	3.0
3	F	162	MET	2.9
1	C	0	MET	2.9
3	E	215	LEU	2.9
3	E	192	GLU	2.8
3	F	188	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	244	THR	2.8
3	E	198	PRO	2.7
1	C	213	CYS	2.6
3	E	24	MET	2.5
3	E	200	ILE	2.4
3	E	161	TYR	2.4
3	F	84	ASP	2.4
3	F	214	LYS	2.3
3	E	148	LEU	2.3
3	F	196	THR	2.3
3	F	183	LYS	2.2
3	E	175	ILE	2.2
3	F	146	ARG	2.2
3	E	203	MET	2.2
3	F	126	VAL	2.2
3	F	24	MET	2.1
3	F	243	PHE	2.1
3	E	191	SER	2.1
3	F	181	THR	2.1
3	F	192	GLU	2.0
3	F	216	ASN	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
6	FUC	I	3	10/11	0.73	0.30	84,87,88,88	0
4	FUC	G	2	10/11	0.76	0.38	85,89,90,92	0
6	NAG	I	2	14/15	0.80	0.21	78,81,84,84	0
5	NAG	J	2	14/15	0.81	0.33	88,90,95,95	0
5	NAG	H	2	14/15	0.82	0.38	95,98,102,103	0
5	NAG	J	1	14/15	0.86	0.24	74,76,79,84	0
5	NAG	H	1	14/15	0.87	0.20	78,80,83,89	0

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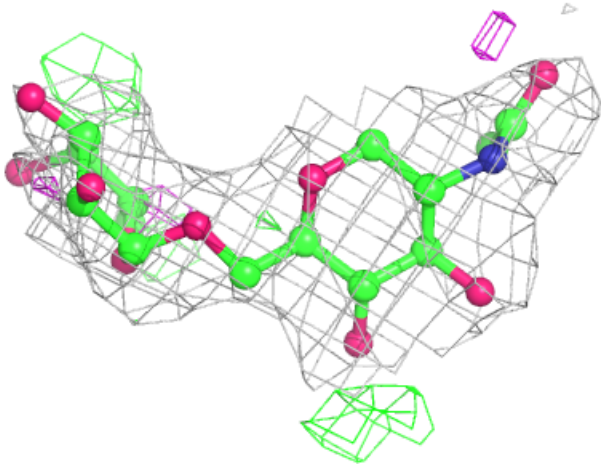
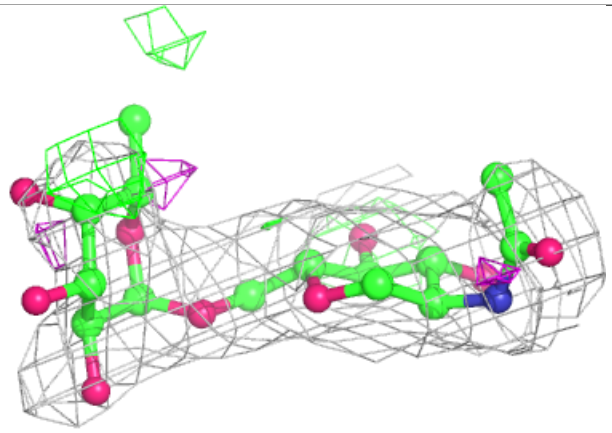
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	1	14/15	0.89	0.16	57,62,71,78	0
6	NAG	I	1	14/15	0.91	0.17	61,68,74,80	0

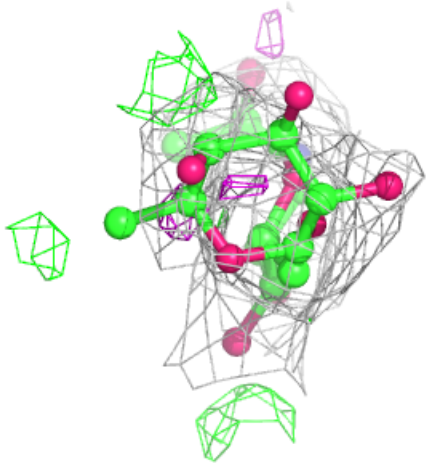
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

