Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 03:07 AM EDT

PDB ID	:	4ENE
Title	:	Structure of the N- and C-terminal trimmed ClC-ec1 Cl-/H+ antiporter and Fab Complex
Authors	:	Lim, H.H.; Shane, T.; Miller, C.
Deposited on	:	2012-04-13
Resolution	:	2.40 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:

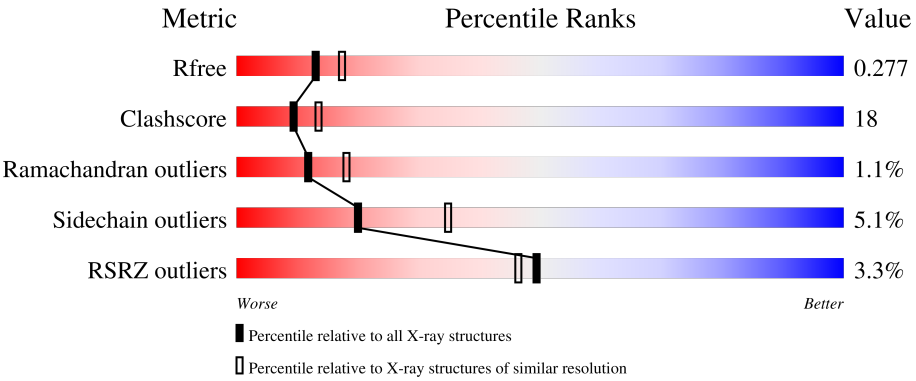
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	446	4% 71% 26%
1	B	446	3% 69% 27%
2	C	222	5% 66% 30%
2	E	222	5% 69% 28%
3	D	211	2% 57% 40%

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Mol	Chain	Length	Quality of chain
3	F	211	2% 74% 22%
4	G	2	100%
4	H	2	100%
4	I	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13691 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	442	Total	C	N	O	S	0	0	0
			3315	2180	557	558	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP P37019
A	461	LYS	-	expression tag	UNP P37019
B	16	MET	-	expression tag	UNP P37019
B	461	LYS	-	expression tag	UNP P37019

- Molecule 2 is a protein called heavy chain of Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1681	1082	275	318	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called light chain of Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

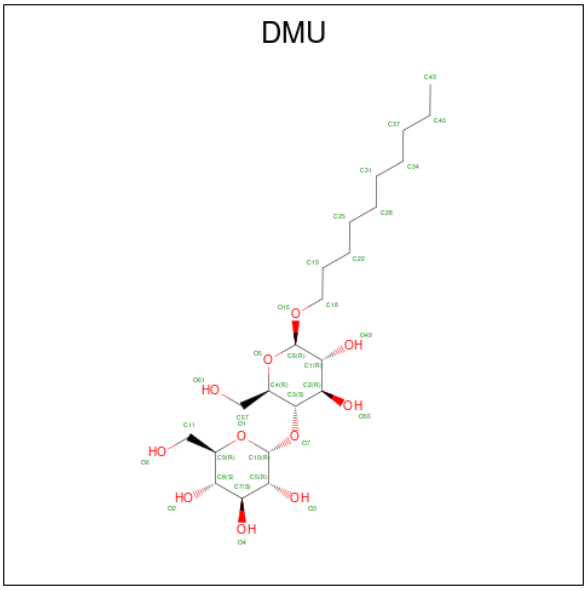
- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	2	Total C O 23 12 11	0	0	0
4	H	2	Total C O 23 12 11	0	0	0
4	I	2	Total C O 23 12 11	0	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	3	Total Cl 3 3	0	0

- Molecule 6 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	B	1	Total C O 33 22 11	0	0
6	B	1	Total C O 33 22 11	0	0

- Molecule 7 is water.

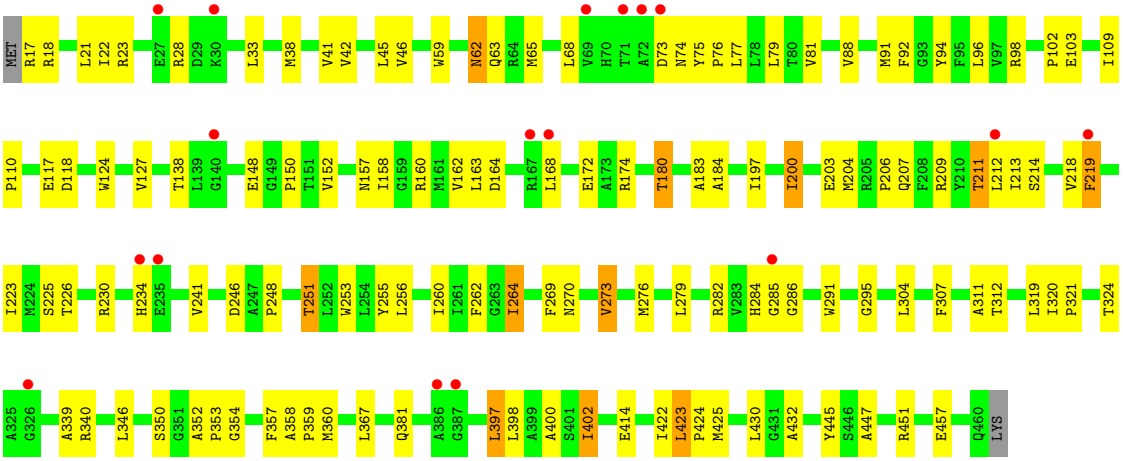
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	17	Total O 17 17	0	0
7	B	34	Total O 34 34	0	0
7	C	45	Total O 45 45	0	0
7	D	24	Total O 24 24	0	0
7	E	22	Total O 22 22	0	0
7	F	34	Total O 34 34	0	0

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.

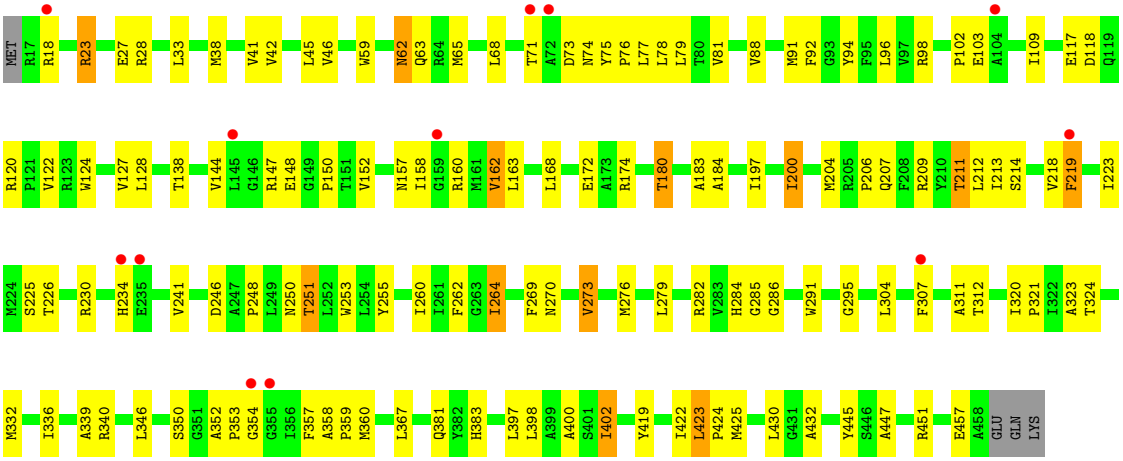
• Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain A:



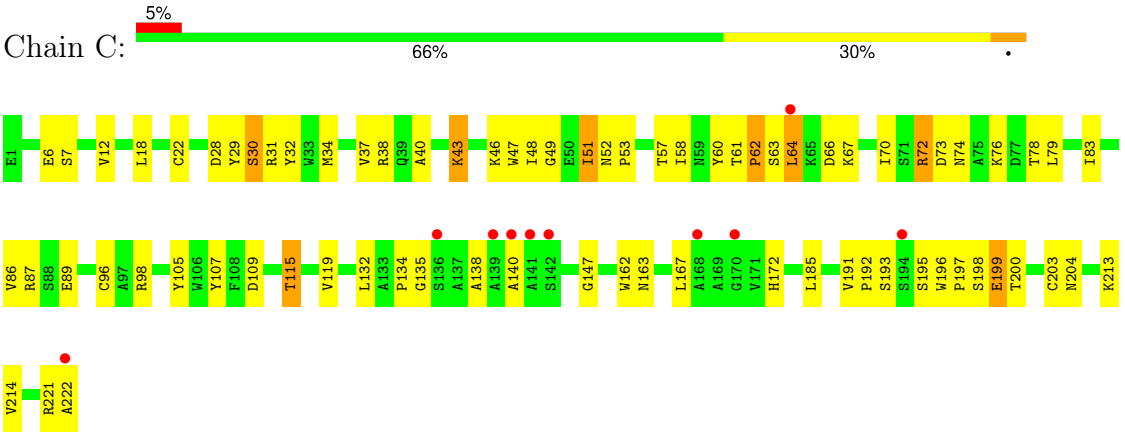
• Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:



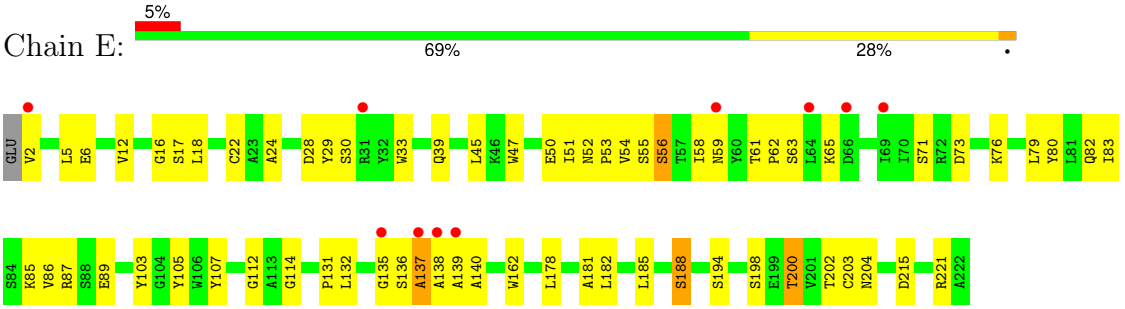
• Molecule 2: heavy chain of Fab fragment

Chain C:



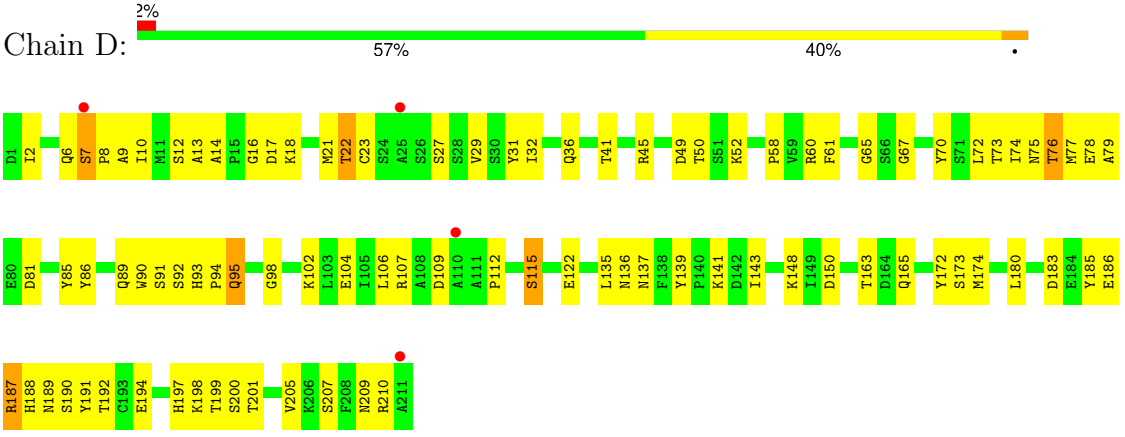
• Molecule 2: heavy chain of Fab fragment

Chain E:



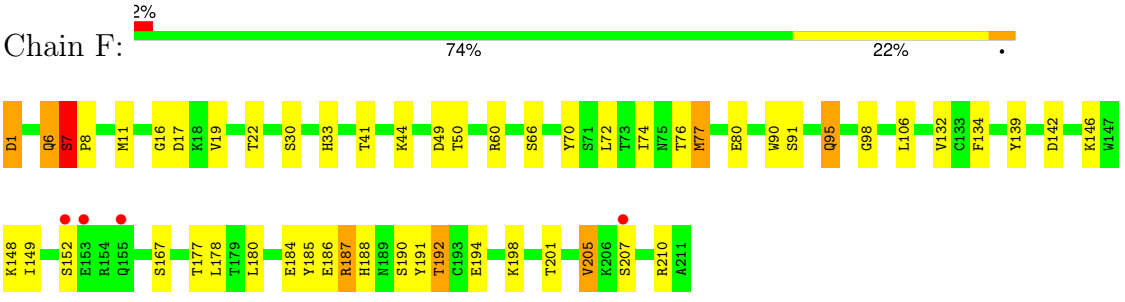
• Molecule 3: light chain of Fab fragment

Chain D:



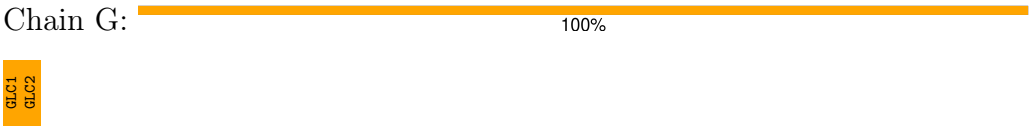
• Molecule 3: light chain of Fab fragment

Chain F:



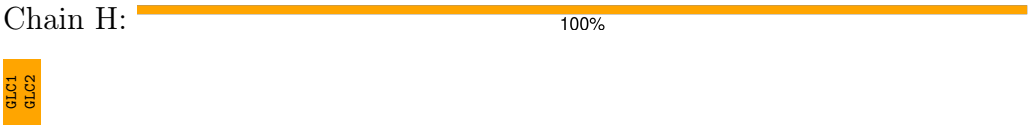
• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:



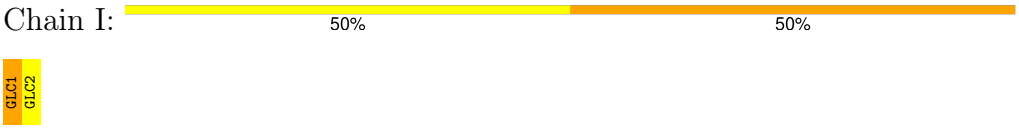
- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:



- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	232.26Å 97.52Å 173.96Å 90.00° 132.87° 90.00°	Depositor
Resolution (Å)	24.87 – 2.40 24.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (24.87-2.40) 97.6 (24.87-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.239 , 0.278 0.236 , 0.277	Depositor DCC
R_{free} test set	5504 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13691	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: CL, GLC, DMU

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	0.37	0/3405	0.50	0/4621
1	B	0.39	0/3387	0.51	0/4597
2	C	0.51	0/1730	0.63	0/2367
2	E	0.43	0/1721	0.61	0/2355
3	D	0.44	0/1660	0.61	0/2257
3	F	0.49	0/1660	0.68	1/2257 (0.0%)
All	All	0.43	0/13563	0.57	1/18454 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	7	SER	C-N-CD	7.37	143.88	128.40

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	3333	0	3484	114	0
1	B	3315	0	3470	120	0
2	C	1681	0	1663	56	0
2	E	1672	0	1654	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1621	0	1546	83	1
3	F	1621	0	1546	55	0
4	G	23	0	21	5	0
4	H	23	0	21	3	0
4	I	23	0	21	2	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
6	A	132	0	168	30	1
6	B	66	0	84	16	0
7	A	17	0	0	2	0
7	B	34	0	0	4	0
7	C	45	0	0	2	1
7	D	24	0	0	3	0
7	E	22	0	0	1	0
7	F	34	0	0	3	1
All	All	13691	0	13678	480	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 18.

