Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 12:22 PM EST

PDB ID	:	4ELM
Title	:	Crystal structure of the mouse CD1d-lysosulfatide-Hy19.3 TCR complex
Authors	:	Girardi, E.; Maricic, I.; Wang, J.; Mac, T.T.; Iyer, P.; Kumar, V.; Zajonc, D.M.
Deposited on	:	2012-04-11
Resolution	:	3.48 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:

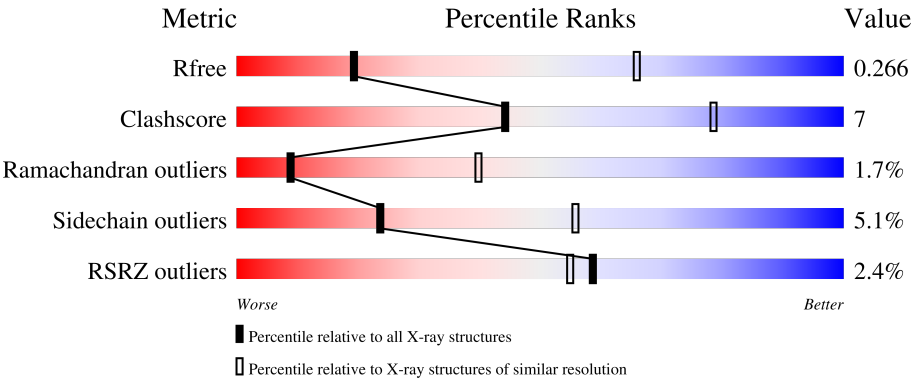
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	285	77% 15% • 7%
1	C	285	77% 15% • 6%
2	B	99	% 85% 12% ••
2	D	99	83% 16% •
3	E	208	4% 74% 9% • 14%

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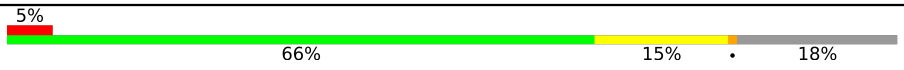
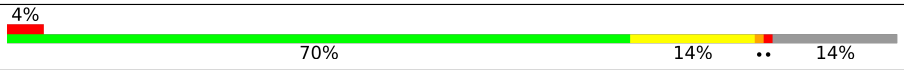
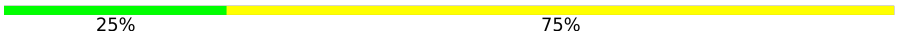
Mol	Chain	Length	Quality of chain
3	G	208	
4	F	244	
4	H	244	
5	I	2	
6	J	4	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11360 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2047	1310	343	382	12			
1	C	269	Total	C	N	O	S	0	0	0
			2093	1340	358	383	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	HIS	-	expression tag	UNP P11609
A	281	HIS	-	expression tag	UNP P11609
A	282	HIS	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	HIS	-	expression tag	UNP P11609
C	201	HIS	ASP	SEE REMARK 999	UNP P11609
C	280	HIS	-	expression tag	UNP P11609
C	281	HIS	-	expression tag	UNP P11609
C	282	HIS	-	expression tag	UNP P11609
C	283	HIS	-	expression tag	UNP P11609
C	284	HIS	-	expression tag	UNP P11609
C	285	HIS	-	expression tag	UNP P11609

- Molecule 2 is a protein called Beta-2 microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			747	471	126	143	7			
2	D	99	Total	C	N	O	S	0	0	0
			777	495	129	146	7			

- Molecule 3 is a protein called Hy19.3 TCR alpha chain (mouse variable domain, human

constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	179	Total	C	N	O	S	0	0	0
			1234	772	217	239	6			
3	G	171	Total	C	N	O	S	0	0	0
			1185	735	207	236	7			

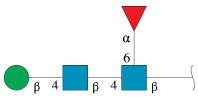
- Molecule 4 is a protein called Hy19.3 TCR beta chain (mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	224	Total	C	N	O	S	0	0	0
			1578	1007	266	296	9			
4	H	211	Total	C	N	O	S	0	0	0
			1459	929	247	274	9			

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

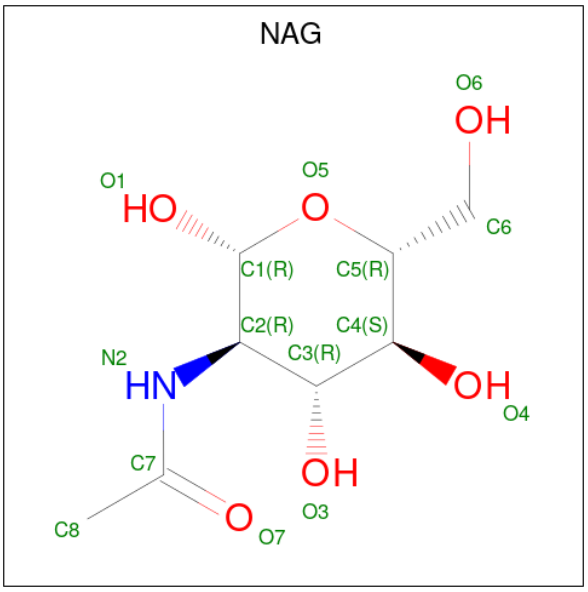
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



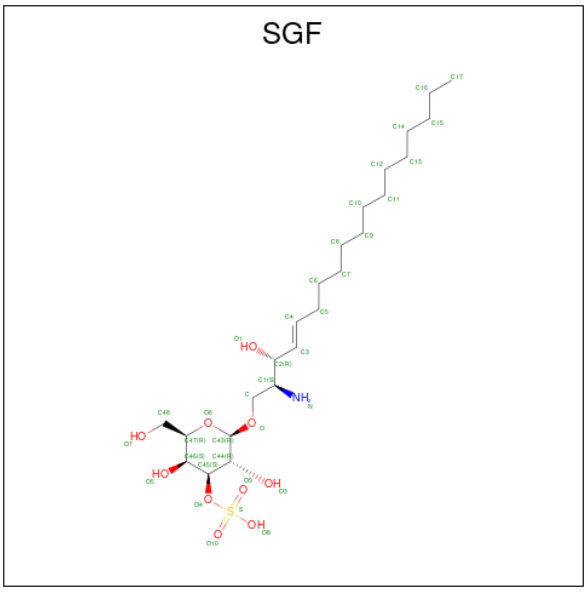
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



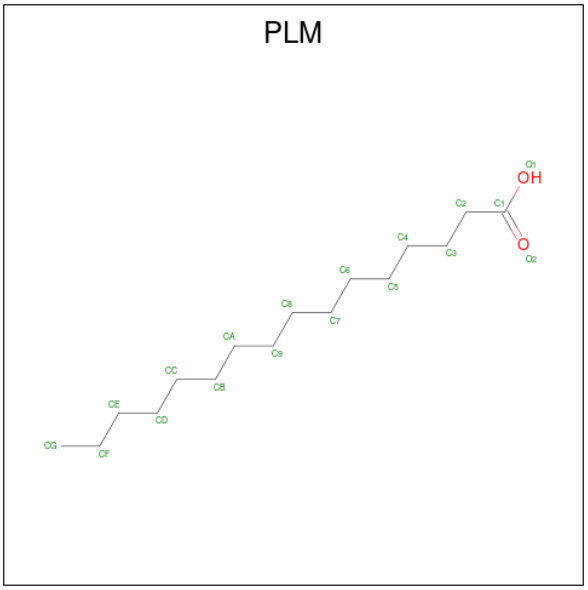
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 13 8 1 4	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is (2S,3R,4E)-2-amino-3-hydroxyoctadec-4-en-1-yl 3-O-sulfo-beta-D-galactopyranoside (three-letter code: SGF) (formula: $C_{24}H_{47}NO_{10}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			36	24	1	10	1		
8	C	1	Total	C	N	O	S	0	0
			36	24	1	10	1		

- Molecule 9 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



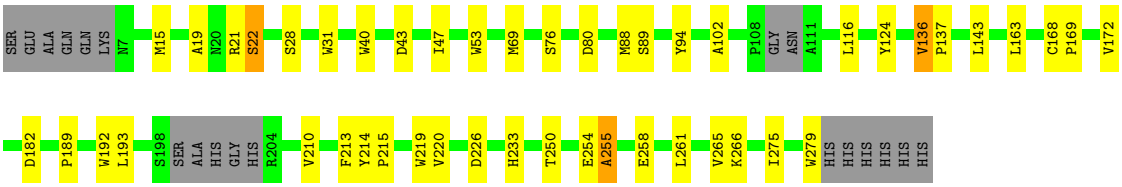
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			18	16	2		
9	C	1	Total	C	O	0	0
			18	16	2		

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.

