Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 08:28 AM EDT

PDB ID	:	5N9Z
Title	:	Rubisco from Thalassiosira hyalina
Authors	:	Andersson, I.; Valegard, K.
Deposited on	:	2017-02-27
Resolution	:	1.90 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

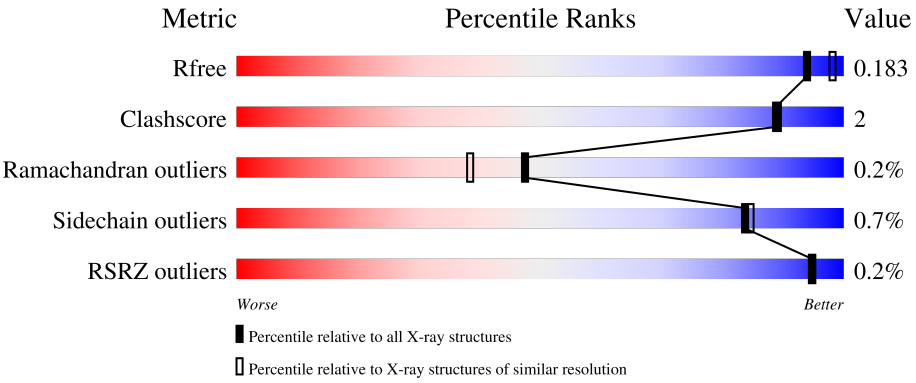
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	490	92% 6% ·
1	B	490	92% 6% ·
1	C	490	92% 6% ·
1	D	490	91% 7% ·
1	E	490	92% 6% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	490	91% 7%
1	G	490	92% 6%
1	H	490	92% 6%
2	I	139	95% 5%
2	J	139	94% 6%
2	K	139	94% 6%
2	L	139	97%
2	M	139	99%
2	N	139	94% 6%
2	O	139	97%
2	P	139	95% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	HLU	A	174	-	X	-	-
1	HLU	B	174	-	X	-	-
1	HLU	C	174	-	X	-	-
1	HLU	D	174	-	X	-	-
1	HLU	E	174	-	X	-	-
1	HLU	F	174	-	X	-	-
1	HLU	G	174	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 42506 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 Ribulose bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	1	0
			3764	2389	647	707	21			
1	H	481	Total	C	N	O	S	0	1	0
			3764	2389	647	707	21			
1	F	481	Total	C	N	O	S	0	1	0
			3764	2389	647	707	21			
1	D	481	Total	C	N	O	S	0	1	0
			3764	2389	647	707	21			
1	B	481	Total	C	N	O	S	0	1	0
			3764	2389	647	707	21			
1	C	481	Total	C	N	O	S	0	1	0
			3764	2389	647	707	21			
1	E	481	Total	C	N	O	S	0	1	0
			3764	2389	647	707	21			
1	G	481	Total	C	N	O	S	0	1	0
			3764	2389	647	707	21			

- Molecule 2 is a protein called Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	139	Total	C	N	O	S	0	1	0
			1130	714	193	215	8			
2	O	139	Total	C	N	O	S	0	0	0
			1122	710	191	213	8			
2	N	139	Total	C	N	O	S	0	1	0
			1130	714	193	215	8			
2	M	139	Total	C	N	O	S	0	1	0
			1130	714	193	215	8			
2	P	139	Total	C	N	O	S	0	1	0
			1130	714	193	215	8			
2	J	139	Total	C	N	O	S	0	1	0
			1130	714	193	215	8			

Continued on next page...

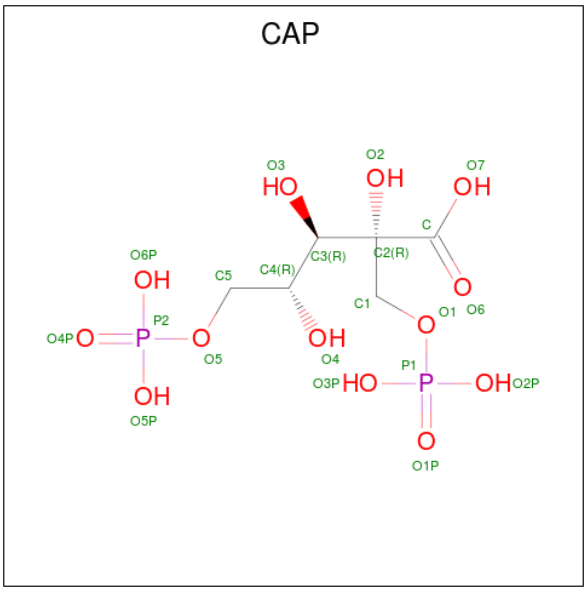
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	139	Total	C	N	O	S	0	1	0
			1130	714	193	215	8			
2	L	139	Total	C	N	O	S	0	1	0
			1130	714	193	215	8			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