All (480) 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:D:95:GLN:OE1	3:D:95:GLN:N	1.69	1.24
1:A:207:GLN:HG2	1:B:28:ARG:HD2	1.17	1.13
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.23	1.11
3:F:95:GLN:OE1	3:F:95:GLN:N	1.90	1.04
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.44	0.99
3:F:7:SER:HB3	3:F:22:THR:HB	1.45	0.99
3:F:95:GLN:H	3:F:95:GLN:CD	1.59	0.97
1:B:422:ILE:HA	1:B:425:MET:HE3	1.47	0.96
3:D:187:ARG:CG	3:D:187:ARG:HH11	1.79	0.95
3:D:192:THR:HG22	3:D:207:SER:CB	1.98	0.94
1:A:422:ILE:HA	1:A:425:MET:HE3	1.52	0.92
6:B:505:DMU:H29	6:B:506:DMU:H11	1.51	0.92
1:B:250:ASN:OD1	7:B:625:HOH:O	1.87	0.90
2:C:51:ILE:HD12	2:C:58:ILE:HG12	1.53	0.89
3:D:187:ARG:HH11	3:D:187:ARG:HG3	1.37	0.88
3:F:95:GLN:N	3:F:95:GLN:CD	2.22	0.87
2:C:163:ASN:HD22	2:C:167:LEU:HD13	1.41	0.85
3:D:192:THR:HG22	3:D:207:SER:HB2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:GLU:HG2	3:F:205:VAL:HB	1.62	0.82
3:F:192:THR:HB	3:F:207:SER:HB3	1.61	0.81
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.62	0.81
3:D:17:ASP:OD1	3:D:18:LYS:N	2.13	0.81
1:B:147:ARG:NH2	7:B:606:HOH:O	1.92	0.80
3:D:95:GLN:H	3:D:95:GLN:CD	1.85	0.79
1:A:207:GLN:HG2	1:B:28:ARG:CD	2.09	0.79
3:D:6:GLN:NE2	3:D:85:TYR:O	2.15	0.79
3:D:197:HIS:CG	3:D:198:LYS:H	2.01	0.78
1:A:241:VAL:HG21	1:A:324:THR:HG21	1.66	0.77
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.66	0.77
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.15	0.76
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.18	0.76
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.68	0.76
1:B:241:VAL:HG21	1:B:324:THR:HG21	1.69	0.75
2:E:135:GLY:O	2:E:137:ALA:N	2.20	0.75
3:D:185:TYR:CZ	3:D:210:ARG:HD3	2.22	0.74
1:A:164:ASP:HB3	6:A:503:DMU:H9	1.70	0.73
6:A:505:DMU:H5	6:A:505:DMU:H10	1.70	0.73
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.71	0.72
3:F:90:TRP:CD2	3:F:95:GLN:HG3	2.25	0.72
3:D:187:ARG:HG3	3:D:187:ARG:NH1	2.03	0.72
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.90	0.71
3:F:7:SER:OG	3:F:8:PRO:CD	2.38	0.71
2:E:85:LYS:HE2	2:E:85:LYS:H	1.56	0.70
6:A:505:DMU:O6	7:A:617:HOH:O	2.09	0.70
3:F:90:TRP:CE2	3:F:95:GLN:HG3	2.27	0.70
6:B:505:DMU:O5	6:B:505:DMU:H8	1.91	0.69
1:A:28:ARG:CD	1:B:207:GLN:HG2	2.12	0.69
1:B:253:TRP:HB3	6:B:505:DMU:H7	1.74	0.69
1:A:160:ARG:HD3	7:A:608:HOH:O	1.91	0.69
1:A:447:ALA:O	1:A:451:ARG:HG3	1.92	0.68
2:C:37:VAL:HG13	2:C:46:LYS:O	1.92	0.68
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.76	0.67
1:A:346:LEU:O	1:A:350:SER:HB3	1.94	0.67
3:F:7:SER:O	3:F:8:PRO:C	2.30	0.67
1:B:346:LEU:O	1:B:350:SER:HB3	1.95	0.67
2:C:7:SER:HA	2:C:115:THR:HG21	1.77	0.67
1:A:253:TRP:HB3	6:A:506:DMU:H7	1.77	0.67
1:A:33:LEU:O	1:A:33:LEU:HD23	1.94	0.66
1:B:447:ALA:O	1:B:451:ARG:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:504:DMU:O49	6:A:504:DMU:H8	1.96	0.66
3:D:31:TYR:HA	3:D:50:THR:OG1	1.95	0.66
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.61	0.66
1:A:241:VAL:CG2	1:A:324:THR:HG21	2.25	0.66
1:B:214:SER:HA	4:G:1:GLC:O3	1.95	0.66
1:B:241:VAL:CG2	1:B:324:THR:HG21	2.26	0.66
2:C:163:ASN:HD22	2:C:167:LEU:CD1	2.09	0.66
2:E:188:SER:HB2	3:F:134:PHE:CE2	2.31	0.66
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.62	0.65
3:F:7:SER:HB2	3:F:8:PRO:HD3	1.79	0.65
6:A:503:DMU:H4	6:A:503:DMU:C5	2.18	0.64
1:B:23:ARG:HH11	1:B:23:ARG:CG	2.10	0.64
3:D:14:ALA:O	3:D:17:ASP:HB3	1.97	0.64
3:F:41:THR:HB	7:F:311:HOH:O	1.97	0.64
1:B:269:PHE:O	1:B:273:VAL:HG12	1.98	0.64
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.33	0.64
2:E:194:SER:O	2:E:198:SER:HB3	1.97	0.64
2:C:86:VAL:CG1	2:C:119:VAL:HG21	2.28	0.63
1:A:270:ASN:O	1:A:273:VAL:HG13	1.99	0.63
1:B:422:ILE:HA	1:B:425:MET:CE	2.26	0.63
6:B:505:DMU:C57	6:B:506:DMU:H11	2.28	0.63
2:E:59:ASN:HB3	7:F:326:HOH:O	1.99	0.63
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.81	0.63
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.64	0.63
1:B:33:LEU:HD23	1:B:33:LEU:O	1.99	0.62
1:A:223:ILE:HD11	1:B:430:LEU:HD22	1.81	0.62
6:B:505:DMU:H29	6:B:506:DMU:O16	1.99	0.62
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.30	0.62
2:C:30:SER:O	2:C:31:ARG:HB2	1.99	0.62
1:A:269:PHE:O	1:A:273:VAL:HG12	2.00	0.62
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.82	0.62
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.68	0.62
1:B:148:GLU:O	1:B:152:VAL:HG23	2.00	0.61
6:A:505:DMU:H10	6:A:505:DMU:C6	2.30	0.61
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.83	0.61
3:F:7:SER:CB	3:F:8:PRO:CD	2.78	0.61
2:C:172:HIS:HE1	3:D:136:ASN:ND2	1.98	0.60
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.66	0.60
2:C:40:ALA:O	2:C:43:LYS:HB2	2.01	0.60
3:D:187:ARG:HH11	3:D:187:ARG:HG2	1.63	0.60
1:A:226:THR:O	1:A:230:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:148:LYS:HA	3:F:152:SER:O	2.01	0.60
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.16	0.60
1:B:457:GLU:O	1:B:457:GLU:HG3	2.02	0.60
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.84	0.59
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.84	0.59
1:B:270:ASN:O	1:B:273:VAL:HG13	2.03	0.59
3:F:185:TYR:O	3:F:191:TYR:OH	2.20	0.59
6:A:503:DMU:O16	6:A:503:DMU:O55	2.16	0.59
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.84	0.59
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.83	0.59
1:B:42:VAL:O	1:B:46:VAL:HG23	2.03	0.59
3:D:189:ASN:O	3:D:209:ASN:HA	2.03	0.59
6:A:503:DMU:H4	6:A:503:DMU:H32	1.85	0.59
6:A:503:DMU:H6	6:A:503:DMU:C57	2.34	0.58
6:A:503:DMU:O3	6:A:503:DMU:O2	2.21	0.58
1:A:17:ARG:HH22	1:A:21:LEU:HD13	1.68	0.58
3:D:150:ASP:HA	3:D:190:SER:OG	2.04	0.58
3:D:197:HIS:CG	3:D:198:LYS:N	2.71	0.58
1:A:206:PRO:HG2	1:A:211:THR:CG2	2.31	0.58
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.19	0.58
1:A:17:ARG:NH2	1:A:21:LEU:HD13	2.19	0.57
1:A:423:LEU:HD13	1:B:230:ARG:CZ	2.34	0.57
3:F:6:GLN:HB3	7:F:331:HOH:O	2.02	0.57
6:B:505:DMU:O49	6:B:505:DMU:H4	2.05	0.57
3:F:187:ARG:O	3:F:188:HIS:CG	2.58	0.57
1:A:207:GLN:HG3	4:G:1:GLC:H61	1.86	0.57
3:D:192:THR:HG22	3:D:207:SER:HB3	1.81	0.57
4:H:1:GLC:O3	4:I:1:GLC:H62	2.05	0.57
1:B:248:PRO:O	1:B:251:THR:HB	2.05	0.57
3:D:75:ASN:O	3:D:76:THR:HG22	2.05	0.57
2:E:85:LYS:HE2	2:E:85:LYS:N	2.18	0.57
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.39	0.56
3:D:12:SER:HA	3:D:104:GLU:O	2.05	0.56
3:D:29:VAL:HG11	3:D:89:GLN:HB2	1.88	0.56
3:F:186:GLU:O	3:F:210:ARG:NH2	2.38	0.56
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.19	0.56
3:D:36:GLN:HG3	3:D:85:TYR:CE2	2.41	0.56
3:F:7:SER:CB	3:F:8:PRO:HD3	2.35	0.56
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.88	0.56
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.40	0.56
3:F:192:THR:HB	3:F:207:SER:CB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD23	1:A:81:VAL:HG23	1.88	0.56
3:F:66:SER:HA	3:F:70:TYR:CZ	2.41	0.56
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.20	0.56
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.41	0.56
3:D:29:VAL:O	3:D:70:TYR:OH	2.17	0.55
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.41	0.55
2:E:24:ALA:HB3	2:E:29:TYR:CD1	2.42	0.55
2:C:12:VAL:HG21	2:C:18:LEU:HD23	1.89	0.55
1:B:68:LEU:HD23	1:B:81:VAL:HG23	1.89	0.55
3:D:141:LYS:HB3	3:D:172:TYR:CD1	2.41	0.55
2:E:50:GLU:HG2	2:E:59:ASN:HB2	1.88	0.55
1:A:248:PRO:O	1:A:251:THR:HB	2.07	0.55
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.89	0.55
1:A:256:LEU:HD23	6:A:505:DMU:H17	1.87	0.55
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.89	0.55
6:B:506:DMU:O1	6:B:506:DMU:C2	2.54	0.55
1:B:284:HIS:C	1:B:286:GLY:H	2.10	0.54
3:D:6:GLN:OE1	3:D:98:GLY:HA3	2.07	0.54
2:C:73:ASP:HB3	2:C:76:LYS:HB2	1.89	0.54
3:F:180:LEU:HD22	3:F:184:GLU:HG2	1.89	0.54
3:F:191:TYR:O	3:F:207:SER:HB2	2.07	0.54
3:D:106:LEU:HD23	3:D:107:ARG:H	1.73	0.54
3:D:115:SER:HB2	7:D:304:HOH:O	2.07	0.54
1:A:62:ASN:O	1:A:65:MET:N	2.40	0.54
3:D:186:GLU:O	3:D:210:ARG:NH2	2.41	0.54
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.90	0.53
6:A:505:DMU:H32	6:A:505:DMU:H4	1.90	0.53
1:A:284:HIS:C	1:A:286:GLY:H	2.12	0.53
6:A:506:DMU:O55	6:A:506:DMU:H32	2.08	0.53
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.07	0.53
2:C:52:ASN:CG	2:C:57:THR:HG22	2.28	0.53
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.24	0.53
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.44	0.53
1:B:23:ARG:HH11	1:B:23:ARG:HG3	1.74	0.53
1:B:226:THR:O	1:B:230:ARG:HG2	2.09	0.53
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.90	0.53
1:B:276:MET:HA	1:B:276:MET:HE2	1.91	0.53
2:C:195:SER:O	2:C:199:GLU:HG3	2.08	0.53
3:D:197:HIS:CD2	3:D:198:LYS:H	2.26	0.53
1:A:230:ARG:CZ	1:B:423:LEU:HD13	2.39	0.53
1:A:276:MET:HE2	1:A:276:MET:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLN:OE1	1:A:381:GLN:N	2.32	0.53
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.43	0.53
2:C:60:TYR:CE2	2:C:70:ILE:HD12	2.44	0.53
2:C:86:VAL:CG1	2:C:119:VAL:CG2	2.87	0.53
1:B:402:ILE:HG13	1:B:402:ILE:O	2.09	0.52
3:D:7:SER:CB	3:D:8:PRO:HD3	2.40	0.52
2:E:204:ASN:HD22	2:E:215:ASP:HB3	1.73	0.52
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.90	0.52
2:E:80:TYR:OH	7:E:307:HOH:O	2.15	0.52
6:B:505:DMU:H29	6:B:506:DMU:C22	2.33	0.52
3:D:58:PRO:HG2	3:D:61:PHE:CE1	2.45	0.52
1:B:23:ARG:CG	1:B:23:ARG:NH1	2.72	0.52
6:A:505:DMU:O61	6:A:506:DMU:H4	2.09	0.52
2:C:51:ILE:HG12	2:C:72:ARG:HG2	1.92	0.52
2:C:86:VAL:HG11	2:C:119:VAL:HG22	1.91	0.52
3:D:106:LEU:HD23	3:D:107:ARG:N	2.24	0.52
2:E:131:PRO:O	2:E:132:LEU:HD23	2.10	0.52
2:C:87:ARG:HH21	2:C:89:GLU:CD	2.12	0.52
3:F:7:SER:OG	3:F:8:PRO:HD2	2.10	0.52
3:D:76:THR:O	3:D:76:THR:HG23	2.10	0.52
1:A:422:ILE:HA	1:A:425:MET:CE	2.33	0.52
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.92	0.52
1:B:197:ILE:HD11	1:B:219:PHE:CD2	2.45	0.51
1:B:206:PRO:HG2	1:B:211:THR:CG2	2.36	0.51
3:D:60:ARG:HD2	3:D:76:THR:O	2.10	0.51
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.44	0.51
1:A:92:PHE:O	1:A:96:LEU:HD23	2.10	0.51
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.92	0.51
3:D:141:LYS:HB3	3:D:172:TYR:CE1	2.44	0.51
1:B:27:GLU:O	4:G:2:GLC:H62	2.11	0.51
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.92	0.51
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.46	0.51
6:A:505:DMU:H9	6:A:506:DMU:O49	2.10	0.51
6:A:504:DMU:H6	6:A:504:DMU:H15	1.93	0.51
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.92	0.51
1:B:214:SER:HA	4:G:1:GLC:HO3	1.76	0.51
1:B:62:ASN:O	1:B:65:MET:N	2.43	0.51
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.93	0.51
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.92	0.50
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.46	0.50
3:F:1:ASP:OD1	3:F:1:ASP:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLU:O	1:A:152:VAL:HG23	2.12	0.50
3:D:76:THR:O	3:D:76:THR:CG2	2.59	0.50
2:E:6:GLU:OE1	2:E:112:GLY:HA3	2.10	0.50
1:A:226:THR:CG2	1:B:423:LEU:HD11	2.41	0.50
1:A:423:LEU:HD11	1:B:226:THR:CG2	2.41	0.50
2:C:213:LYS:N	7:C:342:HOH:O	2.11	0.50
2:C:86:VAL:HG11	2:C:119:VAL:CG2	2.41	0.50
1:A:311:ALA:O	1:A:340:ARG:HD2	2.12	0.50
6:A:503:DMU:H6	6:A:503:DMU:O61	2.11	0.50
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.47	0.50
3:D:136:ASN:HB3	3:D:137:ASN:HD22	1.75	0.50
3:F:95:GLN:O	3:F:95:GLN:NE2	2.45	0.49
6:A:505:DMU:H7	6:A:506:DMU:C2	2.43	0.49
1:B:74:ASN:O	1:B:77:LEU:N	2.45	0.49
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.95	0.49
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.92	0.49
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.27	0.49
3:D:7:SER:O	3:D:9:ALA:N	2.45	0.49
3:D:150:ASP:OD1	3:D:188:HIS:HB3	2.12	0.49
1:A:42:VAL:O	1:A:46:VAL:HG23	2.12	0.49
1:A:109:ILE:HG23	1:A:204:MET:SD	2.52	0.49
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.31	0.49
2:C:32:TYR:CE2	2:C:98:ARG:HD3	2.47	0.49
6:A:505:DMU:C18	6:A:506:DMU:H2	2.43	0.49
2:C:105:TYR:CD2	3:D:91:SER:HA	2.47	0.49
2:E:178:LEU:HD11	2:E:181:ALA:HA	1.94	0.49
2:E:178:LEU:HD12	2:E:182:LEU:O	2.13	0.49
3:F:6:GLN:HA	3:F:22:THR:O	2.13	0.49
2:C:185:LEU:C	2:C:185:LEU:HD12	2.34	0.48
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.28	0.48
1:B:92:PHE:O	1:B:96:LEU:HD23	2.12	0.48
1:B:402:ILE:HD12	1:B:445:TYR:CE1	2.48	0.48
2:C:51:ILE:HD12	2:C:58:ILE:CG1	2.33	0.48
6:A:505:DMU:H7	6:A:506:DMU:H2	1.94	0.48
2:C:7:SER:HA	2:C:115:THR:CG2	2.43	0.48
2:C:172:HIS:HE1	3:D:136:ASN:CG	2.16	0.48
2:E:17:SER:HB2	2:E:83:ILE:O	2.14	0.48
2:E:73:ASP:OD1	2:E:76:LYS:HB2	2.13	0.48
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.96	0.48
1:B:158:ILE:O	1:B:162:VAL:HG13	2.13	0.48
3:F:186:GLU:C	3:F:188:HIS:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:O	1:A:402:ILE:HG13	2.12	0.48
3:D:74:ILE:HD13	3:D:81:ASP:OD2	2.13	0.48
2:E:162:TRP:CH2	2:E:203:CYS:HB3	2.48	0.48
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.95	0.48
6:B:505:DMU:H3	6:B:506:DMU:O49	2.14	0.48
1:A:180:THR:HB	1:A:218:VAL:HA	1.95	0.48
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.95	0.48
3:D:10:ILE:HG23	3:D:102:LYS:HB3	1.95	0.48
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.81	0.47
2:C:29:TYR:HE2	2:C:74:ASN:OD1	1.97	0.47
2:C:87:ARG:NH2	2:C:89:GLU:OE1	2.41	0.47
2:E:54:VAL:HG23	2:E:56:SER:H	1.79	0.47
1:A:262:PHE:CE2	1:A:367:LEU:HD23	2.49	0.47
2:C:18:LEU:HD11	2:C:83:ILE:HD12	1.96	0.47
1:A:197:ILE:HD11	1:A:219:PHE:CD2	2.48	0.47
1:A:158:ILE:O	1:A:162:VAL:HG13	2.13	0.47
1:B:109:ILE:HG23	1:B:204:MET:SD	2.54	0.47
1:B:311:ALA:O	1:B:340:ARG:HD2	2.15	0.47
4:H:1:GLC:C3	4:I:1:GLC:H62	2.44	0.47
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.96	0.47
1:A:414:GLU:HG2	1:B:419:TYR:CZ	2.50	0.47
1:B:381:GLN:OE1	1:B:381:GLN:N	2.33	0.47
1:A:94:TYR:CE1	1:A:295:GLY:HA3	2.50	0.47
1:B:41:VAL:O	1:B:45:LEU:HG	2.14	0.47
1:B:98:ARG:HH21	1:B:102:PRO:HB3	1.78	0.47
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.18	0.47
1:B:172:GLU:HG3	1:B:212:LEU:HB3	1.96	0.47
2:E:47:TRP:CG	3:F:95:GLN:NE2	2.82	0.47
2:E:87:ARG:HE	2:E:89:GLU:CD	2.17	0.47
3:F:6:GLN:O	3:F:7:SER:O	2.33	0.47
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.96	0.47
1:A:75:TYR:O	1:A:79:LEU:HG	2.14	0.47
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.18	0.47
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.93	0.47
1:B:75:TYR:O	1:B:79:LEU:HG	2.14	0.47
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.44	0.47
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.95	0.47
2:C:135:GLY:O	2:C:138:ALA:HB2	2.15	0.47
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.95	0.47
3:D:89:GLN:O	3:D:95:GLN:HB2	2.14	0.47
3:F:184:GLU:HA	3:F:187:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TRP:O	1:B:63:GLN:HG2	2.15	0.47
1:B:197:ILE:CD1	1:B:219:PHE:CD2	2.98	0.47
3:F:6:GLN:OE1	3:F:98:GLY:HA3	2.15	0.47
1:A:255:TYR:CD1	1:A:424:PRO:HB3	2.50	0.46
1:B:117:GLU:O	1:B:118:ASP:HB2	2.14	0.46
1:B:260:ILE:O	1:B:264:ILE:HG23	2.15	0.46
2:C:61:THR:O	2:C:63:SER:N	2.48	0.46
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.84	0.46
1:B:117:GLU:HA	1:B:117:GLU:OE1	2.15	0.46
3:D:191:TYR:O	3:D:207:SER:HB2	2.15	0.46
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.97	0.46
3:F:60:ARG:HG3	3:F:74:ILE:CG2	2.46	0.46
3:F:77:MET:HE2	3:F:77:MET:HB3	1.81	0.46
3:D:109:ASP:HA	3:D:139:TYR:O	2.15	0.46
2:E:18:LEU:O	2:E:82:GLN:HA	2.15	0.46
1:A:74:ASN:O	1:A:77:LEU:N	2.48	0.46
1:A:260:ILE:O	1:A:264:ILE:HG23	2.15	0.46
3:F:72:LEU:C	3:F:72:LEU:HD23	2.35	0.46
1:B:255:TYR:CD1	1:B:424:PRO:HB3	2.51	0.46
2:E:188:SER:HB2	3:F:134:PHE:CD2	2.51	0.46
1:B:262:PHE:CE2	1:B:367:LEU:HD23	2.51	0.46
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.97	0.46
3:F:16:GLY:HA2	3:F:76:THR:HB	1.97	0.46
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.98	0.46
1:B:211:THR:HB	1:B:213:ILE:HG13	1.97	0.46
2:C:28:ASP:O	2:C:30:SER:O	2.34	0.46
7:C:322:HOH:O	3:D:122:GLU:HG2	2.16	0.46
1:A:59:TRP:O	1:A:63:GLN:HG2	2.15	0.46
6:A:503:DMU:H6	6:A:503:DMU:H29	1.97	0.46
2:E:24:ALA:HB3	2:E:29:TYR:HD1	1.81	0.46
1:A:109:ILE:N	1:A:110:PRO:CD	2.79	0.45
3:D:22:THR:CG2	3:D:23:CYS:N	2.79	0.45
3:D:199:THR:O	3:D:200:SER:HB2	2.16	0.45
1:B:120:ARG:HE	1:B:120:ARG:HB3	1.53	0.45
6:B:506:DMU:H10	6:B:506:DMU:H17	1.68	0.45
3:D:143:ILE:HG13	3:D:197:HIS:HA	1.97	0.45
3:F:49:ASP:O	3:F:50:THR:HB	2.16	0.45
3:F:80:GLU:HA	3:F:167:SER:O	2.16	0.45
1:A:360:MET:HB2	1:A:360:MET:HE2	1.81	0.45
2:E:138:ALA:O	2:E:140:ALA:N	2.48	0.45
3:D:89:GLN:NE2	3:D:95:GLN:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:VAL:O	2:E:2:VAL:HG22	2.16	0.45
1:A:160:ARG:HD2	1:A:160:ARG:HA	1.76	0.45
1:B:103:GLU:OE1	1:B:103:GLU:N	2.38	0.45
1:B:183:ALA:HB2	1:B:200:ILE:HG12	1.98	0.45
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.15	0.45
2:E:185:LEU:C	2:E:185:LEU:HD12	2.37	0.45
6:A:506:DMU:H13	6:A:506:DMU:H6	1.65	0.45
1:B:38:MET:O	1:B:42:VAL:HG23	2.17	0.45
6:A:505:DMU:H7	6:A:506:DMU:O55	2.17	0.45
6:A:505:DMU:O16	6:A:506:DMU:H2	2.16	0.45
1:B:445:TYR:HB2	7:B:604:HOH:O	2.17	0.45
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.98	0.45
3:D:79:ALA:C	3:D:81:ASP:H	2.20	0.45
1:B:38:MET:HA	1:B:41:VAL:HG13	1.99	0.45
1:B:94:TYR:CE1	1:B:295:GLY:HA3	2.51	0.45
1:A:211:THR:HB	1:A:213:ILE:HG13	1.98	0.44
1:A:319:LEU:C	1:A:319:LEU:HD12	2.38	0.44
1:A:117:GLU:OE1	1:A:117:GLU:HA	2.17	0.44
6:B:505:DMU:O49	6:B:505:DMU:H36	2.17	0.44
6:A:505:DMU:H4	6:A:505:DMU:C5	2.40	0.44
1:B:180:THR:HB	1:B:218:VAL:HA	2.00	0.44
2:E:28:ASP:O	2:E:30:SER:O	2.35	0.44
1:B:148:GLU:HG3	1:B:357:PHE:HB3	2.00	0.44
2:C:162:TRP:CH2	2:C:203:CYS:HB3	2.52	0.44
3:D:194:GLU:HG2	3:D:205:VAL:CG1	2.29	0.44
1:A:117:GLU:O	1:A:118:ASP:HB2	2.18	0.44
1:A:397:LEU:HA	1:A:397:LEU:HD23	1.66	0.44
3:D:29:VAL:CG1	3:D:89:GLN:HB2	2.46	0.44
1:A:18:ARG:O	1:A:22:ILE:HG13	2.18	0.44
1:B:332:MET:O	1:B:336:ILE:HG13	2.17	0.44
3:D:29:VAL:CG1	3:D:32:ILE:HD11	2.48	0.44
3:D:135:LEU:N	3:D:135:LEU:HD23	2.32	0.44
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.48	0.44
3:F:30:SER:HA	3:F:70:TYR:OH	2.18	0.44
1:A:183:ALA:HB2	1:A:200:ILE:HG12	2.00	0.43
6:B:506:DMU:O1	6:B:506:DMU:H2	2.18	0.43
6:B:506:DMU:O55	6:B:506:DMU:H35	2.18	0.43
3:D:72:LEU:HD23	3:D:73:THR:N	2.33	0.43
3:D:93:HIS:CG	3:D:94:PRO:HA	2.53	0.43
1:A:197:ILE:CD1	1:A:219:PHE:CD2	3.01	0.43
1:A:279:LEU:HA	1:A:282:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.51	0.43
6:B:506:DMU:H21	6:B:506:DMU:H14	1.74	0.43
3:F:149:ILE:HG12	3:F:191:TYR:CD2	2.53	0.43
1:A:172:GLU:HG3	1:A:212:LEU:HB3	1.99	0.43
2:E:6:GLU:CD	2:E:114:GLY:H	2.21	0.43
1:A:163:LEU:HD12	1:A:168:LEU:HB2	2.00	0.43
2:C:132:LEU:HD12	2:C:147:GLY:HA3	2.00	0.43
4:H:1:GLC:H61	4:H:2:GLC:C1	2.47	0.43
1:A:41:VAL:O	1:A:45:LEU:HG	2.19	0.43
1:B:284:HIS:O	1:B:286:GLY:N	2.51	0.43
1:B:312:THR:HG22	1:B:339:ALA:CB	2.49	0.43
2:C:22:CYS:O	2:C:78:THR:HG23	2.19	0.43
2:C:52:ASN:ND2	2:C:57:THR:HG22	2.34	0.43
3:D:104:GLU:HB3	3:D:165:GLN:OE1	2.19	0.43
3:D:112:PRO:HG3	3:D:143:ILE:HD11	2.00	0.43
2:E:47:TRP:CB	3:F:95:GLN:NE2	2.81	0.43
1:A:103:GLU:OE1	1:A:103:GLU:N	2.44	0.43
1:A:226:THR:HG21	1:B:423:LEU:HD11	2.00	0.43
1:B:38:MET:HG3	1:B:168:LEU:HD11	2.00	0.43
3:D:13:ALA:HA	7:D:309:HOH:O	2.17	0.43
2:E:105:TYR:HD2	3:F:91:SER:HA	1.82	0.43
1:A:88:VAL:HA	1:A:91:MET:HE2	2.01	0.43
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.49	0.43
2:E:16:GLY:O	2:E:86:VAL:HB	2.19	0.43
3:F:187:ARG:HG3	3:F:188:HIS:CD2	2.53	0.43
1:A:312:THR:HG22	1:A:339:ALA:CB	2.49	0.42
1:B:88:VAL:HA	1:B:91:MET:HE2	2.00	0.42
2:E:39:GLN:HB2	2:E:45:LEU:HD23	2.01	0.42
1:A:148:GLU:HG3	1:A:357:PHE:HB3	2.00	0.42
2:C:38:ARG:HD3	2:C:48:ILE:HD11	2.01	0.42
3:F:11:MET:CE	3:F:19:VAL:HG13	2.47	0.42
3:F:149:ILE:HD11	3:F:178:LEU:HD21	2.01	0.42
1:A:430:LEU:CD2	1:B:223:ILE:HD12	2.49	0.42
3:F:106:LEU:HA	3:F:139:TYR:OH	2.19	0.42
2:C:61:THR:OG1	2:C:62:PRO:HD2	2.19	0.42
2:C:6:GLU:OE2	2:C:96:CYS:N	2.42	0.42
1:A:98:ARG:HA	1:A:98:ARG:NE	2.35	0.42
3:D:186:GLU:HA	3:D:210:ARG:NH2	2.35	0.42
3:F:187:ARG:O	3:F:188:HIS:CD2	2.73	0.42
1:A:423:LEU:HD11	1:B:226:THR:HG21	2.01	0.42
1:A:62:ASN:O	1:A:63:GLN:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:HD11	1:B:226:THR:HG22	2.02	0.42
2:C:196:TRP:HA	2:C:197:PRO:HA	1.83	0.41
3:D:49:ASP:HB2	3:D:52:LYS:HD3	2.01	0.41
3:D:78:GLU:OE2	3:D:78:GLU:HA	2.20	0.41
1:A:164:ASP:HB3	6:A:503:DMU:C19	2.47	0.41
1:B:279:LEU:HA	1:B:282:ARG:HH11	1.84	0.41
3:F:184:GLU:HA	3:F:187:ARG:NH1	2.35	0.41
1:A:214:SER:O	1:A:218:VAL:HG23	2.20	0.41
2:C:47:TRP:CD2	3:D:95:GLN:NE2	2.87	0.41
2:E:200:THR:HG23	2:E:202:THR:HG23	2.02	0.41
1:B:98:ARG:NE	1:B:98:ARG:HA	2.35	0.41
1:B:160:ARG:HD2	1:B:160:ARG:HA	1.80	0.41
1:B:172:GLU:OE1	4:G:2:GLC:O3	2.35	0.41
2:C:29:TYR:CE2	2:C:74:ASN:OD1	2.72	0.41
1:B:122:VAL:HB	1:B:160:ARG:HG2	2.02	0.41
2:C:221:ARG:O	2:C:222:ALA:HB3	2.21	0.41
2:E:61:THR:O	2:E:63:SER:N	2.54	0.41
6:A:504:DMU:H15	6:A:504:DMU:H21	1.89	0.41
1:A:38:MET:HA	1:A:41:VAL:HG13	2.03	0.41
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.50	0.41
1:A:402:ILE:HD12	1:A:445:TYR:CE1	2.56	0.41
1:A:38:MET:O	1:A:42:VAL:HG23	2.20	0.41
1:A:98:ARG:HH21	1:A:102:PRO:HB3	1.82	0.41
1:A:172:GLU:HG3	1:A:212:LEU:O	2.21	0.41
1:B:68:LEU:HD22	1:B:78:LEU:HD22	2.02	0.41
1:B:323:ALA:HA	7:B:621:HOH:O	2.21	0.41
3:D:7:SER:CB	3:D:8:PRO:CD	2.99	0.41
2:E:204:ASN:ND2	2:E:215:ASP:HB3	2.35	0.41
1:A:226:THR:HG22	1:B:423:LEU:HD11	2.03	0.41
1:B:71:THR:O	1:B:78:LEU:HD23	2.21	0.41
6:B:505:DMU:H30	6:B:505:DMU:O3	2.21	0.41
2:C:53:PRO:O	2:C:74:ASN:ND2	2.53	0.41
3:D:163:THR:OG1	3:D:173:SER:HB2	2.21	0.41
1:A:68:LEU:HD13	1:A:307:PHE:CD1	2.55	0.40
1:A:203:GLU:HA	1:A:203:GLU:OE1	2.21	0.40
6:A:503:DMU:H4	6:A:503:DMU:H36	1.29	0.40
2:C:86:VAL:HG12	2:C:119:VAL:HG11	2.03	0.40
3:F:17:ASP:O	3:F:76:THR:HA	2.20	0.40
1:B:276:MET:HE3	1:B:276:MET:HB2	1.93	0.40
6:B:506:DMU:O55	6:B:506:DMU:C9	2.68	0.40
3:D:16:GLY:N	3:D:77:MET:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:60:ARG:NE	3:D:78:GLU:HG2	2.37	0.40
2:E:52:ASN:HD21	2:E:56:SER:HB3	1.86	0.40
2:C:107:TYR:CD1	3:D:45:ARG:HD3	2.57	0.40
2:C:134:PRO:HA	7:D:318:HOH:O	2.20	0.40
3:D:58:PRO:HG2	3:D:61:PHE:HE1	1.85	0.40
1:B:68:LEU:HD13	1:B:307:PHE:CD1	2.57	0.40
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.87	0.40
1:B:172:GLU:HG3	1:B:212:LEU:O	2.22	0.40
2:C:191:VAL:HB	2:C:192:PRO:CD	2.51	0.40
1:A:253:TRP:HB3	6:A:506:DMU:C18	2.50	0.40
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.22	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)
3:D:183:ASP:OD2	6:A:503:DMU:O2[3_545]	1.78	0.42
7:C:342:HOH:O	7:F:321:HOH:O[2_555]	1.82	0.38