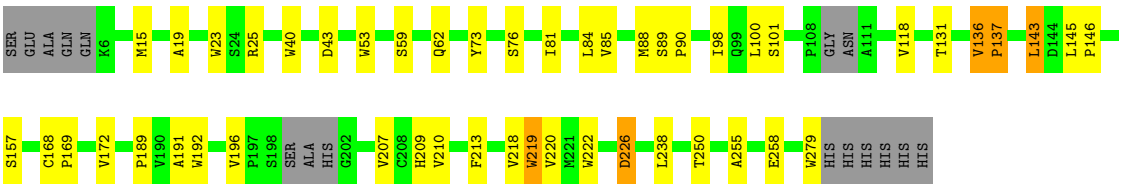
• Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain A:



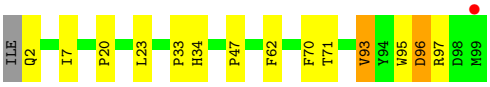
• Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain C:



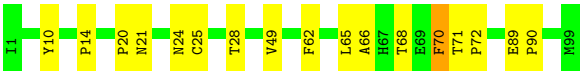
• Molecule 2: Beta-2 microglobulin

Chain B:



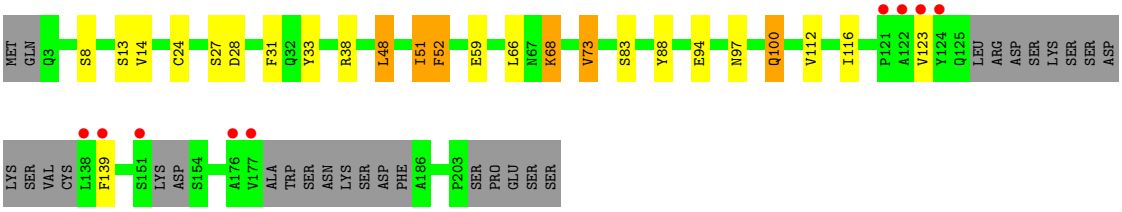
• Molecule 2: Beta-2 microglobulin

Chain D:



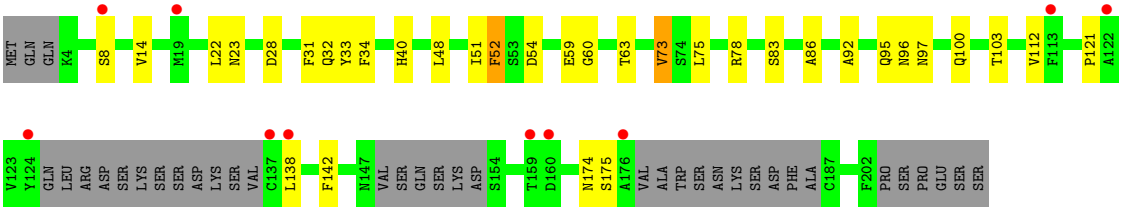
• Molecule 3: Hy19.3 TCR alpha chain (mouse variable domain, human constant domain)

Chain E:



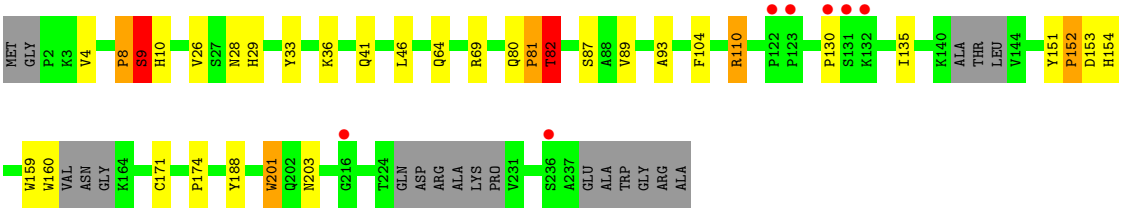
• Molecule 3: Hy19.3 TCR alpha chain (mouse variable domain, human constant domain)

Chain G:



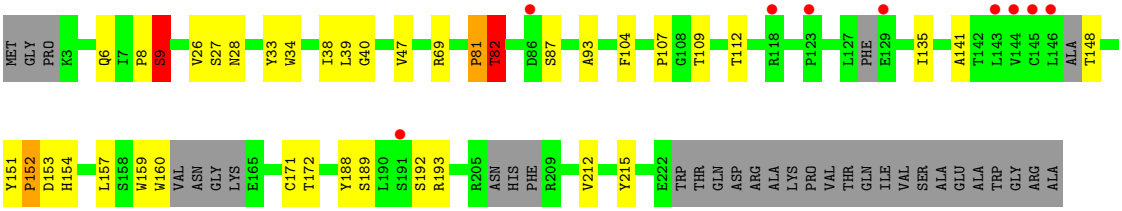
• Molecule 4: Hy19.3 TCR beta chain (mouse variable domain, human constant domain)

Chain F:



• Molecule 4: Hy19.3 TCR beta chain (mouse variable domain, human constant domain)

Chain H:

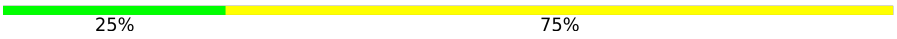


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.51Å 127.00Å 104.35Å 90.00° 110.53° 90.00°	Depositor
Resolution (Å)	92.26 – 3.48 83.22 – 3.48	Depositor EDS
% Data completeness (in resolution range)	99.0 (92.26-3.48) 99.1 (83.22-3.48)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.209 , 0.265 0.208 , 0.266	Depositor DCC
R_{free} test set	1541 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	73.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11360	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.63	3/2108 (0.1%)	0.55	0/2882
1	C	0.62	4/2155 (0.2%)	0.55	0/2943
2	B	0.54	1/773 (0.1%)	0.51	0/1061
2	D	0.55	0/803	0.54	0/1099
3	E	0.48	0/1263	0.54	0/1727
3	G	0.47	0/1211	0.53	0/1654
4	F	0.54	3/1623 (0.2%)	0.60	2/2230 (0.1%)
4	H	0.53	2/1501 (0.1%)	0.57	0/2063
All	All	0.56	13/11437 (0.1%)	0.56	2/15659 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	TRP	CD2-CE2	5.30	1.47	1.41
4	H	160	TRP	CD2-CE2	5.16	1.47	1.41
1	A	53	TRP	CD2-CE2	5.15	1.47	1.41
4	H	159	TRP	CD2-CE2	5.14	1.47	1.41
4	F	160	TRP	CD2-CE2	5.10	1.47	1.41
1	C	53	TRP	CD2-CE2	5.06	1.47	1.41
4	F	201	TRP	CD2-CE2	5.04	1.47	1.41
2	B	95	TRP	CD2-CE2	5.03	1.47	1.41
1	C	40	TRP	CD2-CE2	5.02	1.47	1.41
4	F	159	TRP	CD2-CE2	5.02	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	TRP	CD2-CE2	5.02	1.47	1.41
1	C	222	TRP	CD2-CE2	5.01	1.47	1.41
1	A	192	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	9	SER	N-CA-C	-5.79	95.36	111.00
4	F	82	THR	N-CA-CB	5.08	119.95	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	81	PRO	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	2047	0	1853	20	0
1	C	2093	0	1929	29	0
2	B	747	0	631	7	0
2	D	777	0	703	11	0
3	E	1234	0	986	15	0
3	G	1185	0	953	20	0
4	F	1578	0	1247	21	0
4	H	1459	0	1123	20	0
5	I	28	0	25	0	0
6	J	49	0	43	0	0
7	A	27	0	24	0	0
7	C	28	0	26	1	0
8	A	36	0	47	0	0
8	C	36	0	47	5	0
9	A	18	0	31	0	0
9	C	18	0	31	0	0
All	All	11360	0	9699	139	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 7.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:33:TYR:HD1	3:G:52:PHE:HB3	1.11	1.10
3:G:33:TYR:HD1	3:G:52:PHE:CB	1.68	1.07
3:G:33:TYR:CD1	3:G:52:PHE:HB3	1.90	1.06
4:F:110:ARG:HH11	4:F:110:ARG:HG2	1.23	1.01
4:H:8:PRO:HA	4:H:9:SER:HB3	1.50	0.94
3:E:24:CYS:HB3	3:E:73:VAL:HG23	1.56	0.87
4:H:135:ILE:HG12	4:H:141:ALA:HB2	1.59	0.85
4:F:81:PRO:HA	4:F:82:THR:HG23	1.59	0.84
2:D:20:PRO:HA	2:D:71:THR:HG22	1.61	0.82
4:H:8:PRO:CA	4:H:9:SER:HB3	2.09	0.82
2:B:20:PRO:HA	2:B:71:THR:HG22	1.62	0.80
1:C:168:CYS:HB3	1:C:169:PRO:HD3	1.64	0.79
3:G:33:TYR:CD1	3:G:52:PHE:CB	2.59	0.77
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.72	0.72
4:F:110:ARG:HH11	4:F:110:ARG:CG	2.02	0.70
3:E:97:ASN:HB3	3:E:100:GLN:NE2	2.07	0.70
3:E:33:TYR:HB3	3:E:52:PHE:CD1	2.29	0.66
3:G:97:ASN:HB3	3:G:100:GLN:NE2	2.11	0.66
4:F:33:TYR:HB2	4:F:93:ALA:HB3	1.79	0.63
1:C:118:VAL:HG11	8:C:507:SGF:H17	1.79	0.63
4:H:81:PRO:HA	4:H:82:THR:HG23	1.81	0.63
4:F:64:GLN:HB2	4:F:80:GLN:O	1.99	0.62
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.80	0.62
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.81	0.62
4:F:110:ARG:HG2	4:F:110:ARG:NH1	2.03	0.60
4:H:148:THR:N	4:H:189:SER:HG	2.00	0.60
3:E:33:TYR:HD2	3:E:52:PHE:HA	1.66	0.60
1:A:254:GLU:HG3	1:A:255:ALA:N	2.17	0.59
1:C:84:LEU:O	1:C:88:MET:HG2	2.02	0.59
1:C:89:SER:N	1:C:90:PRO:HA	2.18	0.58
3:E:97:ASN:HB3	3:E:100:GLN:HE21	1.67	0.58
3:G:33:TYR:HD1	3:G:52:PHE:HB2	1.64	0.57
1:C:15:MET:HG2	2:D:62:PHE:HE2	1.68	0.57
3:E:14:VAL:O	3:E:112:VAL:HA	2.05	0.57
1:C:189:PRO:HB3	1:C:213:PHE:HB3	1.86	0.57
4:H:6:GLN:HB2	4:H:107:PRO:HD2	1.87	0.56
1:C:25:ARG:HB3	7:C:502:NAG:H82	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.41	0.55
1:A:254:GLU:HG3	1:A:255:ALA:H	1.71	0.54
1:C:145:LEU:HB3	1:C:146:PRO:HD3	1.89	0.54
4:H:33:TYR:HB2	4:H:93:ALA:HB3	1.90	0.54
4:H:93:ALA:HA	4:H:104:PHE:O	2.09	0.53
4:F:80:GLN:O	4:F:80:GLN:HG3	2.08	0.53
1:A:168:CYS:O	1:A:172:VAL:HG23	2.09	0.53
1:C:73:TYR:HE1	8:C:507:SGF:H26	1.74	0.52
4:H:112:THR:HG21	4:H:152:PRO:HG2	1.91	0.52
1:C:168:CYS:O	1:C:172:VAL:HG23	2.10	0.52
4:F:153:ASP:HB3	4:F:188:TYR:CD1	2.44	0.52
1:C:136:VAL:HG22	1:C:137:PRO:HD2	1.91	0.51
2:B:20:PRO:CA	2:B:71:THR:HG22	2.36	0.51
3:E:123:VAL:HG22	3:E:139:PHE:HD1	1.76	0.51
3:E:66:LEU:HD21	3:E:68:LYS:HD2	1.91	0.51
4:F:110:ARG:CG	4:F:110:ARG:NH1	2.67	0.51
1:C:207:VAL:HG22	1:C:250:THR:HG22	1.92	0.50
1:C:218:VAL:HG22	1:C:219:TRP:H	1.77	0.50
3:G:138:LEU:HD11	3:G:175:SER:HB2	1.94	0.50
1:A:233:HIS:HB2	1:A:250:THR:OG1	2.12	0.50
1:C:19:ALA:HB3	1:C:23:TRP:HB3	1.95	0.49
3:G:14:VAL:O	3:G:112:VAL:HA	2.13	0.49
4:H:27:SER:O	4:H:28:ASN:HB2	2.13	0.49
1:A:265:VAL:HB	1:A:275:ILE:HB	1.93	0.49
1:A:193:LEU:HD23	1:A:279:TRP:HE3	1.77	0.49
4:F:130:PRO:HG2	4:F:201:TRP:CE2	2.48	0.49
1:A:40:TRP:CG	1:A:47:ILE:HG13	2.48	0.48
4:H:9:SER:H	4:H:109:THR:HG23	1.78	0.48
1:A:21:ARG:O	1:A:22:SER:CB	2.62	0.48
3:G:40:HIS:CD2	3:G:86:ALA:HB2	2.48	0.48
2:D:25:CYS:HB3	2:D:66:ALA:HB3	1.96	0.48
4:H:8:PRO:CB	4:H:9:SER:HB3	2.44	0.47
4:F:36:LYS:HB2	4:F:46:LEU:HD11	1.96	0.47
3:E:123:VAL:HG22	3:E:139:PHE:CD1	2.49	0.47
1:C:143:LEU:HD21	8:C:507:SGF:H11	1.97	0.47
3:G:8:SER:HB2	3:G:23:ASN:HB2	1.95	0.47
1:C:59:SER:OG	1:C:62:GLN:HG3	2.14	0.47
1:C:258:GLU:HB3	1:C:279:TRP:CD1	2.50	0.47
2:B:96:ASP:O	2:B:97:ARG:HB3	2.14	0.47
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.79	0.47
4:H:157:LEU:HA	4:H:212:VAL:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:PRO:HD3	2:B:62:PHE:CE1	2.49	0.46
4:F:81:PRO:HA	4:F:82:THR:CG2	2.36	0.46
1:C:136:VAL:CG2	1:C:137:PRO:HD2	2.46	0.46
4:F:151:TYR:CD1	4:F:152:PRO:HB3	2.51	0.46
3:G:28:ASP:HB3	3:G:31:PHE:HD2	1.79	0.46
2:D:89:GLU:HG3	2:D:90:PRO:HD2	1.98	0.46
1:C:98:ILE:HD11	8:C:507:SGF:H9	1.98	0.45
3:E:48:LEU:HD23	3:E:48:LEU:HA	1.76	0.45
3:G:60:GLY:O	3:G:78:ARG:NH1	2.50	0.45
1:C:218:VAL:HG22	1:C:219:TRP:N	2.32	0.45
1:C:191:ALA:HA	1:C:209:HIS:O	2.16	0.45
1:C:192:TRP:CE3	2:D:14:PRO:HG3	2.51	0.45
1:A:258:GLU:HA	1:A:261:LEU:HD12	1.99	0.45
2:D:20:PRO:CA	2:D:71:THR:HG22	2.42	0.45
4:H:153:ASP:HB3	4:H:188:TYR:CD1	2.52	0.45
1:A:19:ALA:O	1:A:94:TYR:HB3	2.16	0.45
1:C:145:LEU:HB3	1:C:146:PRO:CD	2.47	0.44
3:G:33:TYR:CD1	3:G:52:PHE:HB2	2.45	0.44
4:F:93:ALA:HA	4:F:104:PHE:O	2.18	0.44
1:C:81:ILE:O	1:C:85:VAL:HG23	2.17	0.44
1:C:226:ASP:OD1	1:C:226:ASP:N	2.45	0.44
4:H:151:TYR:CD1	4:H:152:PRO:HB3	2.53	0.44
3:G:31:PHE:HB3	3:G:92:ALA:HB1	1.99	0.44
1:C:76:SER:HB3	8:C:507:SGF:H32	1.99	0.43
1:A:124:TYR:CZ	1:A:136:VAL:HG21	2.53	0.43
3:G:142:PHE:CE2	3:G:174:ASN:HB3	2.54	0.43
3:E:94:GLU:HB3	3:E:97:ASN:HD22	1.83	0.43
3:G:48:LEU:HD13	3:G:75:LEU:HD21	1.99	0.43
1:A:214:TYR:CG	1:A:215:PRO:HA	2.54	0.43
1:C:168:CYS:HB3	1:C:169:PRO:CD	2.43	0.43
2:B:7:ILE:HB	2:B:93:VAL:HG11	2.01	0.43
3:G:33:TYR:HB3	3:G:52:PHE:CD1	2.54	0.43
3:G:121:PRO:HB3	3:G:142:PHE:HB3	2.01	0.43
3:E:38:ARG:HD3	3:E:88:TYR:CE2	2.53	0.43
4:H:135:ILE:H	4:H:135:ILE:HG13	1.66	0.42
3:E:51:ILE:HB	3:E:66:LEU:HD22	2.00	0.42
4:H:172:THR:HG23	4:H:192:SER:HB2	2.02	0.42
4:F:89:VAL:HG22	4:F:110:ARG:HG3	2.02	0.42
3:G:95:GLN:O	3:G:96:ASN:HB2	2.20	0.42
1:A:210:VAL:HG21	1:A:220:VAL:HG21	2.02	0.42
1:A:124:TYR:OH	1:A:136:VAL:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:8:PRO:CA	4:F:9:SER:HB3	2.50	0.42
4:H:38:ILE:C	4:H:40:GLY:H	2.23	0.42
4:H:154:HIS:ND1	4:H:215:TYR:HB2	2.34	0.42
1:A:69:MET:HE1	1:A:163:LEU:HD11	2.01	0.41
4:F:10:HIS:HB3	4:F:154:HIS:ND1	2.35	0.41
4:F:151:TYR:HA	4:F:152:PRO:HA	1.95	0.41
3:E:28:ASP:HB3	3:E:31:PHE:HD2	1.84	0.41
1:A:102:ALA:HB2	1:A:116:LEU:HG	2.02	0.41
1:C:210:VAL:HG21	1:C:220:VAL:HG21	2.03	0.41
3:G:34:PHE:CG	3:G:73:VAL:HG21	2.54	0.41
3:E:66:LEU:HD13	3:E:73:VAL:HG13	2.02	0.41
2:D:49:VAL:HG22	2:D:68:THR:HB	2.03	0.41
2:D:71:THR:HA	2:D:72:PRO:HD2	1.92	0.41
4:F:26:VAL:O	4:F:29:HIS:HB2	2.21	0.40
4:F:201:TRP:C	4:F:203:ASN:H	2.25	0.40
1:C:238:LEU:HB3	2:D:10:TYR:CZ	2.55	0.40
2:D:24:ASN:HB3	2:D:65:LEU:HD11	2.04	0.40
2:B:23:LEU:HB2	2:B:70:PHE:CD1	2.57	0.40
4:F:8:PRO:HA	4:F:9:SER:HB3	2.03	0.40
4:H:34:TRP:HB2	4:H:47:VAL:HG12	2.03	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	260/285 (91%)	252 (97%)	3 (1%)	5 (2%)	8 37
1	C	263/285 (92%)	252 (96%)	9 (3%)	2 (1%)	19 57
2	B	96/99 (97%)	86 (90%)	9 (9%)	1 (1%)	15 52
2	D	97/99 (98%)	91 (94%)	6 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	E	171/208 (82%)	146 (85%)	23 (14%)	2 (1%)	13 47
3	G	163/208 (78%)	142 (87%)	20 (12%)	1 (1%)	25 63
4	F	216/244 (88%)	181 (84%)	27 (12%)	8 (4%)	3 24
4	H	201/244 (82%)	173 (86%)	22 (11%)	6 (3%)	4 28
All	All	1467/1672 (88%)	1323 (90%)	119 (8%)	25 (2%)	9 40