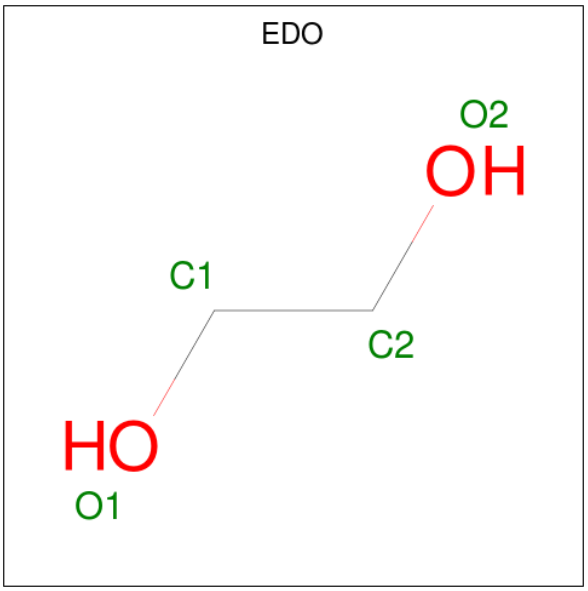
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	H	1	Total	C	O	P	0	0
			21	6	13	2		
4	F	1	Total	C	O	P	0	0
			21	6	13	2		
4	D	1	Total	C	O	P	0	0
			21	6	13	2		
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	C	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	G	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	267	Total O 267 267	0	0
6	I	93	Total O 93 93	0	0
6	H	298	Total O 298 298	0	0
6	O	103	Total O 103 103	0	0
6	F	297	Total O 297 297	0	0
6	N	97	Total O 97 97	0	0
6	D	295	Total O 295 295	0	0
6	M	101	Total O 101 101	0	0
6	B	261	Total O 261 261	0	0
6	P	93	Total O 93 93	0	0
6	C	298	Total O 298 298	0	0
6	J	96	Total O 96 96	0	0
6	E	311	Total O 311 311	0	0
6	K	95	Total O 95 95	0	0

Continued on next page...

Continued from previous page...

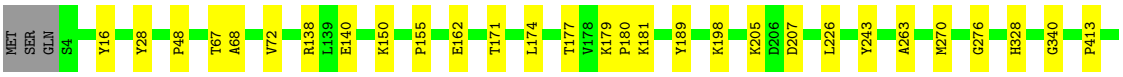
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	307	Total O 307 307	0	0
6	L	96	Total O 96 96	0	0

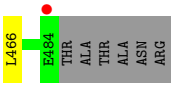
3 Residue-property plots (i)

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: Ribulose bisphosphate carboxylase large chain

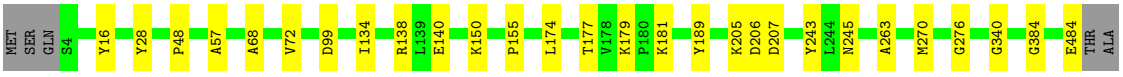
Chain A:





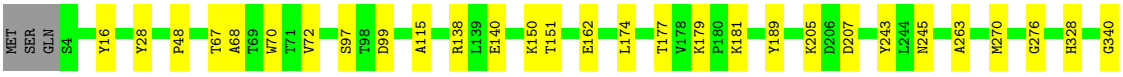
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain H:



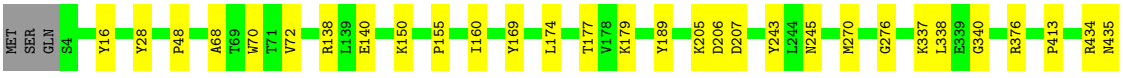
• Molecule 1: Ribulose bisphosphate carboxylase large chain

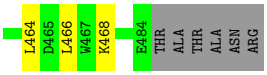
Chain F:



• Molecule 1: Ribulose bisphosphate carboxylase large chain

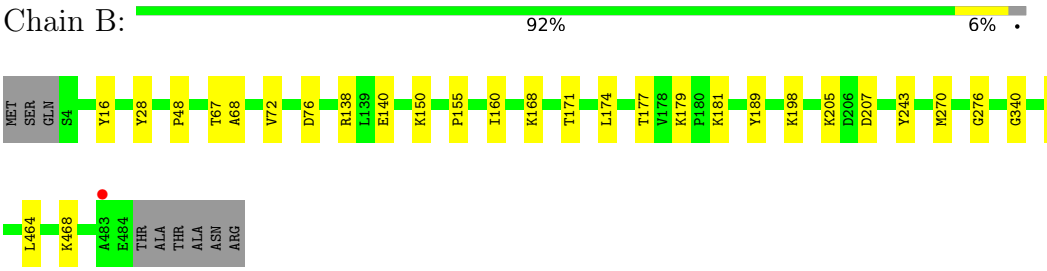
Chain D:





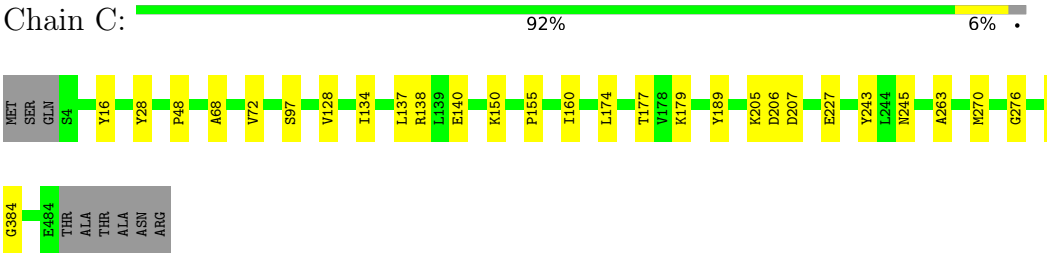
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain B:



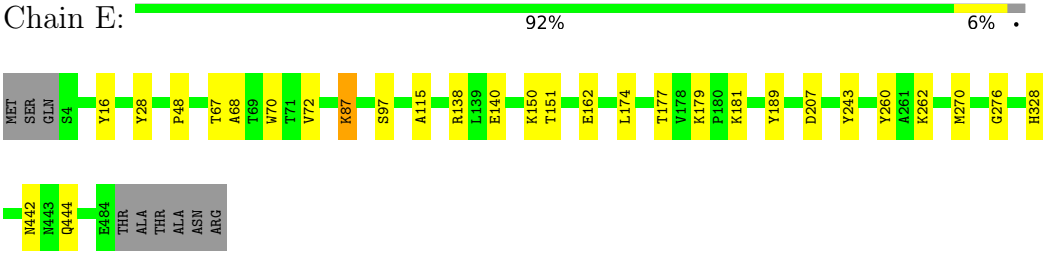
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain C:



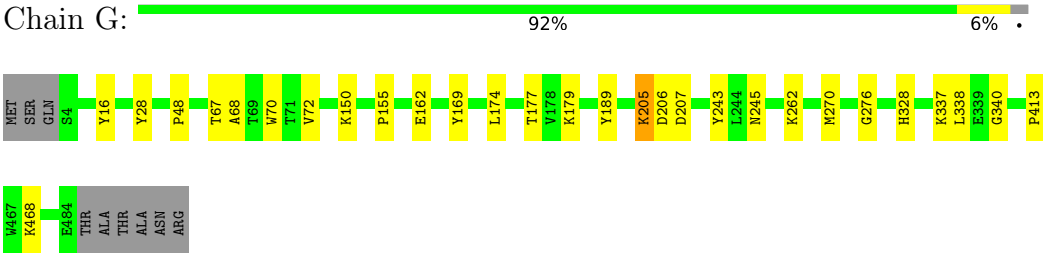
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E:



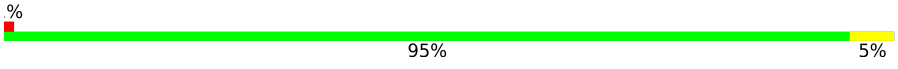
• Molecule 1: Ribulose bisphosphate carboxylase large chain

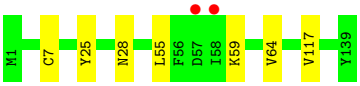
Chain G:



• Molecule 2: Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

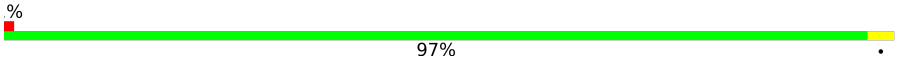
Chain I:

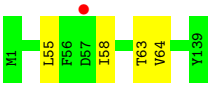




• Molecule 2: Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

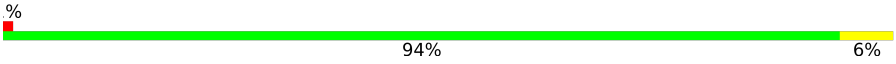
Chain O:

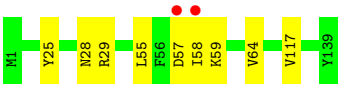




• Molecule 2: Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

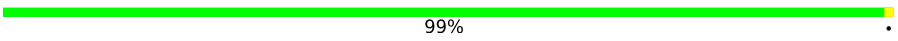
Chain N:





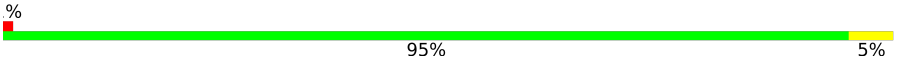
• Molecule 2: Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

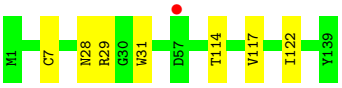
Chain M:



• Molecule 2: Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

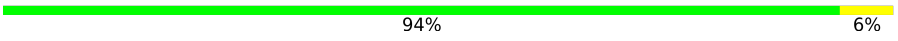
Chain P:

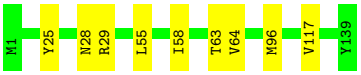




• Molecule 2: Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

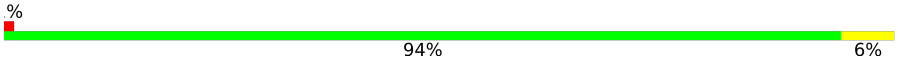
Chain J:

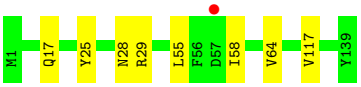




• Molecule 2: Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

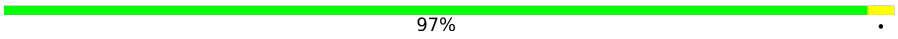
Chain K:





• Molecule 2: Ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.99Å 219.99Å 124.27Å 90.00° 118.34° 90.00°	Depositor
Resolution (Å)	62.03 – 1.90 97.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (62.03-1.90) 99.0 (97.94-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.150 , 0.182 0.152 , 0.183	Depositor DCC
R_{free} test set	21717 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 26.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	42506	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.08% 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: MG, 8RE, HLU, CAP, CSO, KCX, M3L, HYP, LYO, EDO

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	0.36	0/3763	0.55	0/5094
1	B	0.36	0/3763	0.55	0/5094
1	C	0.37	0/3763	0.55	0/5094
1	D	0.38	0/3763	0.57	0/5094
1	E	0.38	0/3763	0.55	0/5094
1	F	0.38	0/3763	0.56	0/5094
1	G	0.38	0/3763	0.57	0/5094
1	H	0.38	0/3763	0.55	0/5094
2	I	0.36	0/1161	0.51	0/1576
2	J	0.39	0/1161	0.53	0/1576
2	K	0.36	0/1161	0.52	0/1576
2	L	0.38	0/1161	0.52	0/1576
2	M	0.36	0/1161	0.52	0/1576
2	N	0.36	0/1161	0.52	0/1576
2	O	0.37	0/1153	0.52	0/1565
2	P	0.37	0/1161	0.53	0/1576
All	All	0.37	0/39384	0.55	0/53349