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	442/446 (99%)	410 (93%)	29 (7%)	3 (1%)	19 29
1	B	440/446 (99%)	413 (94%)	23 (5%)	4 (1%)	14 22
2	C	220/222 (99%)	209 (95%)	8 (4%)	3 (1%)	9 13
2	E	219/222 (99%)	200 (91%)	14 (6%)	5 (2%)	5 6
3	D	209/211 (99%)	182 (87%)	25 (12%)	2 (1%)	13 20
3	F	209/211 (99%)	196 (94%)	11 (5%)	2 (1%)	13 20
All	All	1739/1758 (99%)	1610 (93%)	110 (6%)	19 (1%)	12 18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	LEU
2	E	65	LYS
2	E	136	SER
3	F	7	SER
2	C	140	ALA
3	D	67	GLY
2	E	139	ALA
1	A	457	GLU
1	B	234	HIS
3	D	7	SER
3	F	187	ARG
1	A	234	HIS
2	E	137	ALA
1	B	18	ARG
1	B	285	GLY
1	B	144	VAL
2	E	62	PRO
1	A	285	GLY
2	C	62	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	335/337 (99%)	320 (96%)	15 (4%)	23	40
1	B	333/337 (99%)	317 (95%)	16 (5%)	21	37
2	C	182/182 (100%)	170 (93%)	12 (7%)	14	23
2	E	181/182 (100%)	174 (96%)	7 (4%)	27	46
3	D	185/185 (100%)	174 (94%)	11 (6%)	16	28
3	F	185/185 (100%)	174 (94%)	11 (6%)	16	28
All	All	1401/1408 (100%)	1329 (95%)	72 (5%)	20	35