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	SER
4	F	82	THR
4	F	152	PRO
4	H	81	PRO
4	H	152	PRO
4	F	9	SER
4	H	9	SER
1	A	88	MET
1	A	255	ALA
1	C	255	ALA
4	F	41	GLN
4	F	87	SER
4	H	39	LEU
4	H	87	SER
3	E	52	PHE
4	F	8	PRO
4	F	28	ASN
4	H	82	THR
1	A	137	PRO
1	C	137	PRO
1	A	89	SER
4	F	174	PRO
3	G	83	SER
3	E	116	ILE
2	B	47	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	208/249 (84%)	200 (96%)	8 (4%)	33	64
1	C	215/249 (86%)	206 (96%)	9 (4%)	30	61
2	B	75/93 (81%)	71 (95%)	4 (5%)	22	54
2	D	83/93 (89%)	81 (98%)	2 (2%)	49	75
3	E	104/185 (56%)	94 (90%)	10 (10%)	8	32
3	G	104/185 (56%)	95 (91%)	9 (9%)	10	36
4	F	131/217 (60%)	126 (96%)	5 (4%)	33	64
4	H	118/217 (54%)	112 (95%)	6 (5%)	24	56
All	All	1038/1488 (70%)	985 (95%)	53 (5%)	24	56

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	43	ASP
1	A	76	SER
1	A	80	ASP
1	A	136	VAL
1	A	143	LEU
1	A	182	ASP
1	A	226	ASP
1	C	43	ASP
1	C	100	LEU
1	C	101	SER
1	C	131	THR
1	C	136	VAL
1	C	143	LEU
1	C	157	SER
1	C	196	VAL
1	C	226	ASP
2	B	2	GLN
2	B	34	HIS
2	B	93	VAL
2	B	96	ASP
2	D	28	THR
2	D	70	PHE
3	E	8	SER

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Mol	Chain	Res	Type
3	E	13	SER
3	E	27	SER
3	E	48	LEU
3	E	51	ILE
3	E	59	GLU
3	E	68	LYS
3	E	73	VAL
3	E	83	SER
3	E	100	GLN
4	F	4	VAL
4	F	69	ARG
4	F	110	ARG
4	F	135	ILE
4	F	171	CYS
3	G	22	LEU
3	G	32	GLN
3	G	51	ILE
3	G	52	PHE
3	G	54	ASP
3	G	59	GLU
3	G	63	THR
3	G	73	VAL
3	G	103	THR
4	H	9	SER
4	H	26	VAL
4	H	69	ARG
4	H	82	THR
4	H	171	CYS
4	H	193	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	40	HIS
4	F	22	ASN
3	G	39	GLN
3	G	40	HIS
3	G	65	HIS
4	H	180	GLN

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

6 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	I	1	5,1	14,14,15	0.58	0	17,19,21	0.74	0
5	NAG	I	2	5	14,14,15	0.53	0	17,19,21	1.91	3 (17%)
6	NAG	J	1	1,6	14,14,15	0.62	0	17,19,21	0.80	0
6	NAG	J	2	6	14,14,15	0.63	0	17,19,21	2.23	5 (29%)
6	BMA	J	3	6	11,11,12	0.54	0	15,15,17	1.24	3 (20%)
6	FUC	J	4	6	10,10,11	0.61	0	14,14,16	0.93	1 (7%)

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	2	NAG	C1-O5-C5	5.10	119.10	112.19
6	J	2	NAG	C2-N2-C7	4.98	129.99	122.90
6	J	2	NAG	C4-C3-C2	3.64	116.35	111.02
6	J	2	NAG	C8-C7-N2	3.52	122.06	116.10
6	J	2	NAG	C3-C4-C5	3.50	116.48	110.24
5	I	2	NAG	C3-C4-C5	3.11	115.78	110.24
5	I	2	NAG	C2-N2-C7	2.98	127.15	122.90
6	J	3	BMA	C3-C4-C5	2.47	114.64	110.24
6	J	3	BMA	C2-C3-C4	2.31	114.90	110.89
6	J	4	FUC	O5-C5-C6	2.29	112.26	107.33
6	J	2	NAG	O5-C1-C2	-2.12	107.94	111.29
6	J	3	BMA	C1-O5-C5	-2.09	109.35	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

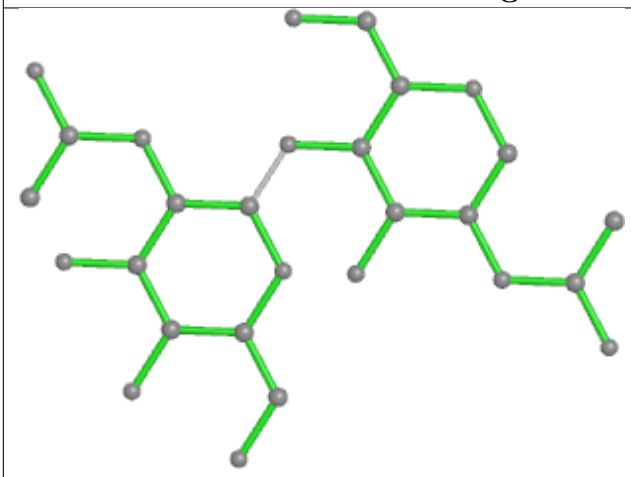
Mol	Chain	Res	Type	Atoms
5	I	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
6	J	3	BMA	C4-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
6	J	2	NAG	C1-C2-N2-C7
5	I	2	NAG	C3-C2-N2-C7

There are no ring outliers.

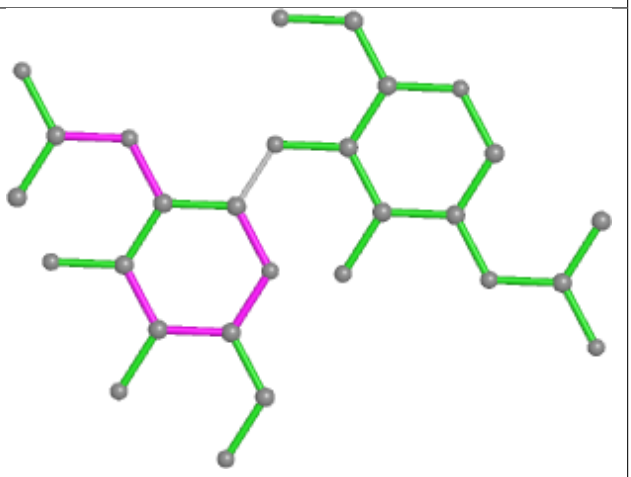
No monomer is involved in short contacts.