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3764	0	3688	14	0
1	B	3764	0	3688	15	0
1	C	3764	0	3688	16	0
1	D	3764	0	3688	14	0
1	E	3764	0	3688	18	0
1	F	3764	0	3688	18	0
1	G	3764	0	3688	15	0
1	H	3764	0	3688	15	0
2	I	1130	0	1061	7	0
2	J	1130	0	1061	7	0
2	K	1130	0	1061	6	0
2	L	1130	0	1061	3	0
2	M	1130	0	1061	2	0
2	N	1130	0	1061	7	0
2	O	1122	0	1056	3	0
2	P	1130	0	1061	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	N	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	8	0	0
4	C	21	0	7	0	0
4	D	21	0	8	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	7	0	0
4	H	21	0	7	0	0
5	A	4	0	6	0	0
5	I	12	0	18	1	0
5	J	8	0	12	0	0
5	K	16	0	24	2	0
5	L	4	0	6	0	0
5	M	12	0	18	0	0
5	N	4	0	6	0	0
5	O	12	0	18	0	0
5	P	4	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	267	0	0	1	0
6	B	261	0	0	1	0
6	C	298	0	0	1	0
6	D	295	0	0	1	0
6	E	311	0	0	2	0
6	F	297	0	0	2	0
6	G	307	0	0	1	0
6	H	298	0	0	3	0
6	I	93	0	0	0	0
6	J	96	0	0	1	0
6	K	95	0	0	1	0
6	L	96	0	0	0	0
6	M	101	0	0	0	0
6	N	97	0	0	1	0
6	O	103	0	0	0	0
6	P	93	0	0	0	0
All	All	42506	0	38159	144	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 2.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:25:TYR:O	2:N:28:ASN:OD1	1.74	1.03
1:A:276:GLY:HA3	1:B:276:GLY:HA3	1.59	0.83
1:H:276:GLY:HA3	1:G:276:GLY:HA3	1.62	0.81
1:C:160:ILE:HD11	1:C:376:ARG:HH11	1.47	0.78
1:D:276:GLY:HA3	1:C:276:GLY:HA3	1.64	0.78
2:J:25:TYR:O	2:J:28:ASN:OD1	2.04	0.75
2:I:25:TYR:O	2:I:28:ASN:ND2	2.20	0.74
1:F:276:GLY:HA3	1:E:276:GLY:HA3	1.72	0.71
2:P:28:ASN:OD1	2:P:29:ARG:HG2	1.91	0.69
2:O:55:LEU:HB3	2:O:58:ILE:HG13	1.79	0.65
1:E:260:TYR:CE1	5:K:203:EDO:H11	2.35	0.62
1:H:263:ALA:HA	2:N:117:VAL:HG12	1.83	0.61
1:C:134:ILE:HD12	1:C:137:LEU:HB2	1.82	0.61
2:O:58:ILE:HD12	2:O:63:THR:HG21	1.82	0.59
2:I:25:TYR:HA	2:I:28:ASN:ND2	2.18	0.59
2:J:58:ILE:HD12	2:J:63:THR:HG21	1.86	0.58
1:C:160:ILE:HD11	1:C:376:ARG:NH1	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:ALA:HB1	1:H:134:ILE:HD11	1.84	0.57
2:P:28:ASN:OD1	2:P:29:ARG:N	2.37	0.57
2:N:57:ASP:O	2:N:59:LYS:NZ	2.38	0.57
1:B:171:THR:HG23	2:P:7:CYS:HB2	1.88	0.56
1:F:243:TYR:HB3	1:F:270:MET:HB3	1.87	0.56
2:K:55:LEU:HD12	2:K:64:VAL:HG22	1.87	0.56
1:B:168:LYS:NZ	6:B:601:HOH:O	2.38	0.55
6:E:900:HOH:O	2:L:117:VAL:HG21	2.06	0.55
1:H:99:ASP:HB3	6:H:670:HOH:O	2.07	0.55
2:K:25:TYR:O	2:K:28:ASN:OD1	2.24	0.55
1:B:16:TYR:HA	1:B:72:VAL:HG11	1.90	0.54
2:N:117:VAL:HG22	6:N:379:HOH:O	2.08	0.54
1:E:243:TYR:HB3	1:E:270:MET:HB3	1.90	0.54
1:H:484:GLU:OE2	6:H:601:HOH:O	2.18	0.54
1:E:87:LYS:NZ	6:E:602:HOH:O	2.40	0.53
1:B:28:TYR:CZ	1:B:68:ALA:HB2	2.43	0.53
1:F:28:TYR:CZ	1:F:68:ALA:HB2	2.44	0.53
1:C:28:TYR:CZ	1:C:68:ALA:HB2	2.44	0.53
1:E:28:TYR:CZ	1:E:68:ALA:HB2	2.43	0.53
1:E:138:ARG:HD3	1:E:140:GLU:OE2	2.09	0.52
1:B:464:LEU:O	1:B:468:LYS:HB3	2.09	0.52
6:H:896:HOH:O	2:N:117:VAL:HG11	2.09	0.52
2:J:55:LEU:HB3	2:J:58:ILE:HG13	1.90	0.52
1:H:28:TYR:CZ	1:H:68:ALA:HB2	2.45	0.51
1:A:243:TYR:HB3	1:A:270:MET:HB3	1.92	0.51
1:D:28:TYR:CZ	1:D:68:ALA:HB2	2.45	0.51
1:B:243:TYR:HB3	1:B:270:MET:HB3	1.91	0.51
1:H:16:TYR:HA	1:H:72:VAL:HG11	1.92	0.51
1:A:181:LYS:HB2	1:B:67:THR:HA	1.93	0.50
1:A:28:TYR:CZ	1:A:68:ALA:HB2	2.47	0.50
1:A:16:TYR:HA	1:A:72:VAL:HG11	1.92	0.50
2:I:117:VAL:HG21	6:G:889:HOH:O	2.11	0.50
1:F:138:ARG:HD3	1:F:140:GLU:OE2	2.11	0.50
1:A:67:THR:HA	1:B:181:LYS:HB2	1.93	0.50
1:A:171:THR:HG23	2:I:7:CYS:HB2	1.92	0.50
6:C:895:HOH:O	2:K:117:VAL:HG11	2.11	0.50
2:I:25:TYR:HA	2:I:28:ASN:HD22	1.76	0.50
1:E:442:ASN:OD1	1:E:444:GLN:HG2	2.11	0.50
1:G:28:TYR:CE1	1:G:68:ALA:HB2	2.47	0.50
1:E:262:LYS:HE2	2:L:117:VAL:HG22	1.94	0.50
1:G:28:TYR:CZ	1:G:68:ALA:HB2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:TYR:CE1	1:D:68:ALA:HB2	2.47	0.50
1:D:16:TYR:HA	1:D:72:VAL:HG11	1.93	0.49
2:O:55:LEU:HD12	2:O:64:VAL:HG22	1.95	0.49
1:C:16:TYR:HA	1:C:72:VAL:HG11	1.94	0.49
1:E:16:TYR:HA	1:E:72:VAL:HG11	1.95	0.49
2:I:117:VAL:HG22	1:G:262:LYS:HE2	1.94	0.48
1:B:28:TYR:CE1	1:B:68:ALA:HB2	2.48	0.48
1:E:260:TYR:CD1	5:K:203:EDO:H11	2.48	0.48
1:G:16:TYR:HA	1:G:72:VAL:HG11	1.94	0.48
1:F:442:ASN:OD1	1:F:444:GLN:HG2	2.14	0.48
1:H:138:ARG:HD3	1:H:140:GLU:OE2	2.14	0.47
6:D:891:HOH:O	2:P:117:VAL:HG11	2.13	0.47
2:J:55:LEU:HD12	2:J:64:VAL:HG22	1.95	0.47