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	62	ASN
1	A	73	ASP
1	A	180	THR
1	A	200	ILE
1	A	211	THR
1	A	219	PHE
1	A	246	ASP
1	A	251	THR
1	A	264	ILE
1	A	273	VAL
1	A	304	LEU
1	A	397	LEU
1	A	402	ILE
1	A	423	LEU
1	B	23	ARG
1	B	62	ASN
1	B	73	ASP
1	B	162	VAL
1	B	180	THR
1	B	200	ILE
1	B	211	THR
1	B	219	PHE
1	B	246	ASP
1	B	251	THR
1	B	264	ILE
1	B	273	VAL
1	B	304	LEU
1	B	397	LEU
1	B	402	ILE
1	B	423	LEU
2	C	30	SER
2	C	43	LYS
2	C	51	ILE
2	C	66	ASP
2	C	72	ARG
2	C	115	THR
2	C	193	SER
2	C	198	SER
2	C	199	GLU
2	C	200	THR
2	C	204	ASN
2	C	214	VAL

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Mol	Chain	Res	Type
3	D	21	MET
3	D	22	THR
3	D	41	THR
3	D	76	THR
3	D	92	SER
3	D	95	GLN
3	D	115	SER
3	D	174	MET
3	D	180	LEU
3	D	187	ARG
3	D	201	THR
2	E	5	LEU
2	E	55	SER
2	E	56	SER
2	E	71	SER
2	E	103	TYR
2	E	188	SER
2	E	200	THR
3	F	1	ASP
3	F	6	GLN
3	F	44	LYS
3	F	77	MET
3	F	95	GLN
3	F	142	ASP
3	F	190	SER
3	F	192	THR
3	F	198	LYS
3	F	201	THR
3	F	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	157	ASN
1	A	207	GLN
1	A	270	ASN
1	B	157	ASN
1	B	250	ASN
1	B	270	ASN
2	C	163	ASN
2	C	172	HIS

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Mol	Chain	Res	Type
3	D	136	ASN
3	D	137	ASN
3	D	144	ASN
3	D	188	HIS
2	E	172	HIS
2	E	179	GLN
3	F	136	ASN
3	F	137	ASN
3	F	188	HIS

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	$\#\|Z\| > 2$
4	GLC	G	1	4	12,12,12	0.67	0	17,17,17	1.40	3 (17%)
4	GLC	G	2	4	11,11,12	0.49	0	15,15,17	1.83	2 (13%)
4	GLC	H	1	4	12,12,12	0.56	0	17,17,17	0.94	1 (5%)
4	GLC	H	2	4	11,11,12	0.38	0	15,15,17	1.22	1 (6%)
4	GLC	I	1	4	12,12,12	0.64	0	17,17,17	1.03	1 (5%)
4	GLC	I	2	4	11,11,12	0.66	0	15,15,17	2.34	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	G	1	4	-	2/2/22/22	0/1/1/1
4	GLC	G	2	4	-	2/2/19/22	0/1/1/1
4	GLC	H	1	4	-	0/2/22/22	0/1/1/1
4	GLC	H	2	4	-	0/2/19/22	0/1/1/1
4	GLC	I	1	4	-	1/2/22/22	0/1/1/1
4	GLC	I	2	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2	GLC	C1-O5-C5	6.00	120.22	112.19
4	I	2	GLC	C1-O5-C5	5.90	120.09	112.19
4	I	2	GLC	C1-C2-C3	5.77	118.05	109.64
4	H	2	GLC	C1-O5-C5	3.89	117.41	112.19
4	G	1	GLC	C4-C3-C2	3.39	116.78	110.83
4	I	1	GLC	C3-C4-C5	-2.58	105.55	110.23
4	G	1	GLC	C3-C4-C5	2.51	114.78	110.23
4	I	2	GLC	O5-C1-C2	2.43	116.59	110.79
4	G	1	GLC	O5-C5-C4	2.41	114.05	109.70
4	G	2	GLC	C1-C2-C3	2.15	112.78	109.64
4	H	1	GLC	O4-C4-C3	-2.06	105.53	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	GLC	C4-C5-C6-O6
4	G	1	GLC	O5-C5-C6-O6
4	G	2	GLC	O5-C5-C6-O6
4	I	1	GLC	O5-C5-C6-O6
4	I	2	GLC	O5-C5-C6-O6
4	G	1	GLC	C4-C5-C6-O6

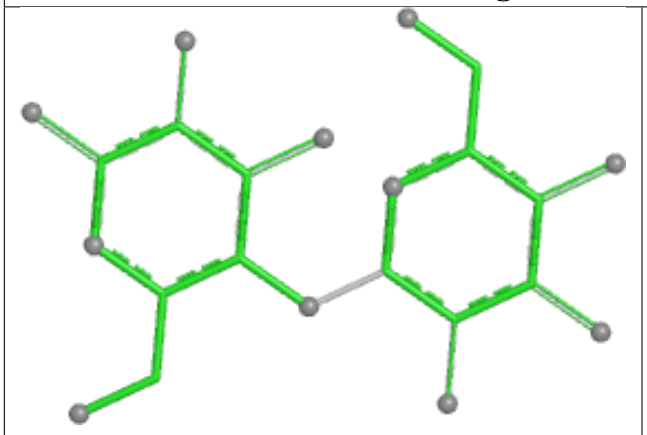
There are no ring outliers.