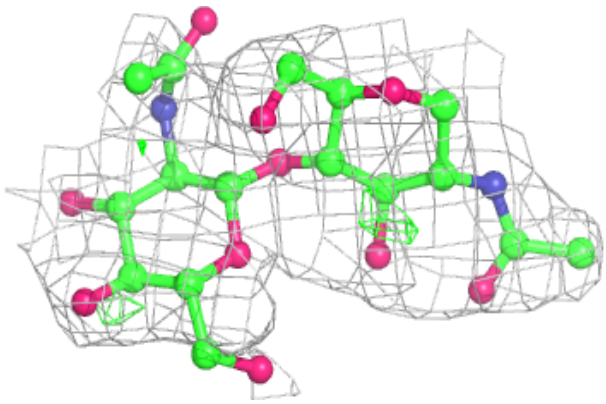


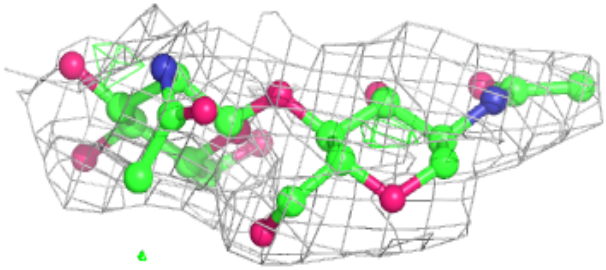


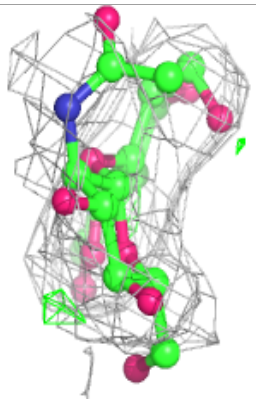


Electron density around Chain H:

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

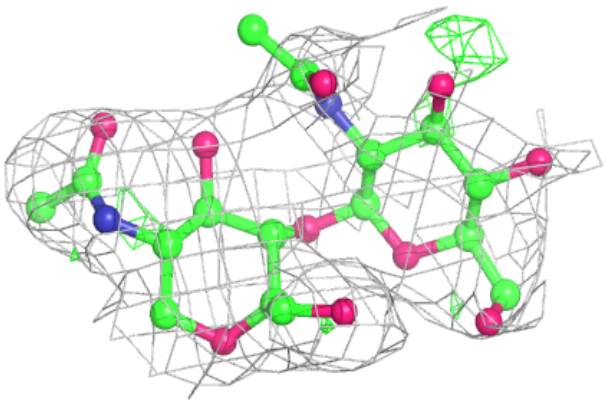


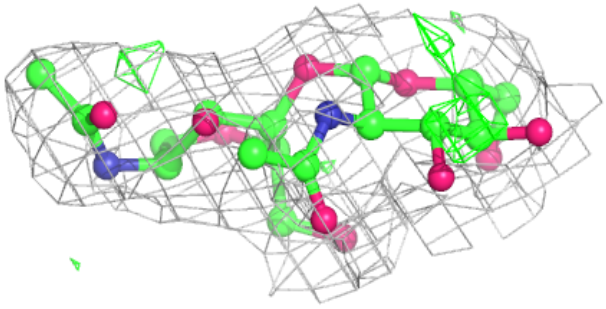


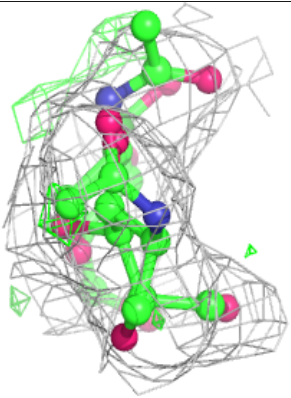


Electron density around Chain J:

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

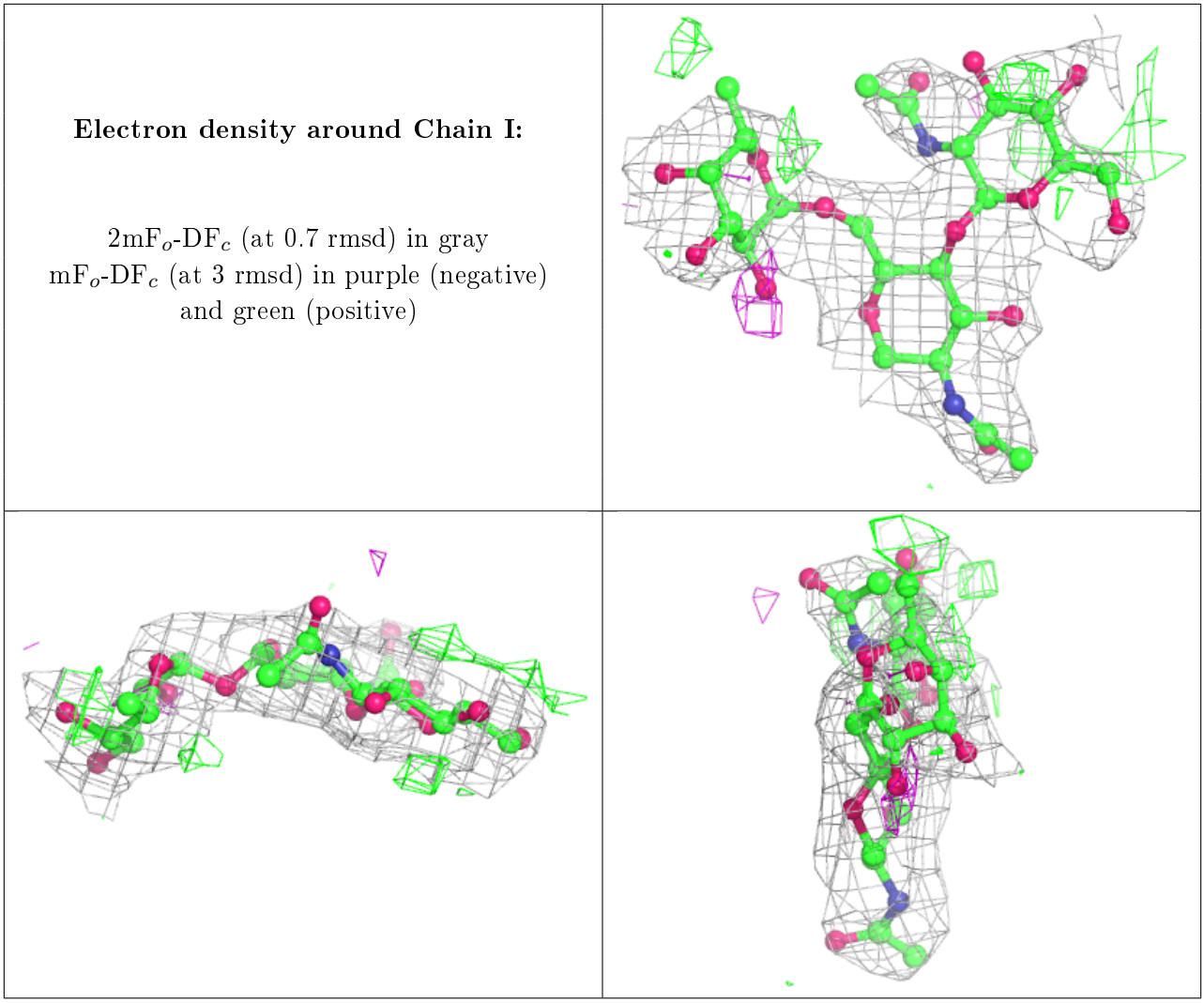






Electron density around Chain I:

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



6.4 Ligands

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
8	ACY	E	305	4/4	0.86	0.24	54,55,57,57	0
8	ACY	F	306	4/4	0.94	0.24	56,56,57,57	0
7	SO4	B	501	5/5	0.97	0.10	83,83,83,84	0
7	SO4	D	601	5/5	0.97	0.12	87,88,88,88	0

6.5 Other polymers

There are no such residues in this entry.