1:H:243:TYR:HB3	1:H:270:MET:HB3	1.96	0.47
1:B:138:ARG:HD3	1:B:140:GLU:OE2	2.15	0.47
1:A:28:TYR:CE1	1:A:68:ALA:HB2	2.49	0.47
1:C:243:TYR:HB3	1:C:270:MET:HB3	1.97	0.47
2:P:29:ARG:HD3	2:P:31:TRP:CZ2	2.49	0.47
1:F:99:ASP:HB3	6:F:622:HOH:O	2.14	0.46
1:C:128:VAL:O	1:C:134:ILE:HD11	2.14	0.46
1:G:337:LYS:HG3	1:G:338:LEU:HD22	1.97	0.46
1:H:28:TYR:CE1	1:H:68:ALA:HB2	2.51	0.46
1:F:70:TRP:CD1	1:E:384:GLY:HA2	2.50	0.46
1:F:263:ALA:HA	2:M:117:VAL:HG12	1.98	0.46
1:H:384:GLY:HA2	1:G:70:TRP:CD1	2.50	0.46
1:D:243:TYR:HB3	1:D:270:MET:HB3	1.97	0.46
6:A:865:HOH:O	2:J:117:VAL:HG11	2.16	0.46
1:F:384:GLY:HA2	1:E:70:TRP:CD1	2.51	0.46
1:F:452:ASP:O	1:F:455:LYS:HG3	2.16	0.45
5:I:204:EDO:H21	1:C:227:GLU:HB2	1.99	0.45
1:E:177:THR:HB	1:E:179:LYS:HE2	1.99	0.45
1:C:263:ALA:HA	2:K:117:VAL:HG12	1.99	0.45
1:F:28:TYR:CE1	1:F:68:ALA:HB2	2.51	0.45
1:D:337:LYS:HG3	1:D:338:LEU:HD22	1.98	0.45
1:C:28:TYR:CE1	1:C:68:ALA:HB2	2.52	0.45
1:C:138:ARG:HD3	1:C:140:GLU:OE2	2.17	0.45
1:F:16:TYR:HA	1:F:72:VAL:HG11	1.99	0.45
2:K:117:VAL:HG22	6:K:382:HOH:O	2.16	0.45
1:E:28:TYR:CE1	1:E:68:ALA:HB2	2.51	0.45
1:A:177:THR:HB	1:A:179:LYS:HE2	1.99	0.44
1:F:67:THR:HA	1:E:181:LYS:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:LYS:HB2	1:E:67:THR:HA	2.00	0.44
1:B:177:THR:HB	1:B:179:LYS:HE2	1.99	0.44
1:A:263:ALA:HA	2:J:117:VAL:HG12	1.97	0.44
1:H:181:LYS:HB2	1:G:67:THR:HA	2.00	0.44
1:G:243:TYR:HB3	1:G:270:MET:HB3	1.98	0.44
6:F:892:HOH:O	2:M:117:VAL:HG11	2.17	0.43
1:F:162:GLU:CD	1:F:328:HIS:HE2	2.19	0.43
1:A:138:ARG:HD3	1:A:140:GLU:OE2	2.19	0.43
1:B:160:ILE:HD11	1:B:376:ARG:NH1	2.33	0.43
1:C:206:ASP:HB2	1:C:245:ASN:HB2	2.01	0.43
1:D:177:THR:HB	1:D:179:LYS:HE2	2.00	0.43
1:A:162:GLU:CD	1:A:328:HIS:HE2	2.21	0.43
1:H:57:ALA:HB1	1:H:134:ILE:CD1	2.49	0.42
2:N:55:LEU:HD12	2:N:64:VAL:HG22	2.01	0.42
1:H:177:THR:HB	1:H:179:LYS:HE2	2.00	0.42
1:D:464:LEU:O	1:D:468:LYS:HB3	2.20	0.42
2:L:114:THR:HB	2:L:122:ILE:HB	2.01	0.42
1:D:160:ILE:HD11	1:D:376:ARG:NH1	2.34	0.42
1:F:245:ASN:HA	1:F:270:MET:HG2	2.02	0.42
1:C:160:ILE:HD13	6:J:354:HOH:O	2.20	0.42
2:P:114:THR:HB	2:P:122:ILE:HB	2.02	0.42
1:G:177:THR:HB	1:G:179:LYS:HE2	2.02	0.42
1:A:180:PRO:HB3	1:B:76:ASP:OD1	2.20	0.41
1:E:115:ALA:HB2	1:E:151:THR:O	2.20	0.41
1:D:413:PRO:HD3	1:D:466:LEU:HD22	2.02	0.41
1:G:464:LEU:O	1:G:468:LYS:HB2	2.19	0.41
1:D:138:ARG:HD3	1:D:140:GLU:OE2	2.20	0.41
2:K:55:LEU:HB3	2:K:58:ILE:HG13	2.02	0.41
2:N:55:LEU:HB3	2:N:58:ILE:HD13	2.03	0.41
1:G:162:GLU:CD	1:G:328:HIS:HE2	2.22	0.41
1:G:413:PRO:HD3	1:G:466:LEU:HD22	2.01	0.41
1:F:177:THR:HB	1:F:179:LYS:HE2	2.02	0.41
1:D:206:ASP:HB2	1:D:245:ASN:HB2	2.03	0.41
1:C:177:THR:HB	1:C:179:LYS:HE2	2.03	0.41
1:H:206:ASP:HB2	1:H:245:ASN:HB2	2.03	0.41
1:F:115:ALA:HB2	1:F:151:THR:O	2.20	0.41
1:D:434:ARG:HD2	1:D:435:ASN:OD1	2.21	0.41
1:D:70:TRP:CD1	1:C:384:GLY:HA2	2.55	0.40
1:G:205:KCX:HB2	1:G:243:TYR:CD1	2.55	0.40
1:A:413:PRO:HD3	1:A:466:LEU:HD22	2.04	0.40
1:G:206:ASP:HB2	1:G:245:ASN:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ARG:HD2	1:B:435:ASN:OD1	2.21	0.40
2:J:29:ARG:HA	2:J:29:ARG:HD3	1.96	0.40
2:I:55:LEU:HD12	2:I:64:VAL:HG22	2.03	0.40
1:E:162:GLU:CD	1:E:328:HIS:HE2	2.21	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	472/490 (96%)	461 (98%)	10 (2%)	1 (0%)	47	38
1	B	472/490 (96%)	460 (98%)	11 (2%)	1 (0%)	47	38
1	C	472/490 (96%)	460 (98%)	11 (2%)	1 (0%)	47	38
1	D	472/490 (96%)	461 (98%)	10 (2%)	1 (0%)	47	38
1	E	472/490 (96%)	460 (98%)	11 (2%)	1 (0%)	47	38
1	F	472/490 (96%)	459 (97%)	12 (2%)	1 (0%)	47	38
1	G	472/490 (96%)	458 (97%)	13 (3%)	1 (0%)	47	38
1	H	472/490 (96%)	460 (98%)	11 (2%)	1 (0%)	47	38
2	I	138/139 (99%)	137 (99%)	1 (1%)	0	100	100
2	J	138/139 (99%)	136 (99%)	2 (1%)	0	100	100
2	K	138/139 (99%)	137 (99%)	1 (1%)	0	100	100
2	L	138/139 (99%)	136 (99%)	1 (1%)	1 (1%)	22	12
2	M	138/139 (99%)	136 (99%)	2 (1%)	0	100	100
2	N	138/139 (99%)	137 (99%)	1 (1%)	0	100	100
2	O	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	P	138/139 (99%)	137 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4879/5032 (97%)	4771 (98%)	99 (2%)	9 (0%)	47 38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	57	ASP
1	A	340	GLY
1	H	340	GLY
1	F	340	GLY
1	C	340	GLY
1	B	340	GLY
1	E	340	GLY
1	D	340	GLY
1	G	340	GLY