5 monomers are involved in 8 short contacts:

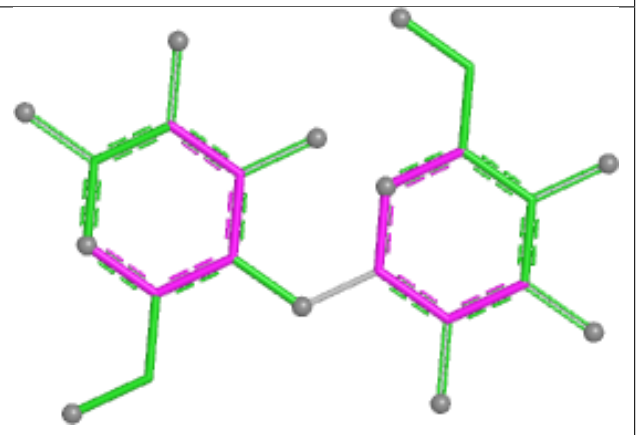
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	GLC	3	0
4	I	1	GLC	2	0
4	H	2	GLC	1	0
4	G	2	GLC	2	0
4	H	1	GLC	3	0

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

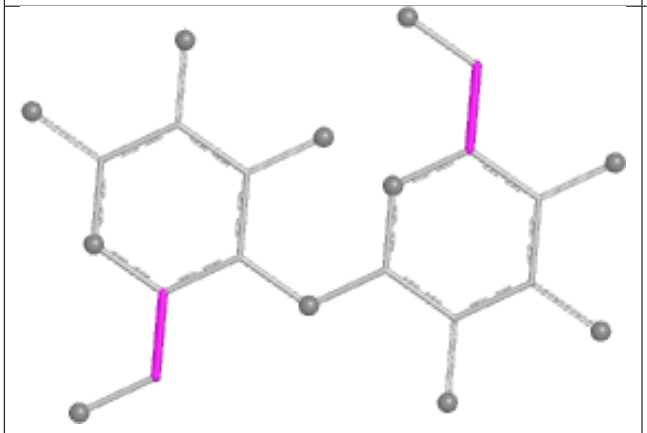
Oligosaccharide Chain G



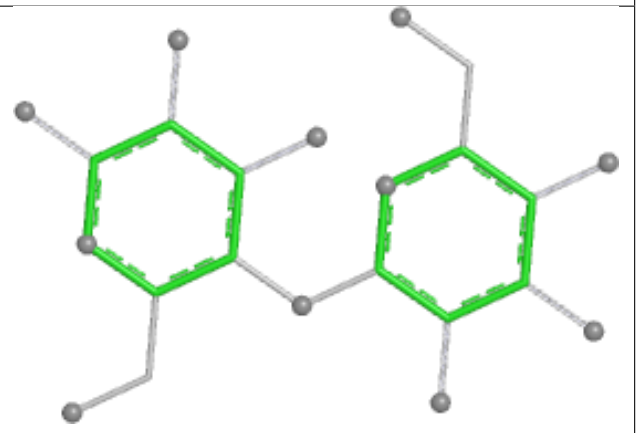
Bond lengths



Bond angles

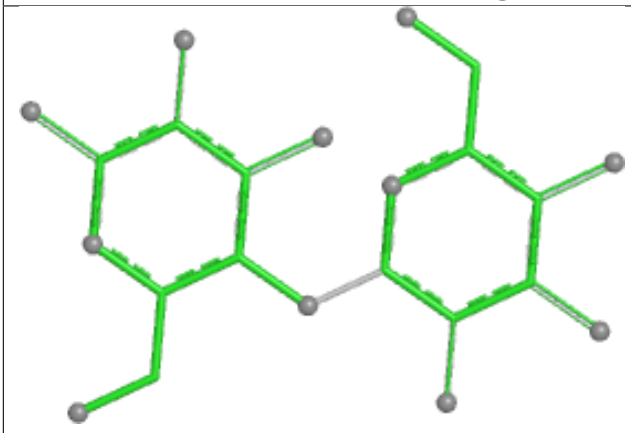


Torsions

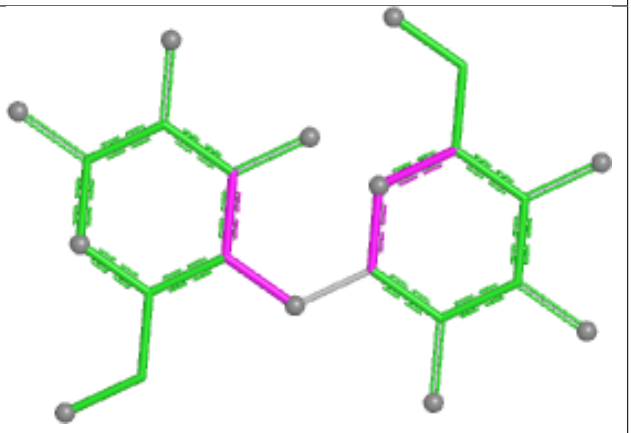


Rings

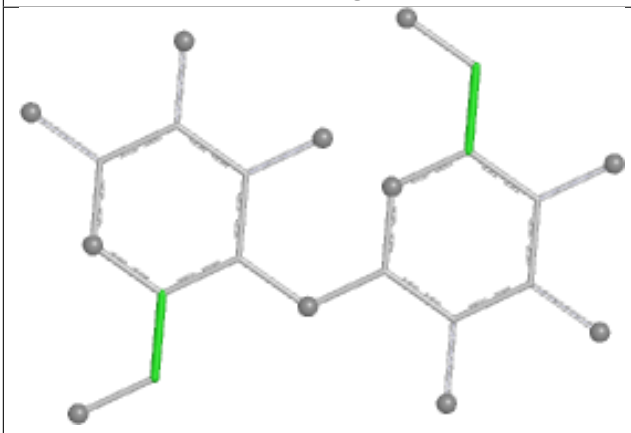
Oligosaccharide Chain H



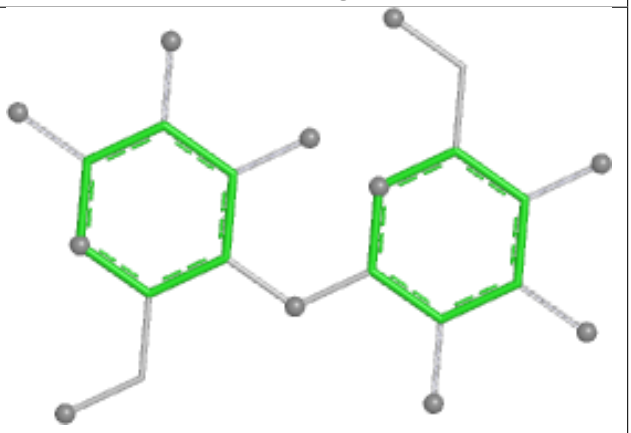
Bond lengths



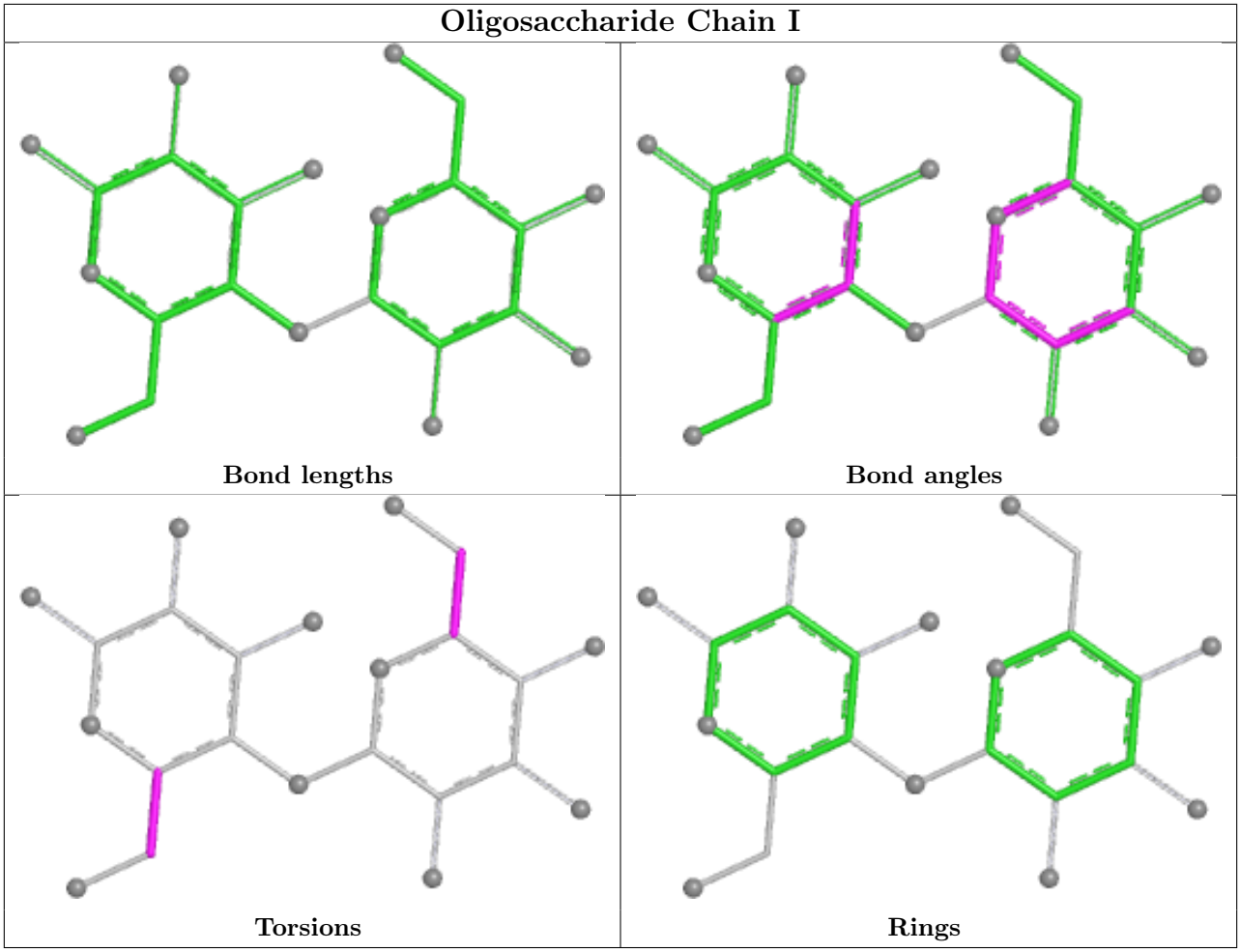
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	DMU	A	504	-	34,34,34	0.55	1 (2%)	45,45,45	1.17	3 (6%)
6	DMU	A	503	-	34,34,34	0.50	0	45,45,45	1.32	5 (11%)
6	DMU	B	505	-	34,34,34	0.45	0	45,45,45	1.08	3 (6%)
6	DMU	B	506	-	34,34,34	0.47	0	45,45,45	1.05	2 (4%)
6	DMU	A	505	-	34,34,34	0.49	0	45,45,45	1.11	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	DMU	A	506	-	34,34,34	0.42	0	45,45,45	1.19	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DMU	A	504	-	-	10/19/59/59	0/2/2/2
6	DMU	A	503	-	-	9/19/59/59	0/2/2/2
6	DMU	B	505	-	-	11/19/59/59	0/2/2/2
6	DMU	B	506	-	-	15/19/59/59	0/2/2/2
6	DMU	A	505	-	-	14/19/59/59	0/2/2/2
6	DMU	A	506	-	-	11/19/59/59	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	504	DMU	O16-C6	2.11	1.43	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	503	DMU	C8-C7-C5	-3.91	103.97	110.83
6	A	506	DMU	C2-C3-C4	-3.40	103.39	110.93
6	A	504	DMU	C6-O5-C4	3.37	120.30	113.72
6	A	503	DMU	O5-C4-C3	3.02	115.97	109.72
6	A	505	DMU	C7-C8-C9	3.00	115.67	110.23
6	A	503	DMU	C10-O7-C3	-2.80	111.35	117.98
6	B	505	DMU	C10-O1-C9	-2.73	108.39	113.72
6	A	503	DMU	O2-C8-C7	-2.67	104.09	110.38
6	A	505	DMU	O1-C9-C8	2.66	114.48	109.70
6	B	506	DMU	C6-O5-C4	-2.60	108.64	113.72
6	A	504	DMU	C10-O7-C3	-2.59	111.83	117.98
6	B	505	DMU	C7-C8-C9	2.57	114.89	110.23
6	B	506	DMU	C1-C2-C3	2.43	115.20	109.68
6	B	505	DMU	C18-O16-C6	-2.31	109.74	113.68
6	A	506	DMU	C18-O16-C6	-2.24	109.85	113.68
6	A	506	DMU	C6-C1-C2	2.19	114.61	110.01
6	A	503	DMU	C6-C1-C2	-2.18	105.42	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	504	DMU	O16-C6-C1	2.15	111.54	108.27
6	A	506	DMU	C6-O5-C4	-2.12	109.58	113.72
6	A	505	DMU	O7-C3-C4	2.04	114.83	109.48

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	504	DMU	C19-C18-O16-C6
6	A	505	DMU	C1-C6-O16-C18
6	A	505	DMU	O5-C6-O16-C18
6	A	506	DMU	C1-C6-O16-C18
6	B	505	DMU	C19-C18-O16-C6
6	B	506	DMU	C19-C18-O16-C6
6	A	503	DMU	C4-C3-O7-C10
6	A	505	DMU	C4-C3-O7-C10
6	B	506	DMU	C5-C10-O7-C3
6	B	506	DMU	C2-C3-O7-C10
6	A	503	DMU	C5-C10-O7-C3
6	A	503	DMU	O1-C10-O7-C3
6	A	504	DMU	O5-C6-O16-C18
6	A	506	DMU	O1-C10-O7-C3
6	A	505	DMU	O6-C11-C9-O1
6	A	505	DMU	O1-C10-O7-C3
6	A	504	DMU	O6-C11-C9-O1
6	A	504	DMU	C1-C6-O16-C18
6	A	503	DMU	O6-C11-C9-O1
6	A	506	DMU	C5-C10-O7-C3
6	A	505	DMU	O6-C11-C9-C8
6	A	506	DMU	O5-C6-O16-C18
6	B	505	DMU	C2-C3-O7-C10
6	A	505	DMU	C5-C10-O7-C3
6	B	506	DMU	C3-C4-C57-O61
6	B	506	DMU	O1-C10-O7-C3
6	B	505	DMU	C4-C3-O7-C10
6	B	505	DMU	C25-C28-C31-C34
6	B	505	DMU	C31-C34-C37-C40
6	A	504	DMU	C19-C22-C25-C28
6	A	505	DMU	O16-C18-C19-C22
6	A	506	DMU	C31-C34-C37-C40
6	B	506	DMU	C1-C6-O16-C18
6	A	505	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
6	B	506	DMU	C22-C25-C28-C31
6	B	505	DMU	C19-C22-C25-C28
6	B	506	DMU	C25-C28-C31-C34
6	B	506	DMU	O6-C11-C9-O1
6	A	503	DMU	C28-C31-C34-C37
6	B	505	DMU	C34-C37-C40-C43
6	A	506	DMU	C4-C3-O7-C10
6	A	504	DMU	C18-C19-C22-C25
6	B	506	DMU	C4-C3-O7-C10
6	B	506	DMU	O16-C18-C19-C22
6	B	505	DMU	C3-C4-C57-O61
6	B	505	DMU	C18-C19-C22-C25
6	B	506	DMU	O5-C4-C57-O61
6	A	505	DMU	C19-C22-C25-C28
6	B	505	DMU	O16-C18-C19-C22
6	A	506	DMU	C34-C37-C40-C43
6	A	503	DMU	O5-C4-C57-O61
6	A	504	DMU	C2-C3-O7-C10
6	A	503	DMU	C31-C34-C37-C40
6	A	506	DMU	C2-C3-O7-C10
6	B	506	DMU	C28-C31-C34-C37
6	A	504	DMU	C4-C3-O7-C10
6	B	505	DMU	O5-C4-C57-O61
6	A	505	DMU	C19-C18-O16-C6
6	A	506	DMU	C19-C18-O16-C6
6	B	506	DMU	C34-C37-C40-C43
6	A	506	DMU	C19-C22-C25-C28
6	A	504	DMU	O6-C11-C9-C8
6	A	504	DMU	C31-C34-C37-C40
6	B	506	DMU	O5-C6-O16-C18
6	A	505	DMU	C31-C34-C37-C40
6	A	505	DMU	C34-C37-C40-C43
6	A	506	DMU	C18-C19-C22-C25
6	A	503	DMU	C19-C22-C25-C28
6	A	503	DMU	O16-C18-C19-C22
6	A	505	DMU	C28-C31-C34-C37

There are no ring outliers.