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

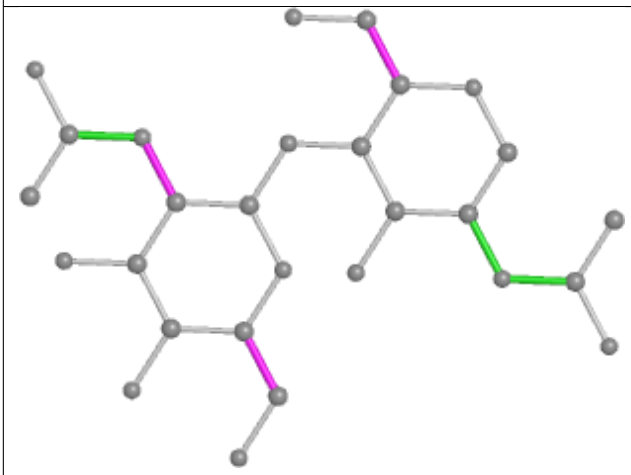
Oligosaccharide Chain I



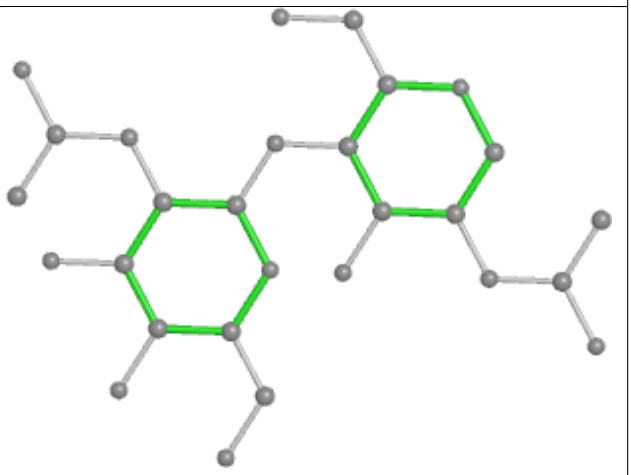
Bond lengths



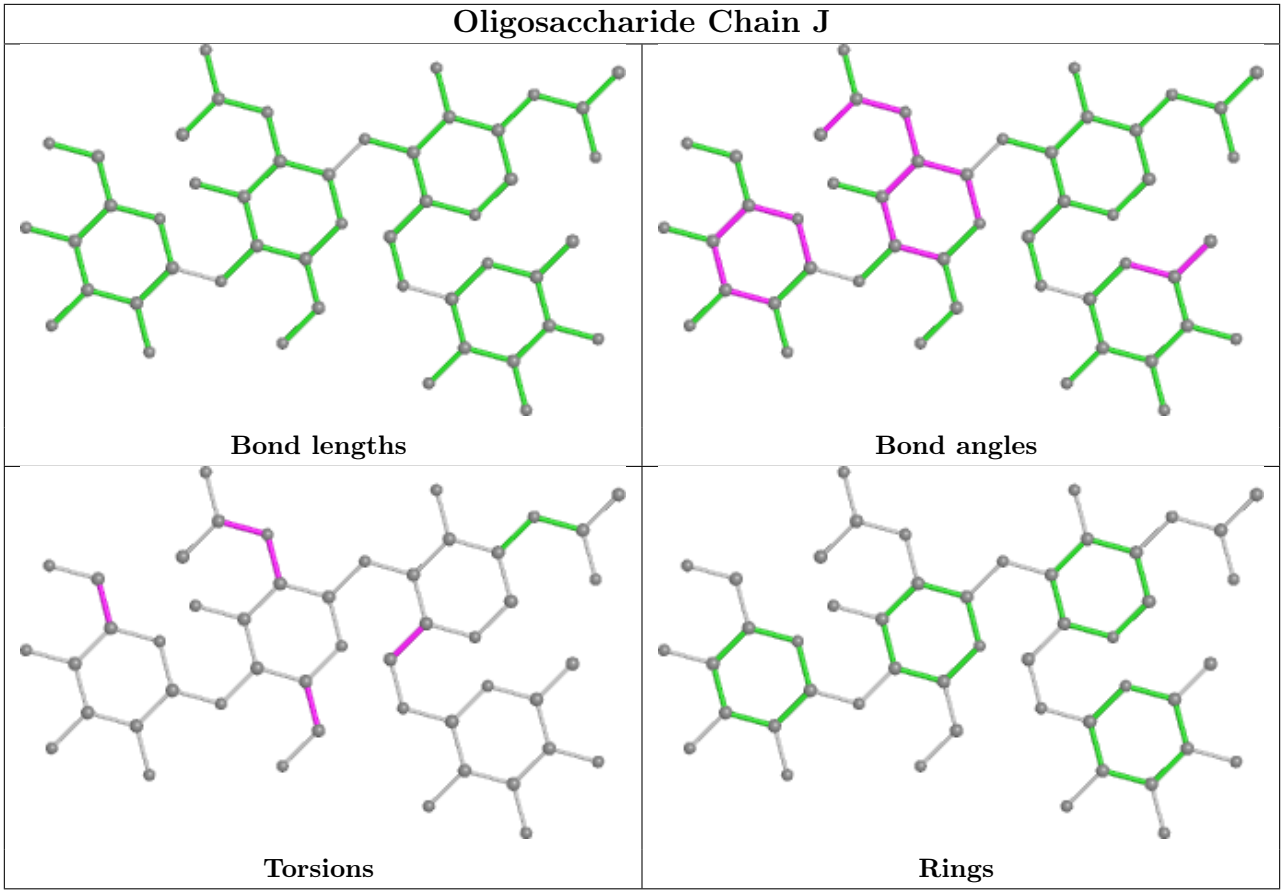
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

8 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	NAG	A	304	1	14,14,15	0.49	0	17,19,21	1.13	1 (5%)
8	SGF	C	507	-	35,36,36	1.09	2 (5%)	37,46,46	1.23	5 (13%)
8	SGF	A	305	-	35,36,36	1.12	1 (2%)	37,46,46	1.23	5 (13%)
7	NAG	A	303	1	13,13,15	0.58	0	14,17,21	0.93	0
9	PLM	C	508	-	17,17,17	0.59	0	17,17,17	0.63	0
7	NAG	C	501	1	14,14,15	0.57	0	17,19,21	0.67	0
9	PLM	A	306	-	17,17,17	0.56	0	17,17,17	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	C	502	1	14,14,15	0.58	0	17,19,21	1.31	2 (11%)

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
7	NAG	A	304	1	-	0/6/23/26	0/1/1/1
8	SGF	C	507	-	-	10/31/51/51	0/1/1/1
8	SGF	A	305	-	-	14/31/51/51	0/1/1/1
7	NAG	A	303	1	-	0/6/19/26	0/1/1/1
9	PLM	C	508	-	-	11/15/15/15	-
7	NAG	C	501	1	-	2/6/23/26	0/1/1/1
9	PLM	A	306	-	-	11/15/15/15	-
7	NAG	C	502	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	305	SGF	O4-S	-4.41	1.44	1.57
8	C	507	SGF	O4-S	-4.23	1.44	1.57
8	C	507	SGF	C2-C3	2.23	1.53	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	507	SGF	C-O-C43	-3.57	106.76	113.74
7	A	304	NAG	C1-O5-C5	3.44	116.85	112.19
8	A	305	SGF	C45-O4-S	-3.42	112.27	118.88
8	A	305	SGF	C-O-C43	-3.18	107.53	113.74
7	C	502	NAG	C1-O5-C5	3.16	116.48	112.19
8	C	507	SGF	O-C-C1	2.89	115.00	108.87
7	C	502	NAG	C1-C2-N2	-2.62	106.02	110.49
8	A	305	SGF	C2-C3-C4	-2.60	118.98	124.79
8	C	507	SGF	C45-O4-S	-2.58	113.88	118.88
8	A	305	SGF	O-C43-C44	2.43	112.09	108.30
8	A	305	SGF	O-C-C1	2.22	113.57	108.87
8	C	507	SGF	C2-C3-C4	-2.12	120.05	124.79
8	C	507	SGF	O-C43-C44	2.01	111.45	108.30

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	305	SGF	C-C1-C2-C3
7	C	502	NAG	O5-C5-C6-O6
8	C	507	SGF	C44-C43-O-C
7	C	502	NAG	C4-C5-C6-O6
9	A	306	PLM	C1-C2-C3-C4
8	C	507	SGF	O6-C43-O-C
8	C	507	SGF	C4-C5-C6-C7
8	C	507	SGF	C11-C10-C9-C8
9	A	306	PLM	C5-C6-C7-C8
9	A	306	PLM	C6-C7-C8-C9
9	C	508	PLM	C3-C4-C5-C6
8	A	305	SGF	C7-C8-C9-C10
8	A	305	SGF	C5-C6-C7-C8
8	A	305	SGF	C9-C10-C11-C12
8	C	507	SGF	C11-C12-C13-C14
8	A	305	SGF	C11-C12-C13-C14
9	A	306	PLM	CB-CC-CD-CE
9	C	508	PLM	CA-CB-CC-CD
9	C	508	PLM	CB-CC-CD-CE
8	A	305	SGF	C12-C13-C14-C15
9	A	306	PLM	C3-C4-C5-C6
9	A	306	PLM	C8-C9-CA-CB
8	C	507	SGF	C10-C11-C12-C13
8	C	507	SGF	C12-C13-C14-C15
9	C	508	PLM	C4-C5-C6-C7
8	C	507	SGF	C6-C7-C8-C9
9	A	306	PLM	CA-CB-CC-CD
9	C	508	PLM	C9-CA-CB-CC
8	A	305	SGF	C4-C5-C6-C7
9	C	508	PLM	C8-C9-CA-CB
9	C	508	PLM	CD-CE-CF-CG
8	C	507	SGF	C7-C8-C9-C10
9	C	508	PLM	C5-C6-C7-C8
7	C	501	NAG	C4-C5-C6-O6
8	A	305	SGF	C11-C10-C9-C8
9	A	306	PLM	C9-CA-CB-CC
8	A	305	SGF	C-C1-C2-O1
9	A	306	PLM	C2-C3-C4-C5
8	A	305	SGF	C44-C43-O-C
9	A	306	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	A	306	PLM	O1-C1-C2-C3
8	A	305	SGF	O6-C43-O-C
9	C	508	PLM	C2-C3-C4-C5
8	A	305	SGF	C1-C-O-C43
8	C	507	SGF	C1-C-O-C43
8	A	305	SGF	O-C-C1-N
8	A	305	SGF	N-C1-C2-O1
9	C	508	PLM	O1-C1-C2-C3
7	C	501	NAG	O5-C5-C6-O6
9	C	508	PLM	O2-C1-C2-C3