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	382/388 (98%)	378 (99%)	4 (1%)	76 76
1	B	382/388 (98%)	380 (100%)	2 (0%)	88 89
1	C	382/388 (98%)	379 (99%)	3 (1%)	81 82
1	D	382/388 (98%)	379 (99%)	3 (1%)	81 82
1	E	382/388 (98%)	378 (99%)	4 (1%)	76 76
1	F	382/388 (98%)	379 (99%)	3 (1%)	81 82
1	G	382/388 (98%)	379 (99%)	3 (1%)	81 82
1	H	382/388 (98%)	380 (100%)	2 (0%)	88 89
2	I	120/120 (100%)	119 (99%)	1 (1%)	81 82
2	J	120/120 (100%)	119 (99%)	1 (1%)	81 82
2	K	120/120 (100%)	118 (98%)	2 (2%)	60 57
2	L	120/120 (100%)	120 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	M	120/120 (100%)	120 (100%)	0	100 100
2	N	120/120 (100%)	119 (99%)	1 (1%)	81 82
2	O	119/120 (99%)	119 (100%)	0	100 100
2	P	120/120 (100%)	120 (100%)	0	100 100
All	All	4015/4064 (99%)	3986 (99%)	29 (1%)	84 84

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	TYR
1	A	207	ASP
1	A	226[A]	LEU
1	A	226[B]	LEU
2	I	59	LYS
1	H	189	TYR
1	H	207	ASP
1	F	97	SER
1	F	189	TYR
1	F	207	ASP
2	N	29	ARG
1	D	169	TYR
1	D	189	TYR
1	D	207	ASP
1	B	189	TYR
1	B	207	ASP
1	C	97	SER
1	C	189	TYR
1	C	207	ASP
2	J	96	MET
1	E	87	LYS
1	E	97	SER
1	E	189	TYR
1	E	207	ASP
2	K	17	GLN
2	K	29	ARG
1	G	169	TYR
1	G	189	TYR
1	G	207	ASP

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

Mol	Chain	Res	Type
2	I	28	ASN
2	N	28	ASN
2	J	28	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