6 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	504	DMU	3	0

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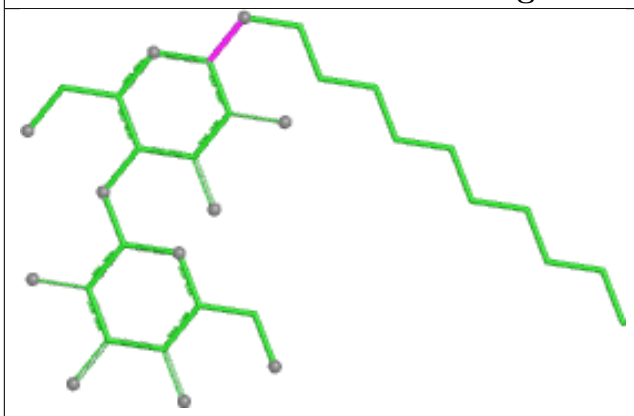
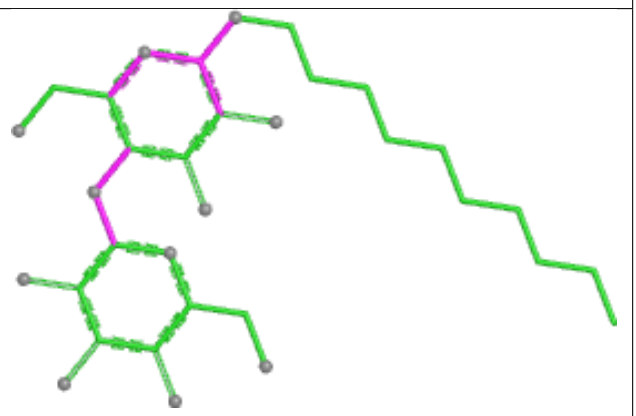
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	503	DMU	10	1
6	B	505	DMU	10	0
6	B	506	DMU	11	0
6	A	505	DMU	13	0
6	A	506	DMU	11	0

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.