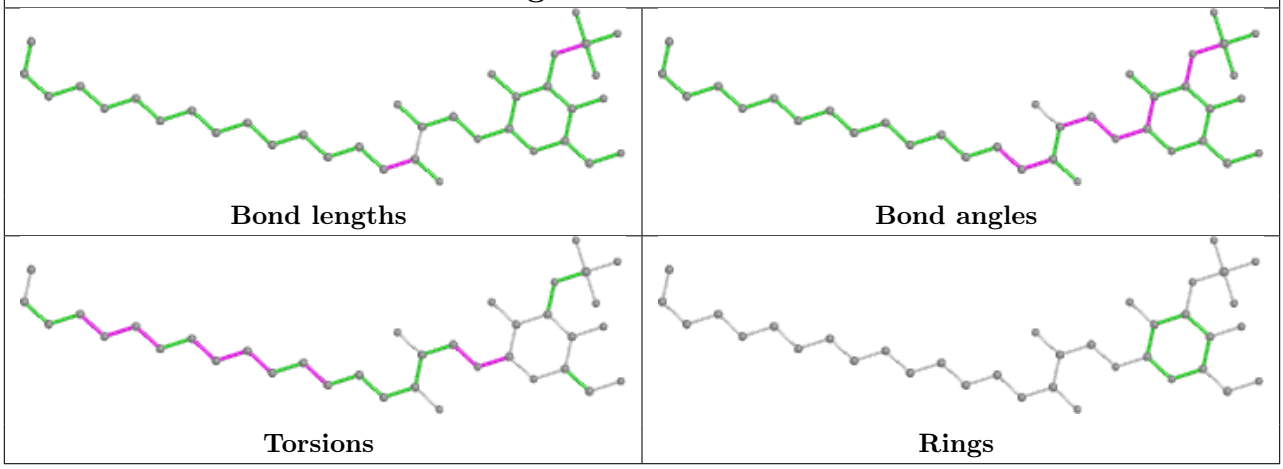
There are no ring outliers.

2 monomers are involved in 6 short contacts:

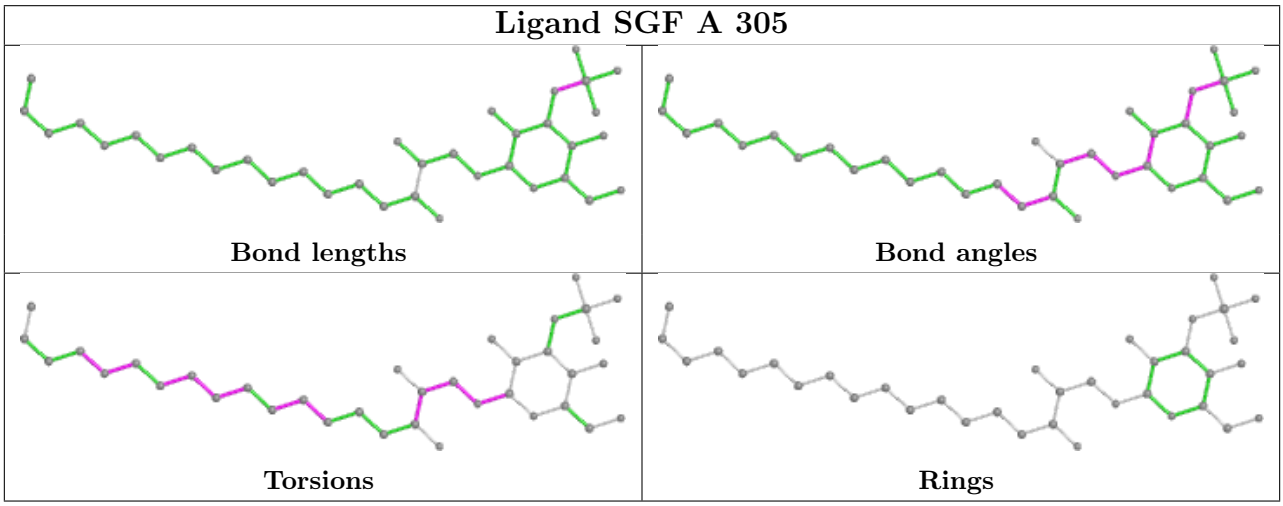
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	507	SGF	5	0
7	C	502	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

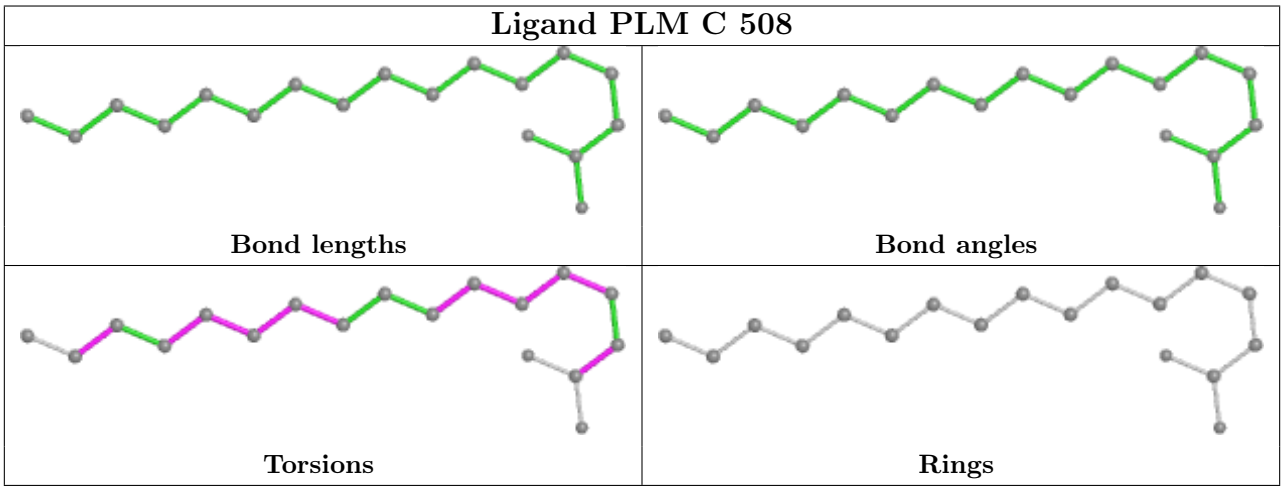
Ligand SGF C 507

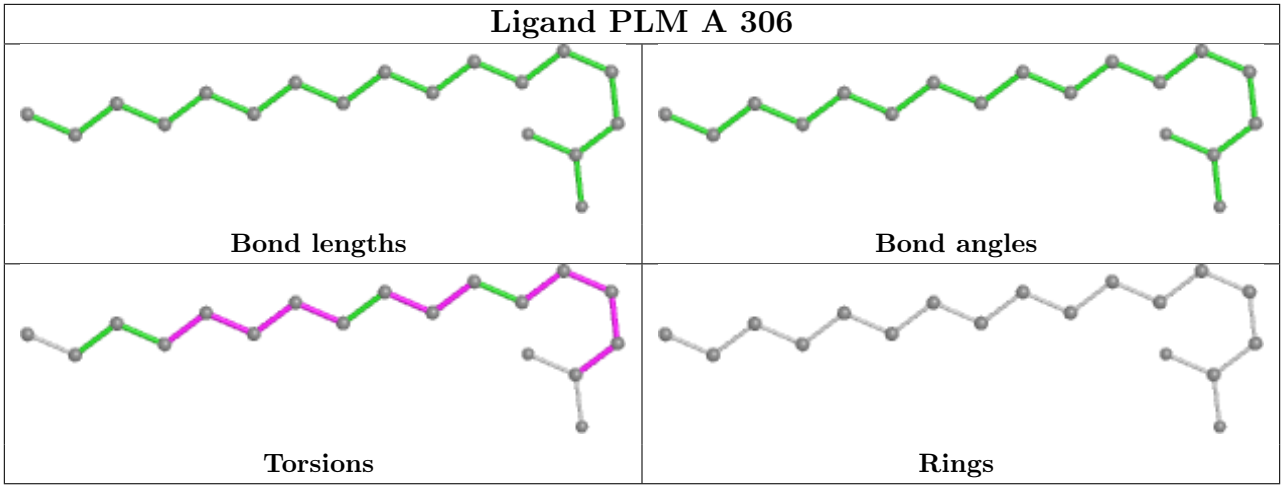


Ligand SGF A 305



Ligand PLM C 508





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	266/285 (93%)	-0.21	0 100 100	46, 61, 99, 152	0
1	C	269/285 (94%)	-0.13	0 100 100	38, 54, 95, 133	0
2	B	98/99 (98%)	-0.24	1 (1%) 82 78	55, 85, 108, 117	0
2	D	99/99 (100%)	-0.25	0 100 100	36, 49, 72, 78	0
3	E	179/208 (86%)	0.14	9 (5%) 28 27	40, 62, 171, 193	0
3	G	171/208 (82%)	0.18	10 (5%) 23 22	52, 81, 174, 203	0
4	F	224/244 (91%)	-0.01	7 (3%) 49 45	40, 101, 169, 221	0
4	H	211/244 (86%)	0.08	9 (4%) 35 33	53, 127, 189, 236	0
All	All	1517/1672 (90%)	-0.05	36 (2%) 59 55	36, 71, 162, 236	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	122	ALA	5.3
3	E	176	ALA	4.6
3	G	138	LEU	4.4
3	E	138	LEU	4.4
4	F	216	GLY	4.0
4	H	144	VAL	3.8
3	E	151	SER	3.8
3	E	122	ALA	3.7
4	F	123	PRO	3.6
3	G	137	CYS	3.6
4	F	130	PRO	3.5
3	G	176	ALA	3.5
3	E	177	VAL	3.4
4	H	123	PRO	3.0
4	H	143	LEU	3.0
3	G	113	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	123	VAL	2.9
3	E	124	TYR	2.8
4	F	122	PRO	2.5
4	F	131	SER	2.5
4	H	118	ARG	2.5
3	E	139	PHE	2.4
3	E	121	PRO	2.4
4	F	132	LYS	2.4
4	H	146	LEU	2.4
3	G	8	SER	2.4
3	G	19	MET	2.4
3	G	160	ASP	2.3
4	H	86	ASP	2.2
4	H	191	SER	2.2
4	H	145	CYS	2.1
2	B	99	MET	2.1
3	G	124	TYR	2.1
4	H	129	GLU	2.1
3	G	159	THR	2.0
4	F	236	SER	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.