64 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	HYP	B	155	1	6,8,9	0.57	0	5,10,12	1.41	1 (20%)
1	HYP	F	155	1	6,8,9	0.61	0	5,10,12	1.21	0
1	HYP	D	155	1	6,8,9	0.73	0	5,10,12	1.78	2 (40%)
1	HYP	C	48	1	6,8,9	0.68	0	5,10,12	2.14	2 (40%)
1	HYP	A	155	1	6,8,9	0.59	0	5,10,12	1.51	1 (20%)
1	CSO	F	109	1	3,6,7	0.70	0	0,6,8	-	-
1	CSO	A	109	1	3,6,7	0.78	0	0,6,8	-	-
1	CSO	B	109	1	3,6,7	0.73	0	0,6,8	-	-
1	HLU	E	174	1	7,8,9	0.71	0	7,10,12	2.59	4 (57%)
1	8RE	D	150	1	9,10,11	0.62	0	6,12,14	2.15	2 (33%)
1	HYP	H	155	1	6,8,9	0.77	0	5,10,12	1.49	2 (40%)
1	HYP	G	155	1	6,8,9	0.74	0	5,10,12	1.57	2 (40%)
1	M3L	H	346	1	10,11,12	0.51	0	9,14,16	0.48	0
1	HYP	D	48	1	6,8,9	0.75	0	5,10,12	2.06	2 (40%)
1	KCX	D	205	3,1	9,11,12	1.09	1 (11%)	5,12,14	1.72	1 (20%)
1	LYO	E	198	1	7,9,10	0.36	0	6,10,12	0.76	0
1	M3L	A	346	1	10,11,12	0.54	0	9,14,16	0.38	0
1	KCX	A	205	3,1	9,11,12	1.02	1 (11%)	5,12,14	1.67	1 (20%)
1	M3L	F	346	1	10,11,12	0.51	0	9,14,16	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HLU	A	174	1	7,8,9	0.77	0	7,10,12	2.53	4 (57%)
1	KCX	F	205	3,1	9,11,12	0.93	0	5,12,14	0.99	1 (20%)
1	CSO	D	109	1	3,6,7	0.79	0	0,6,8	-	-
1	M3L	B	346	1	10,11,12	0.50	0	9,14,16	0.38	0
1	HYP	E	48	1	6,8,9	0.70	0	5,10,12	1.70	1 (20%)
1	HYP	F	48	1	6,8,9	0.68	0	5,10,12	1.82	1 (20%)
1	M3L	G	346	1	10,11,12	0.55	0	9,14,16	0.51	0
1	KCX	G	205	3,1	9,11,12	1.12	2 (22%)	5,12,14	1.70	1 (20%)
1	CSO	C	109	1	3,6,7	0.82	0	0,6,8	-	-
1	8RE	B	150	1	9,10,11	0.55	0	6,12,14	2.11	2 (33%)
1	8RE	G	150	1	9,10,11	0.64	0	6,12,14	2.14	2 (33%)
1	LYO	H	198	1	7,9,10	0.36	0	6,10,12	0.90	0
1	HYP	A	48	1	6,8,9	0.76	0	5,10,12	2.02	2 (40%)
1	KCX	H	205	3,1	9,11,12	1.00	1 (11%)	5,12,14	1.04	1 (20%)
1	CSO	H	109	1	3,6,7	0.84	0	0,6,8	-	-
1	CSO	E	109	1	3,6,7	0.72	0	0,6,8	-	-
1	8RE	F	150	1	9,10,11	0.73	0	6,12,14	2.45	3 (50%)
1	HLU	D	174	1	7,8,9	0.85	0	7,10,12	2.16	4 (57%)
1	CSO	G	109	1	3,6,7	0.81	0	0,6,8	-	-
1	HLU	H	174	1	7,8,9	0.77	0	7,10,12	2.10	3 (42%)
1	KCX	C	205	3,1	9,11,12	1.03	0	5,12,14	0.96	1 (20%)
1	M3L	D	346	1	10,11,12	0.54	0	9,14,16	0.48	0
1	HLU	B	174	1	7,8,9	0.79	0	7,10,12	2.23	4 (57%)
1	HYP	E	155	1	6,8,9	0.57	0	5,10,12	1.20	0
1	KCX	E	205	3,1	9,11,12	0.95	0	5,12,14	0.93	0
1	M3L	E	346	1	10,11,12	0.52	0	9,14,16	0.57	0
1	8RE	C	150	1	9,10,11	0.65	0	6,12,14	2.12	2 (33%)
1	LYO	C	198	1	7,9,10	0.37	0	6,10,12	0.93	0
1	8RE	E	150	1	9,10,11	0.71	0	6,12,14	2.33	2 (33%)
1	HLU	G	174	1	7,8,9	0.85	0	7,10,12	2.32	4 (57%)
1	LYO	F	198	1	7,9,10	0.39	0	6,10,12	0.71	0
1	LYO	D	198	1	7,9,10	0.37	0	6,10,12	0.97	0
1	HLU	F	174	1	7,8,9	0.73	0	7,10,12	2.73	6 (85%)
1	LYO	A	198	1	7,9,10	0.48	0	6,10,12	1.64	1 (16%)
1	LYO	B	198	1	7,9,10	0.45	0	6,10,12	1.38	1 (16%)
1	KCX	B	205	3,1	9,11,12	0.99	1 (11%)	5,12,14	1.80	1 (20%)
1	HYP	H	48	1	6,8,9	0.67	0	5,10,12	2.09	2 (40%)
1	HYP	C	155	1	6,8,9	0.80	0	5,10,12	1.52	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HLU	C	174	1	7,8,9	0.78	0	7,10,12	2.20	4 (57%)
1	8RE	A	150	1	9,10,11	0.52	0	6,12,14	2.15	2 (33%)