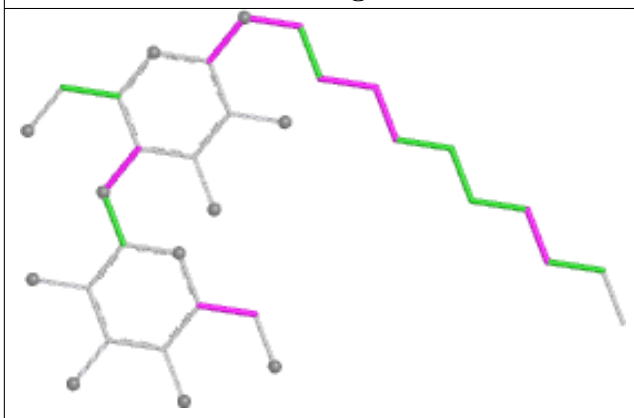
Ligand DMU A 504



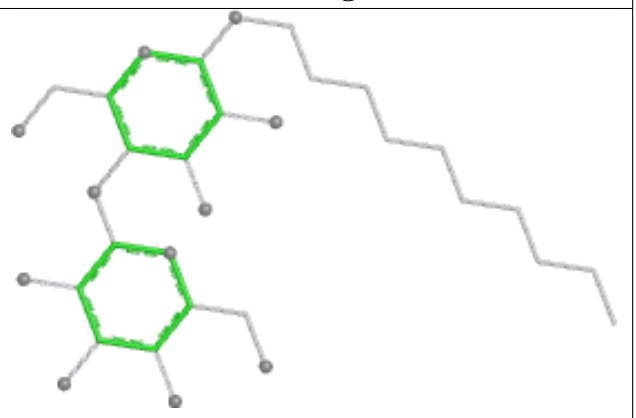
Bond lengths



Bond angles

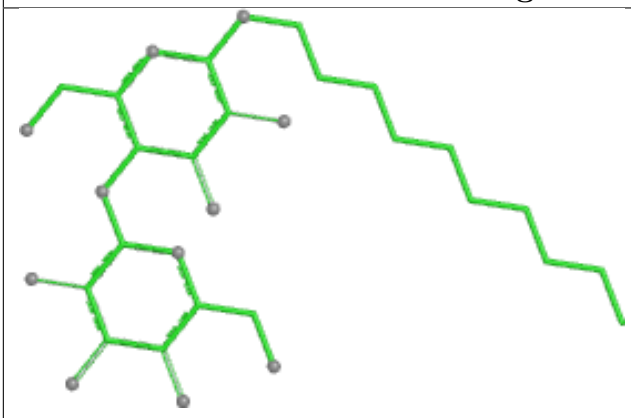


Torsions

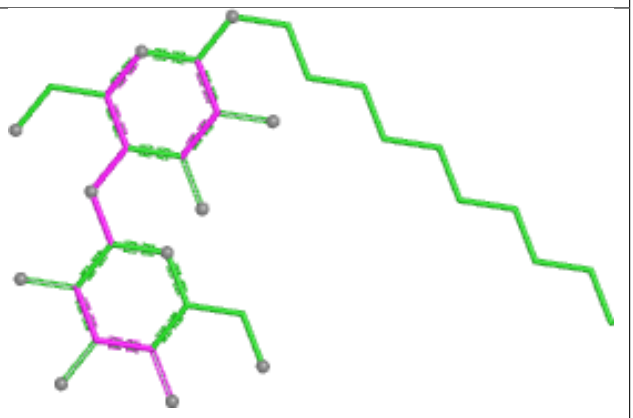


Rings

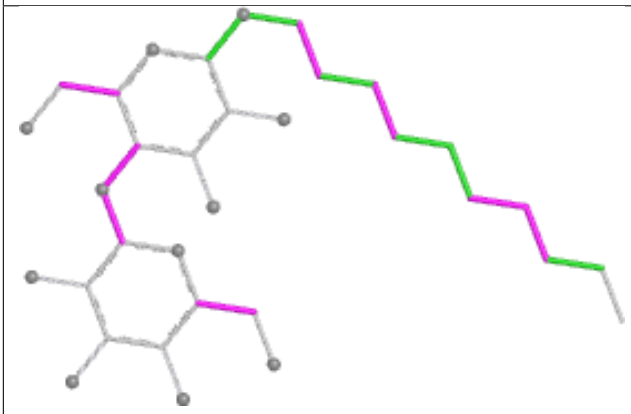
Ligand DMU A 503



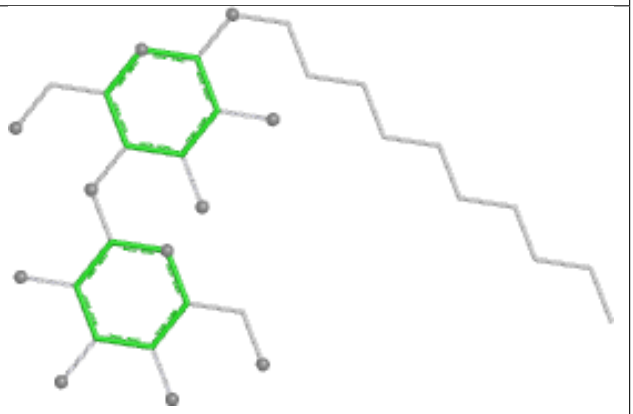
Bond lengths



Bond angles

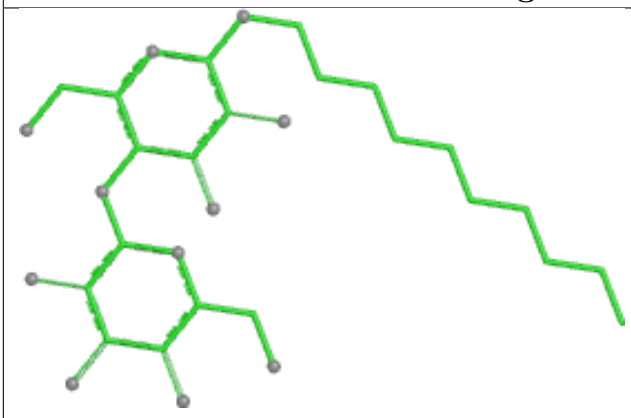


Torsions

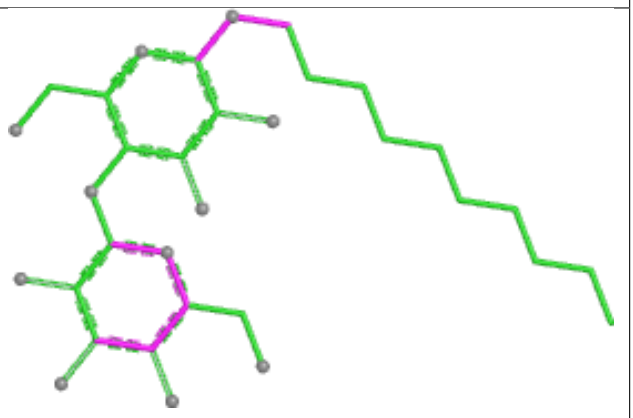


Rings

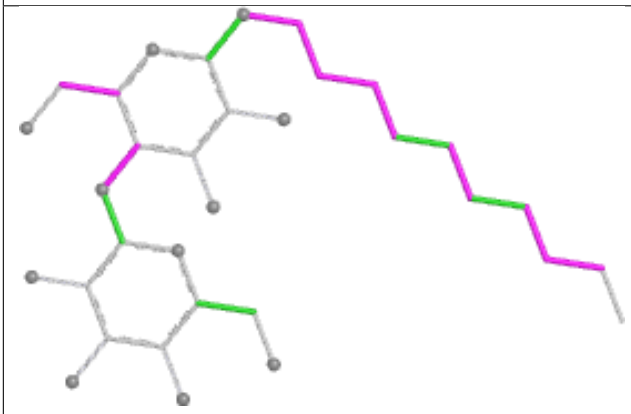
Ligand DMU B 505



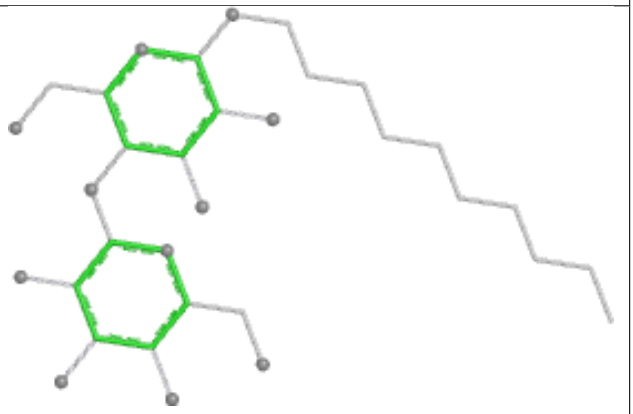
Bond lengths



Bond angles

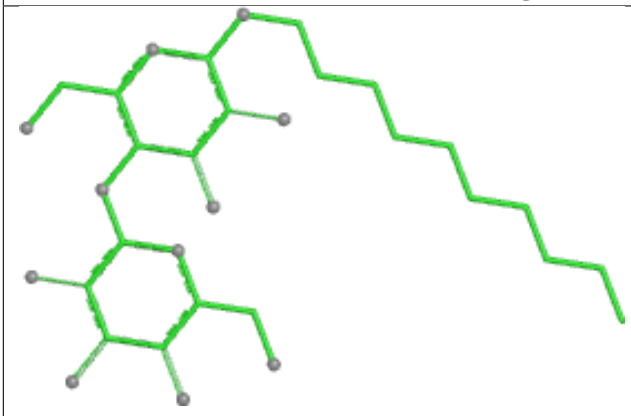


Torsions

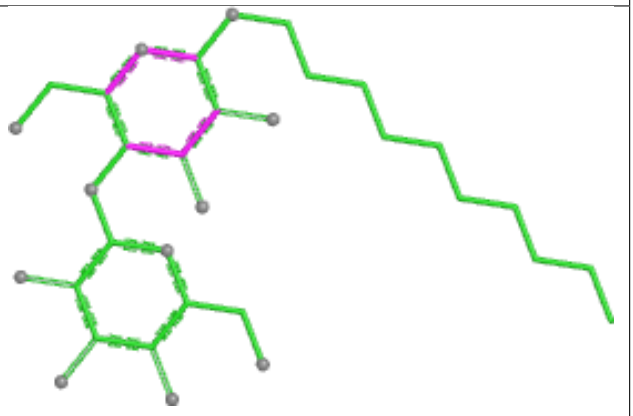


Rings

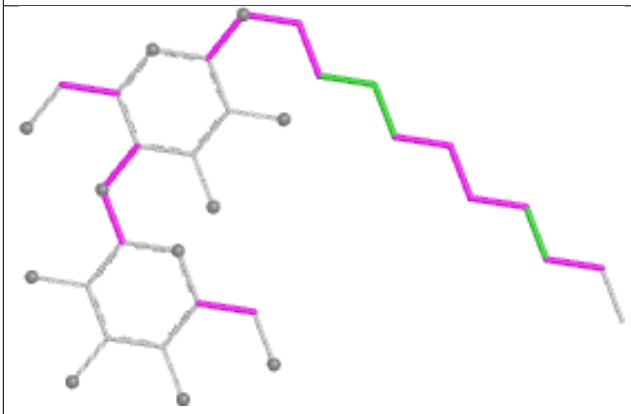
Ligand DMU B 506



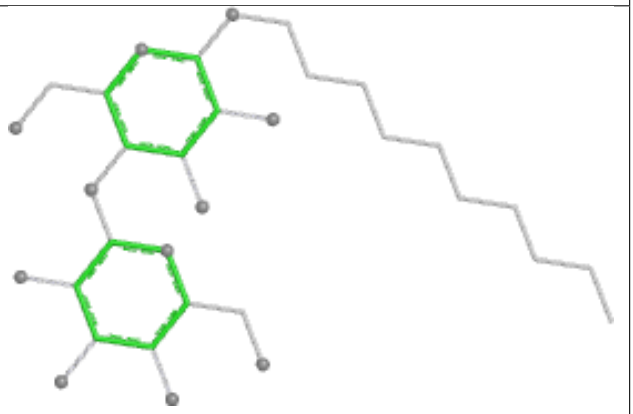
Bond lengths



Bond angles

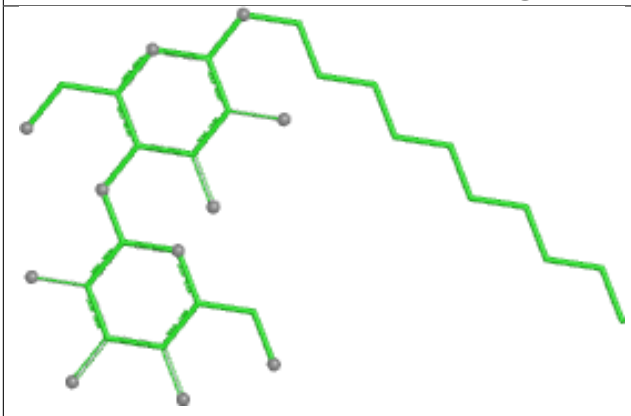


Torsions

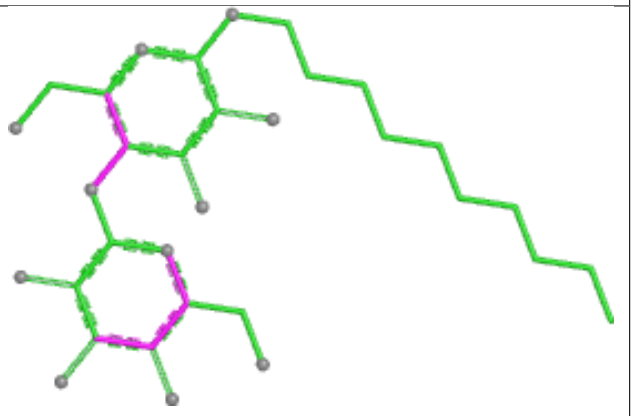


Rings

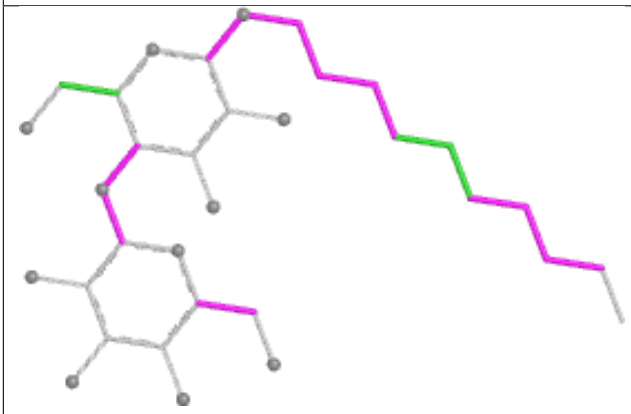
Ligand DMU A 505



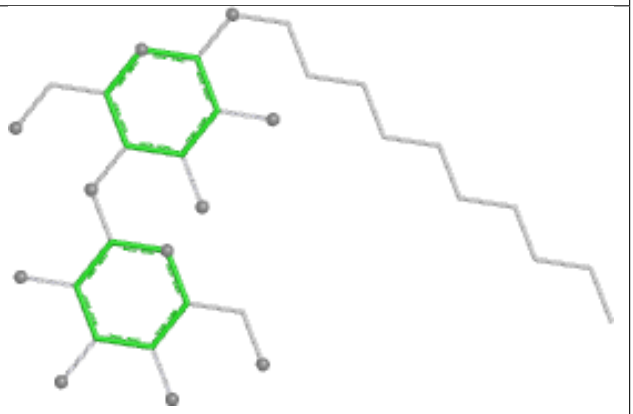
Bond lengths



Bond angles

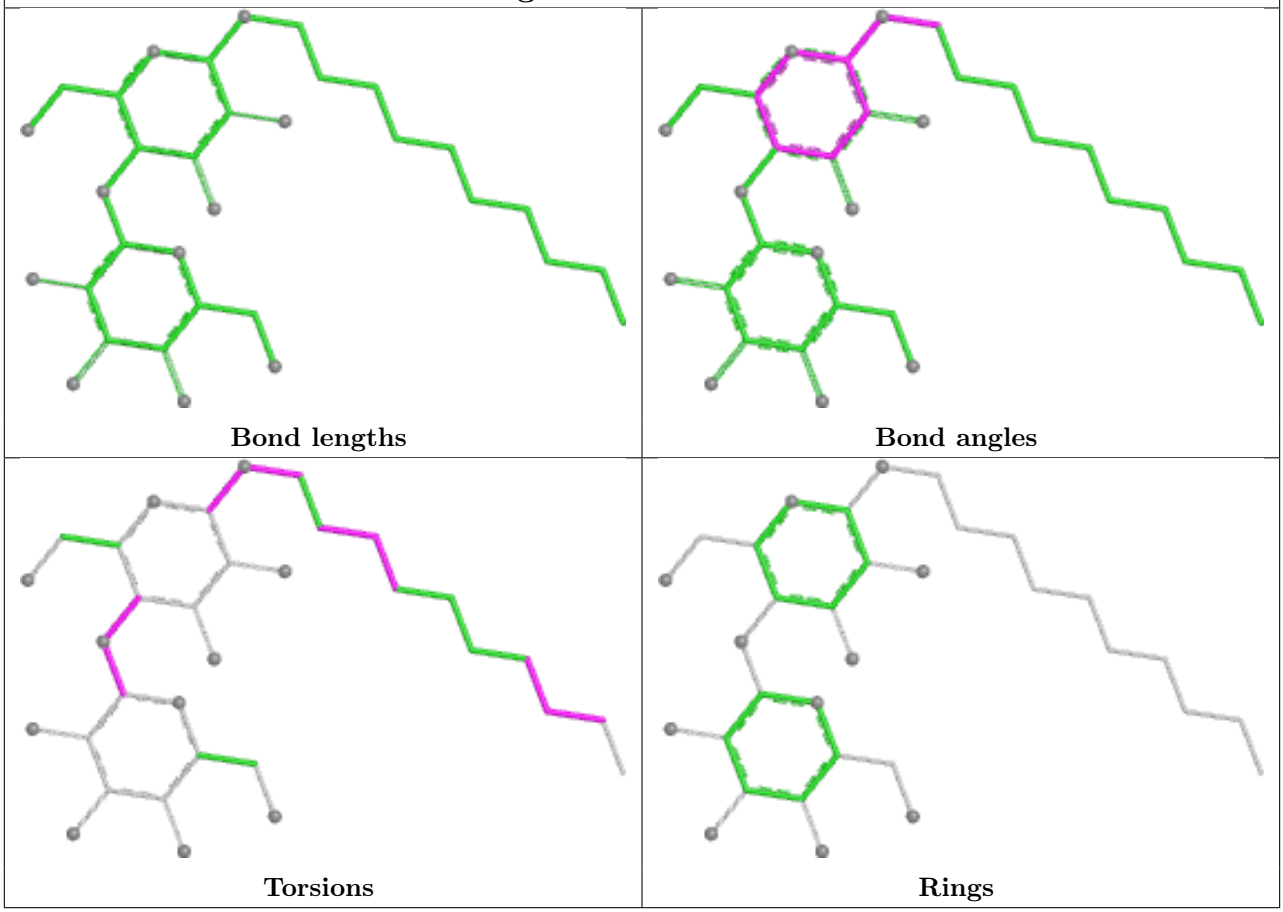


Torsions



Rings

Ligand DMU A 506



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	444/446 (99%)	0.33	17 (3%)	44	42	27, 47, 78, 118	0
1	B	442/446 (99%)	0.34	12 (2%)	56	53	27, 46, 79, 106	0
2	C	222/222 (100%)	-0.02	10 (4%)	39	36	15, 40, 76, 102	0
2	E	221/222 (99%)	0.07	10 (4%)	39	36	19, 43, 75, 124	0
3	D	211/211 (100%)	0.29	4 (1%)	66	62	26, 48, 70, 86	0
3	F	211/211 (100%)	-0.07	4 (1%)	66	62	16, 37, 76, 98	0
All	All	1751/1758 (99%)	0.20	57 (3%)	49	46	15, 45, 78, 124	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ALA	4.7
1	B	354	GLY	4.7
1	A	140	GLY	4.6
1	B	235	GLU	4.5
3	D	211	ALA	4.3
2	E	66	ASP	3.9
1	B	307	PHE	3.7
1	B	355	GLY	3.5
1	A	72	ALA	3.5
1	A	71	THR	3.5
1	A	167	ARG	3.4
2	E	69	ILE	3.4
1	A	168	LEU	3.4
3	F	155	GLN	3.2
1	A	235	GLU	3.0
2	E	138	ALA	3.0
1	A	326	GLY	3.0
3	F	207	SER	3.0
1	A	234	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	73	ASP	2.9
1	B	18	ARG	2.9
3	D	7	SER	2.9
1	A	212	LEU	2.8
1	B	72	ALA	2.8
2	E	31	ARG	2.8
2	C	140	ALA	2.6
2	C	64	LEU	2.6
3	F	152	SER	2.6
2	C	141	ALA	2.6
2	C	170	GLY	2.6
1	B	145	LEU	2.5
2	E	135	GLY	2.5
2	C	139	ALA	2.5
2	C	136	SER	2.3
3	D	110	ALA	2.3
1	A	285	GLY	2.3
1	B	234	HIS	2.3
1	A	219	PHE	2.3
2	E	2	VAL	2.3
2	E	139	ALA	2.3
1	A	27	GLU	2.2
1	B	219	PHE	2.2
3	F	153	GLU	2.2
2	E	137	ALA	2.2
1	B	159	GLY	2.2
2	C	142	SER	2.2
2	C	194	SER	2.1
1	A	30	LYS	2.1
1	A	386	ALA	2.1
2	C	168	ALA	2.1
1	B	71	THR	2.1
3	D	25	ALA	2.1
2	E	64	LEU	2.1
1	A	69	VAL	2.0
2	C	222	ALA	2.0
1	A	387	GLY	2.0
2	E	59	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)

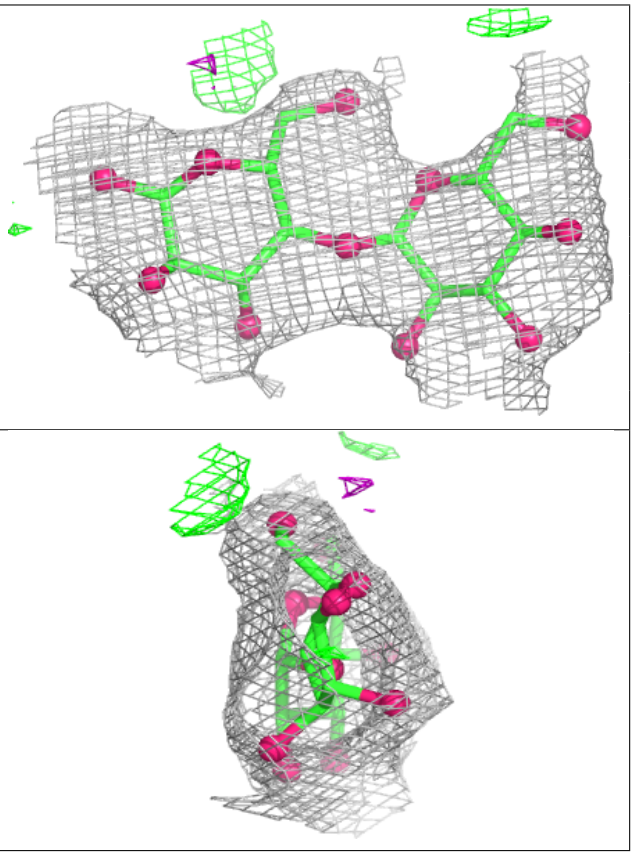
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GLC	H	2	11/12	0.57	0.14	80,91,105,105	0
4	GLC	H	1	12/12	0.63	0.12	85,91,97,99	0
4	GLC	I	1	12/12	0.64	0.14	74,87,97,100	0
4	GLC	G	1	12/12	0.73	0.11	59,74,85,85	0
4	GLC	I	2	11/12	0.74	0.13	72,85,86,99	0
4	GLC	G	2	11/12	0.85	0.10	65,77,83,84	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.