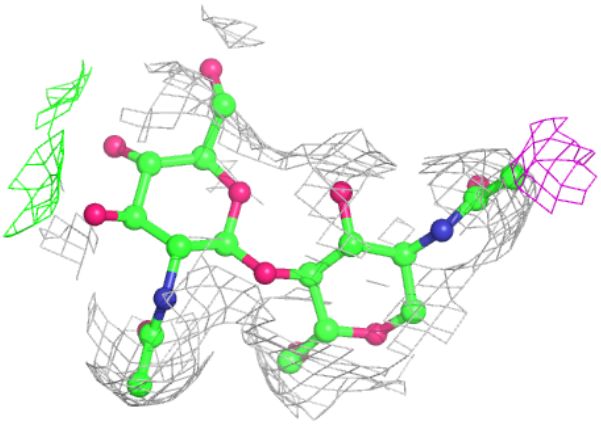
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	I	2	14/15	0.82	0.18	72,76,85,85	0
6	BMA	J	3	11/12	0.82	0.18	105,111,116,117	0
6	NAG	J	2	14/15	0.92	0.15	82,86,95,99	0
6	NAG	J	1	14/15	0.94	0.18	63,67,77,79	0
6	FUC	J	4	10/11	0.94	0.24	72,76,80,84	0
5	NAG	I	1	14/15	0.95	0.16	60,62,67,69	0

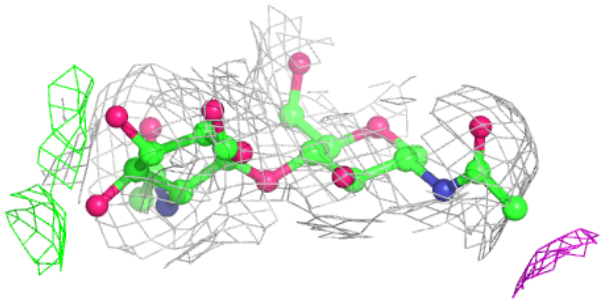
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

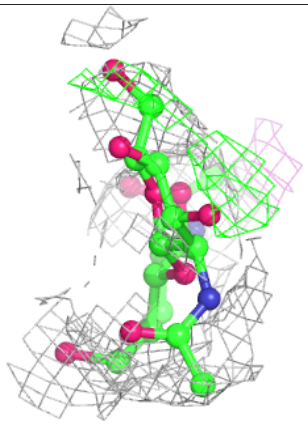
charide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

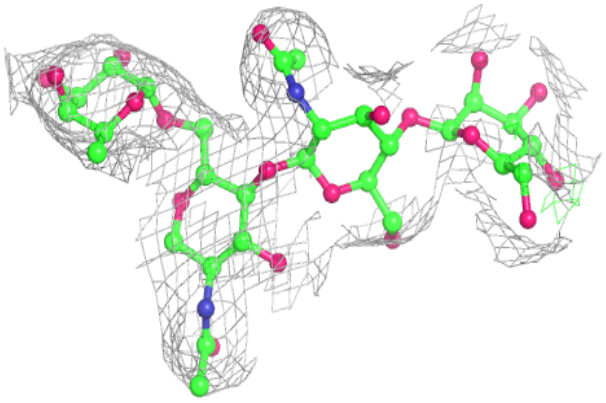


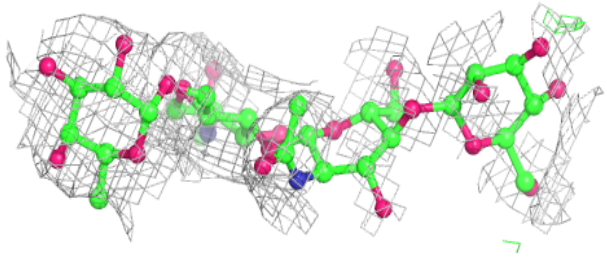


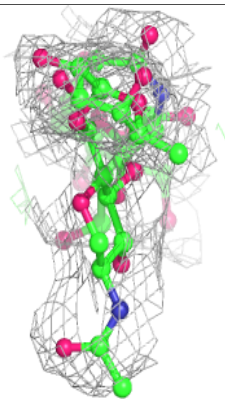


Electron density around Chain J:

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







6.4 Ligands (i)

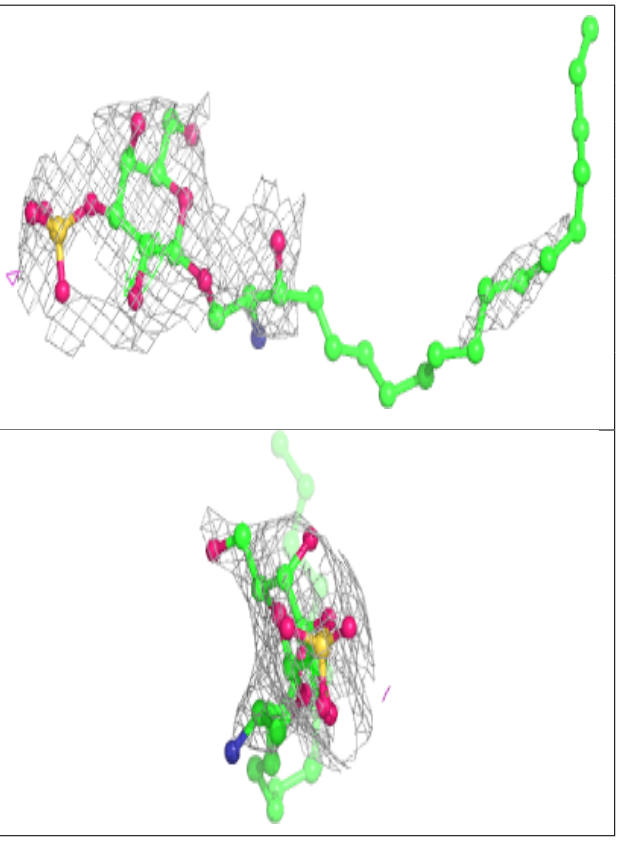
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
8	SGF	A	305	36/36	0.81	0.61	169,222,273,280	0
7	NAG	C	501	14/15	0.83	0.24	83,88,98,99	0
8	SGF	C	507	36/36	0.88	0.53	126,173,216,221	0
7	NAG	C	502	14/15	0.90	0.21	53,58,61,62	0
7	NAG	A	304	14/15	0.90	0.21	77,83,86,90	0
7	NAG	A	303	13/15	0.90	0.24	102,109,118,118	0
9	PLM	C	508	18/18	0.90	0.77	52,69,98,100	0
9	PLM	A	306	18/18	0.92	0.66	64,69,87,87	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

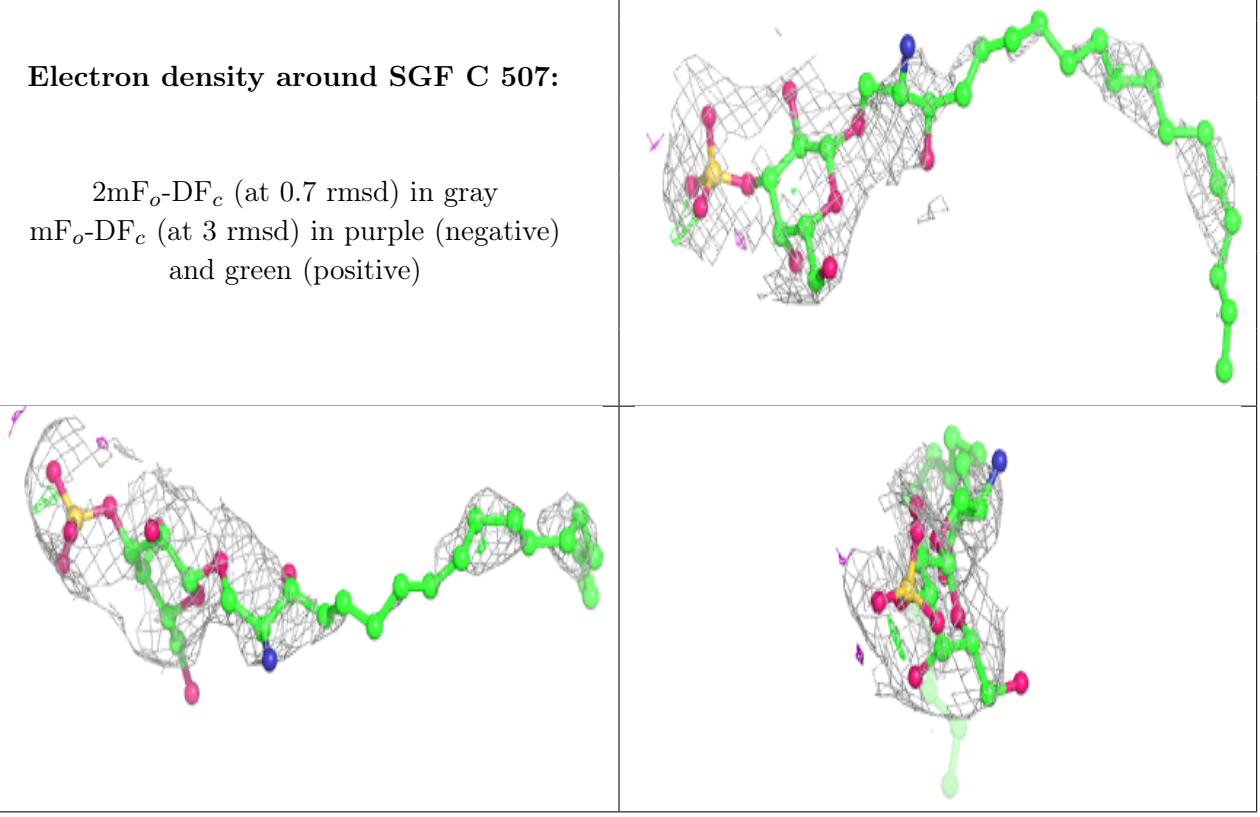
Electron density around SGF A 305:

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



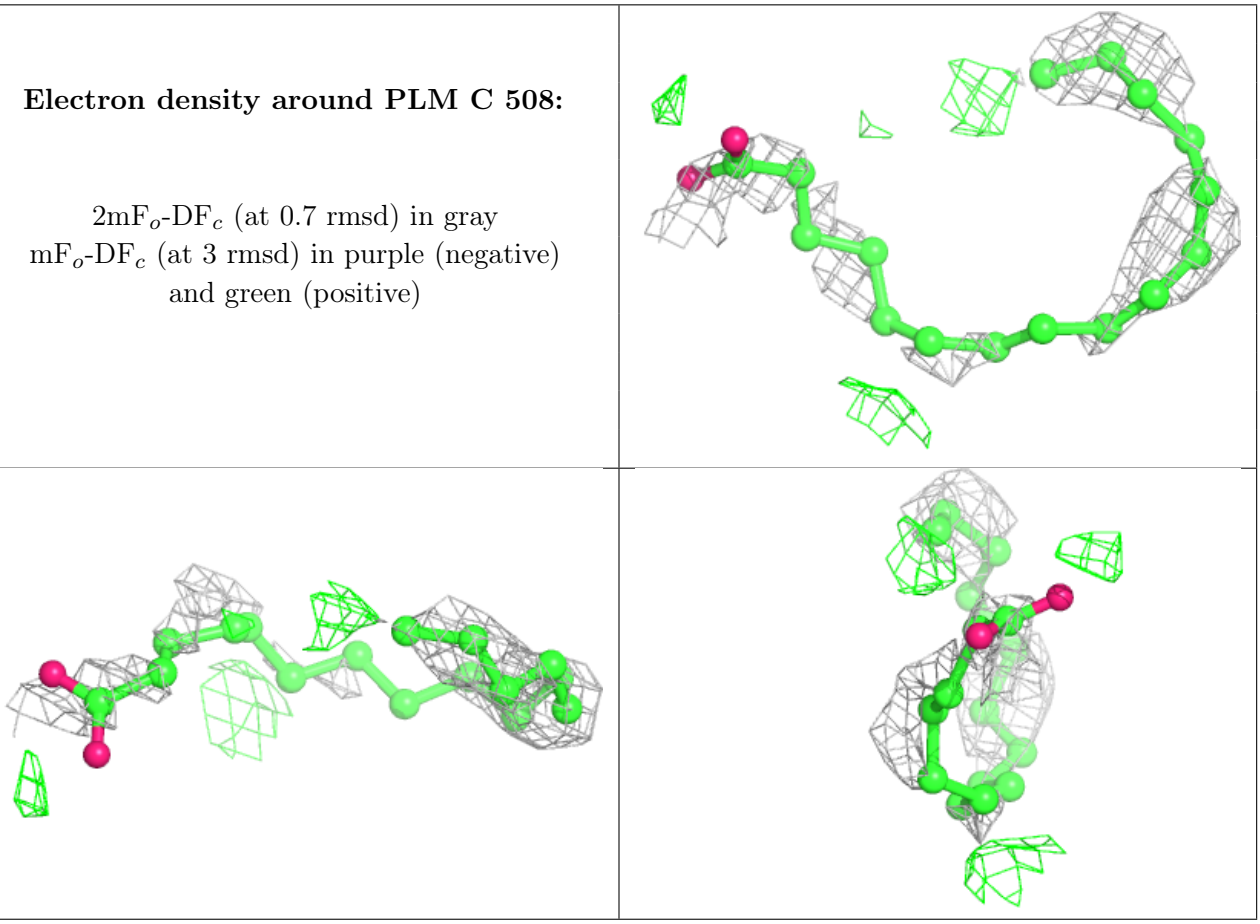
Electron density around SGF C 507:

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



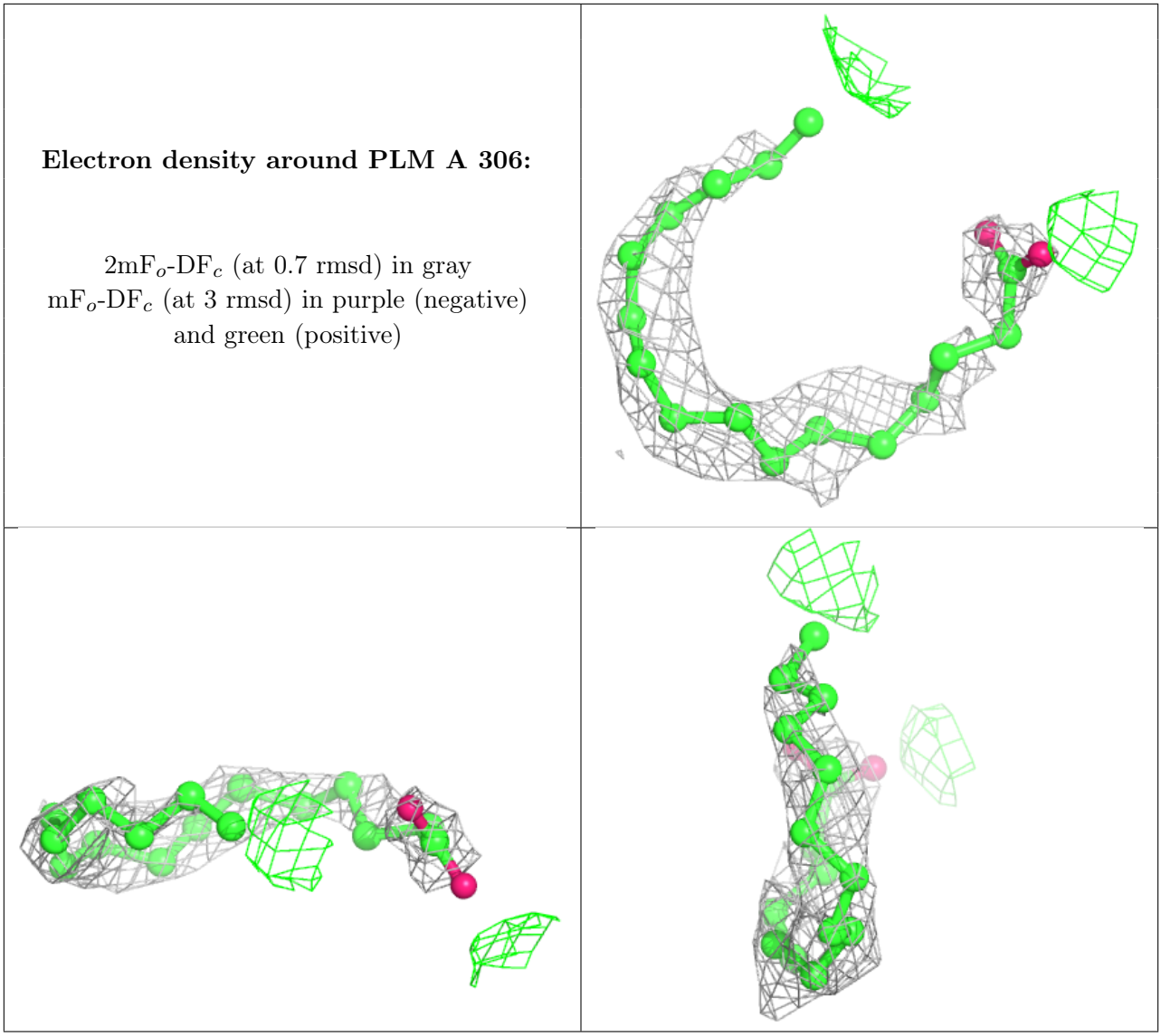
Electron density around PLM C 508:

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



Electron density around PLM A 306:

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



6.5 Other polymers

There are no such residues in this entry.