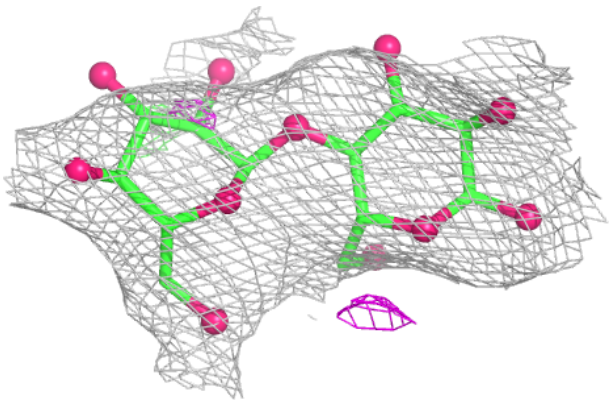
Electron density around Chain G:

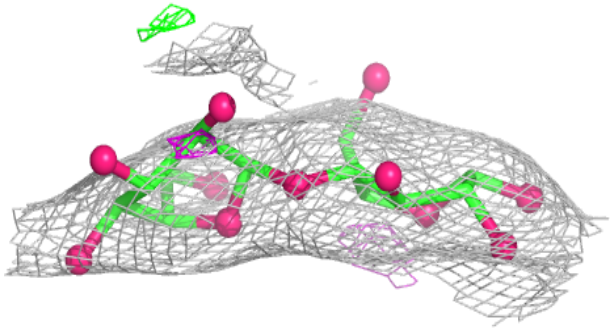
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

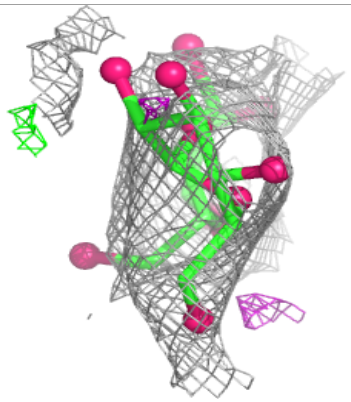


Electron density around Chain H:

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

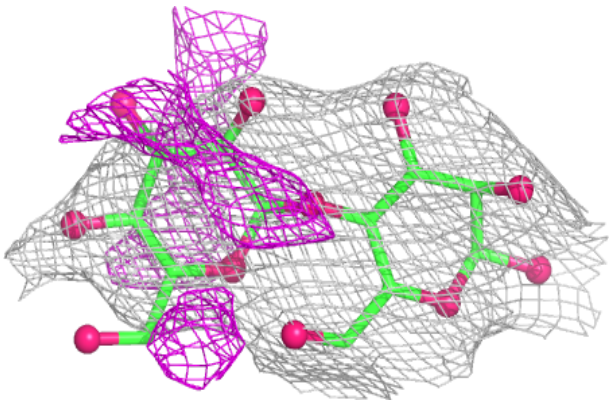


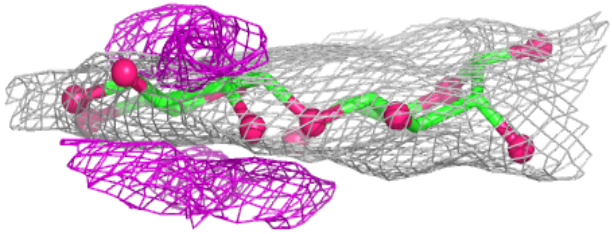


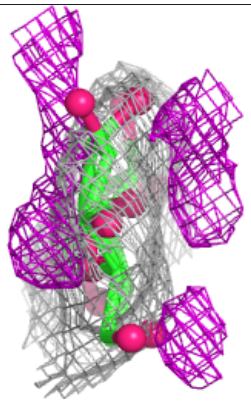


Electron density around Chain I:

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







6.4 Ligands (i)

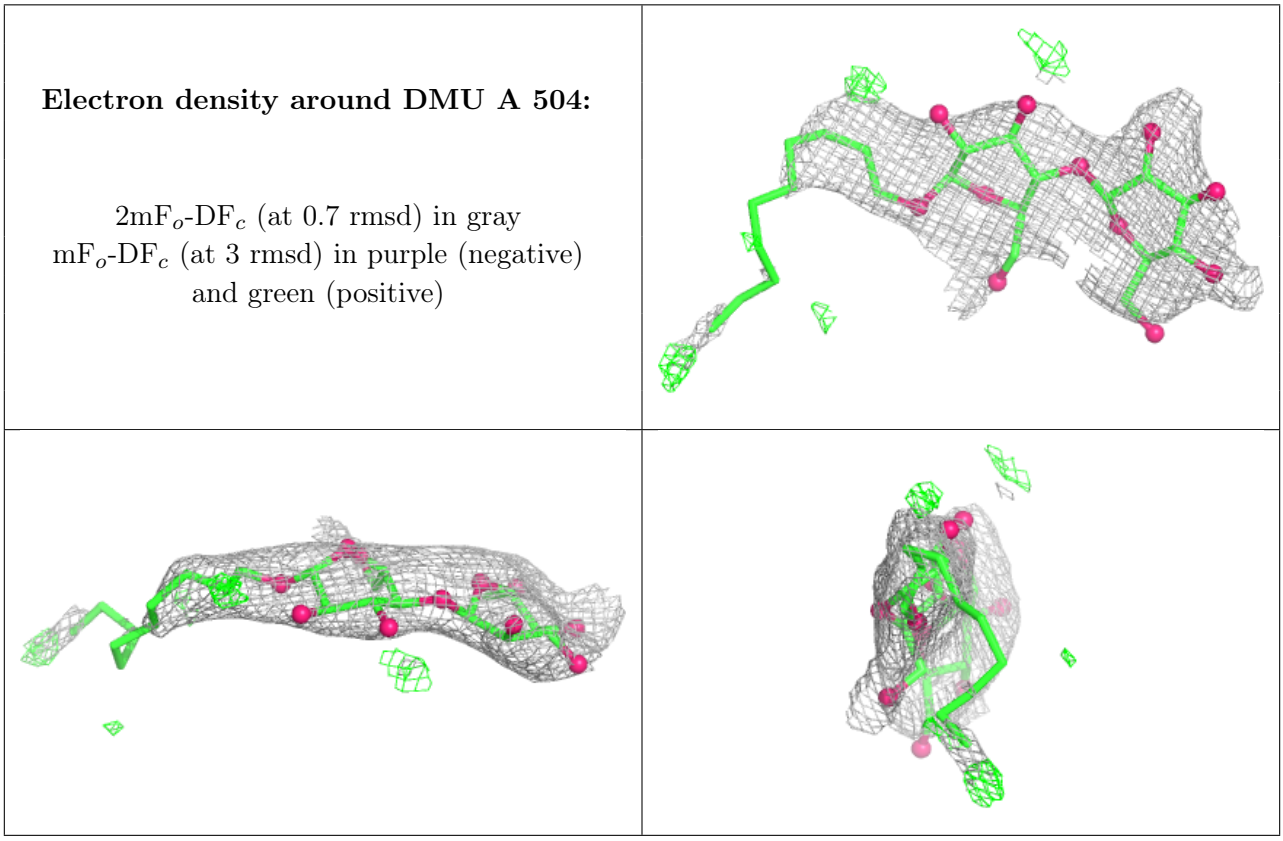
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	DMU	A	504	33/33	0.68	0.15	69,81,91,92	0
6	DMU	A	505	33/33	0.80	0.11	61,72,80,83	0
6	DMU	A	503	33/33	0.81	0.15	43,72,80,83	0
6	DMU	B	505	33/33	0.83	0.12	38,68,90,95	0
6	DMU	A	506	33/33	0.85	0.10	48,72,96,98	0
6	DMU	B	506	33/33	0.89	0.10	54,65,84,87	0
5	CL	A	502	1/1	0.90	0.13	60,60,60,60	0
5	CL	B	504	1/1	0.91	0.08	49,49,49,49	0
5	CL	B	503	1/1	0.92	0.07	43,43,43,43	0
5	CL	B	501	1/1	0.92	0.11	65,65,65,65	0
5	CL	A	501	1/1	0.94	0.09	42,42,42,42	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.

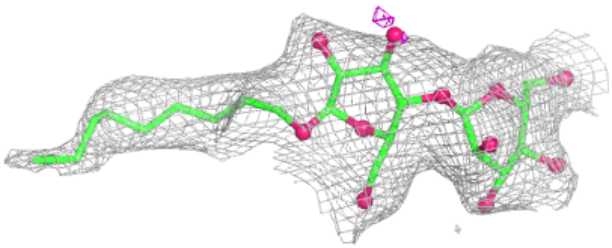
Electron density around DMU A 504:

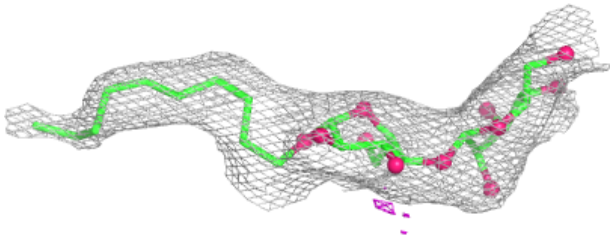
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

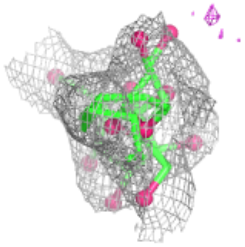


Electron density around DMU A 505:

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

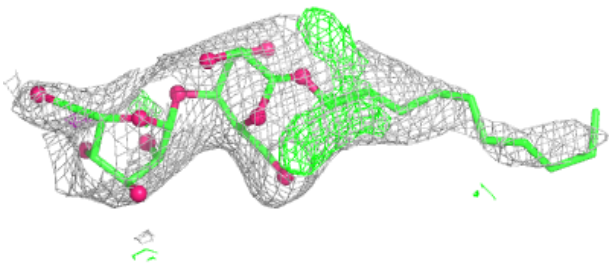


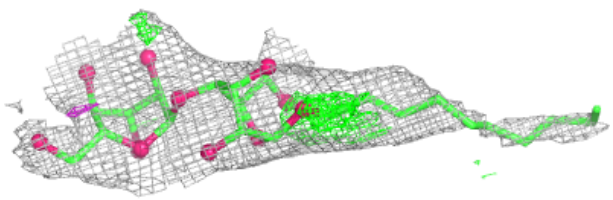


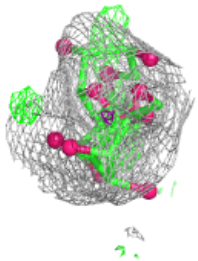


Electron density around DMU A 503:

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

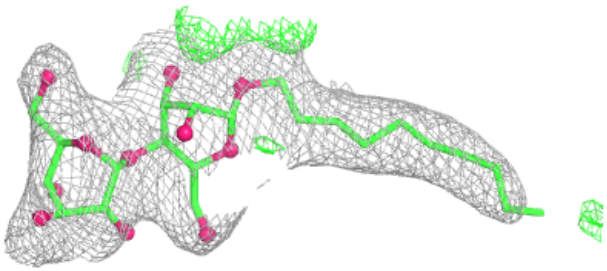


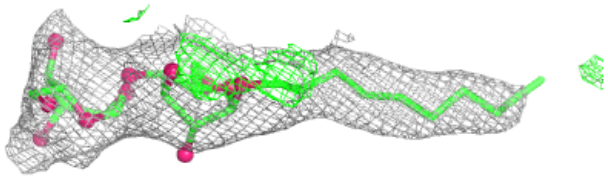


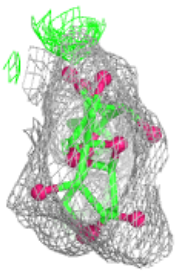


Electron density around DMU B 505:

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

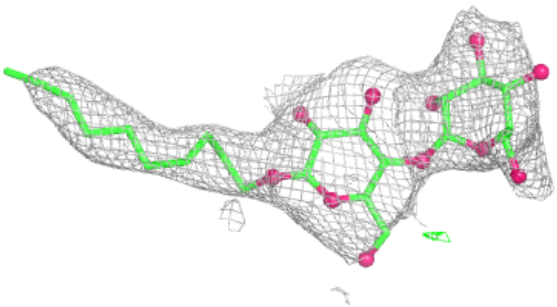


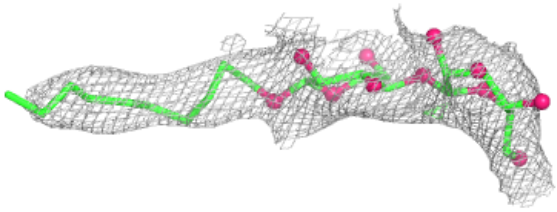


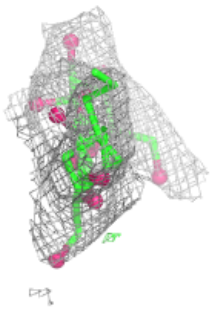


Electron density around DMU A 506:

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

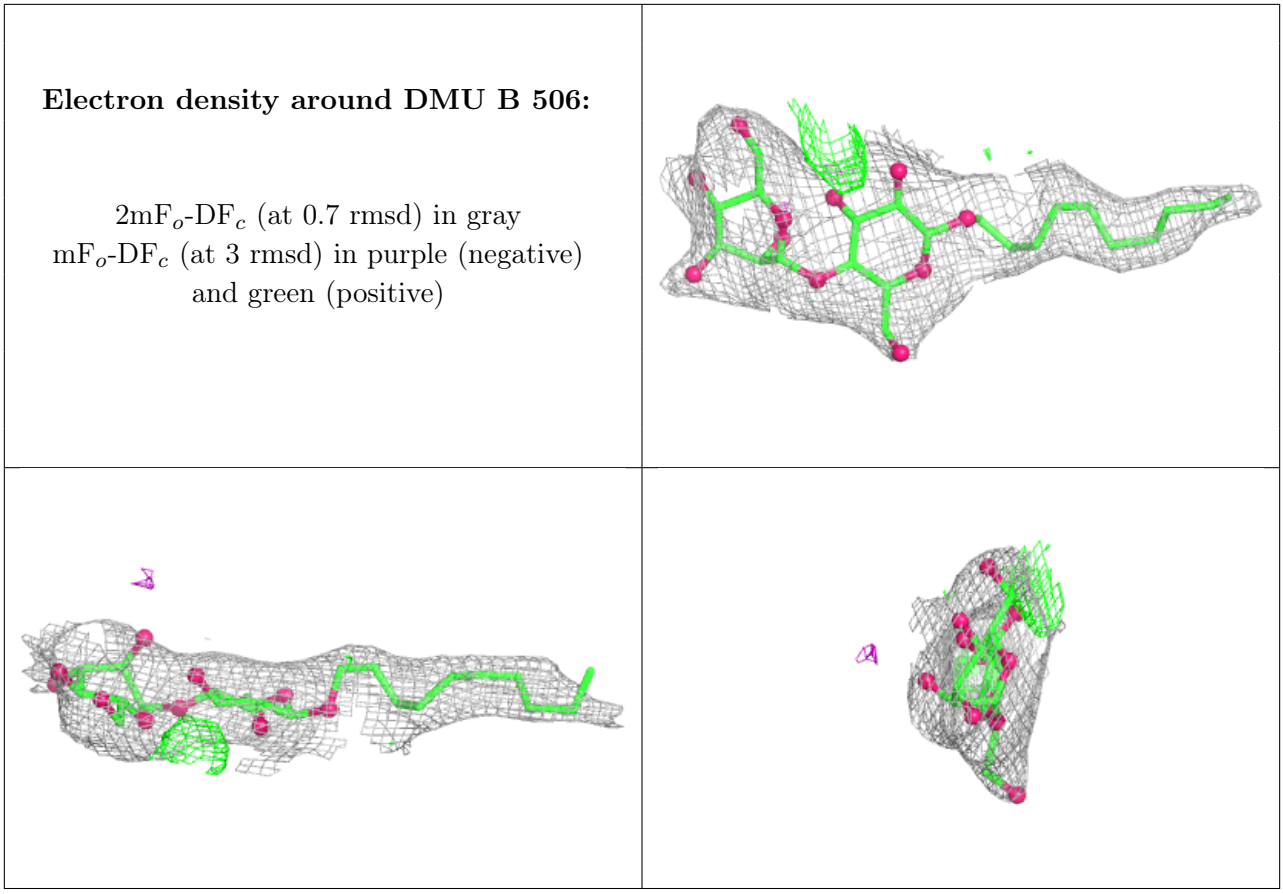






Electron density around DMU B 506:

$2mF_o$-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.