1	HYP	B	48	1	6,8,9	0.78	0	5,10,12	2.07	2 (40%)
1	8RE	H	150	1	9,10,11	0.68	0	6,12,14	2.14	2 (33%)
1	LYO	G	198	1	7,9,10	0.40	0	6,10,12	0.90	0
1	HYP	G	48	1	6,8,9	0.68	0	5,10,12	2.06	2 (40%)
1	M3L	C	346	1	10,11,12	0.53	0	9,14,16	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	155	1	-	0/0/11/13	0/1/1/1
1	HYP	F	155	1	-	0/0/11/13	0/1/1/1
1	HYP	D	155	1	-	0/0/11/13	0/1/1/1
1	HYP	C	48	1	-	0/0/11/13	0/1/1/1
1	HYP	A	155	1	-	0/0/11/13	0/1/1/1
1	CSO	F	109	1	-	0/1/5/7	-
1	CSO	A	109	1	-	0/1/5/7	-
1	CSO	B	109	1	-	0/1/5/7	-
1	HLU	E	174	1	-	8/9/10/12	-
1	8RE	D	150	1	-	9/12/13/15	-
1	HYP	H	155	1	-	0/0/11/13	0/1/1/1
1	HYP	G	155	1	-	0/0/11/13	0/1/1/1
1	M3L	H	346	1	-	2/9/10/12	-
1	HYP	D	48	1	-	0/0/11/13	0/1/1/1
1	KCX	D	205	3,1	-	0/9/10/12	-
1	LYO	E	198	1	-	1/8/9/11	-
1	M3L	A	346	1	-	2/9/10/12	-
1	KCX	A	205	3,1	-	0/9/10/12	-
1	M3L	F	346	1	-	2/9/10/12	-
1	HLU	A	174	1	-	8/9/10/12	-
1	KCX	F	205	3,1	-	0/9/10/12	-
1	CSO	D	109	1	-	0/1/5/7	-
1	M3L	B	346	1	-	2/9/10/12	-
1	HYP	E	48	1	-	0/0/11/13	0/1/1/1
1	HYP	F	48	1	-	0/0/11/13	0/1/1/1
1	M3L	G	346	1	-	2/9/10/12	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	G	205	3,1	-	0/9/10/12	-
1	CSO	C	109	1	-	0/1/5/7	-
1	8RE	B	150	1	-	9/12/13/15	-
1	8RE	G	150	1	-	9/12/13/15	-
1	LYO	H	198	1	-	1/8/9/11	-
1	HYP	A	48	1	-	0/0/11/13	0/1/1/1
1	KCX	H	205	3,1	-	0/9/10/12	-
1	CSO	H	109	1	-	0/1/5/7	-
1	CSO	E	109	1	-	0/1/5/7	-
1	8RE	F	150	1	-	9/12/13/15	-
1	HLU	D	174	1	-	8/9/10/12	-
1	CSO	G	109	1	-	0/1/5/7	-
1	HLU	H	174	1	-	8/9/10/12	-
1	KCX	C	205	3,1	-	0/9/10/12	-
1	M3L	D	346	1	-	1/9/10/12	-
1	HLU	B	174	1	-	8/9/10/12	-
1	HYP	E	155	1	-	0/0/11/13	0/1/1/1
1	KCX	E	205	3,1	-	0/9/10/12	-
1	M3L	E	346	1	-	1/9/10/12	-
1	8RE	C	150	1	-	9/12/13/15	-
1	LYO	C	198	1	-	1/8/9/11	-
1	8RE	E	150	1	-	9/12/13/15	-
1	HLU	G	174	1	-	8/9/10/12	-
1	LYO	F	198	1	-	1/8/9/11	-
1	LYO	D	198	1	-	1/8/9/11	-
1	HLU	F	174	1	-	8/9/10/12	-
1	LYO	A	198	1	-	2/8/9/11	-
1	LYO	B	198	1	-	2/8/9/11	-
1	KCX	B	205	3,1	-	0/9/10/12	-
1	HYP	H	48	1	-	0/0/11/13	0/1/1/1
1	HYP	C	155	1	-	0/0/11/13	0/1/1/1
1	HLU	C	174	1	-	8/9/10/12	-
1	8RE	A	150	1	-	9/12/13/15	-
1	HYP	B	48	1	-	0/0/11/13	0/1/1/1
1	8RE	H	150	1	-	9/12/13/15	-
1	LYO	G	198	1	-	1/8/9/11	-
1	HYP	G	48	1	-	0/0/11/13	0/1/1/1
1	M3L	C	346	1	-	1/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	KCX	CE-NZ	2.29	1.51	1.46
1	A	205	KCX	CE-NZ	2.13	1.51	1.46
1	G	205	KCX	CE-NZ	2.06	1.50	1.46
1	H	205	KCX	OQ1-CX	2.04	1.25	1.21
1	D	205	KCX	OQ1-CX	2.01	1.25	1.21
1	G	205	KCX	OQ1-CX	2.00	1.25	1.21

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	174	HLU	OH-CB-CG	4.35	118.98	109.89
1	E	174	HLU	OH-CB-CG	4.26	118.79	109.89
1	A	174	HLU	OH-CB-CG	4.25	118.77	109.89
1	F	150	8RE	OH1-CB-CG	4.21	118.97	108.81
1	B	205	KCX	OQ1-CX-NZ	-4.00	118.76	124.96
1	G	174	HLU	OH-CB-CG	3.99	118.23	109.89
1	E	150	8RE	OH1-CB-CG	3.98	118.43	108.81
1	D	174	HLU	OH-CB-CG	3.88	117.99	109.89
1	C	174	HLU	OH-CB-CG	3.84	117.92	109.89
1	B	174	HLU	OH-CB-CG	3.84	117.91	109.89
1	A	198	LYO	CE-CD-CG	-3.81	105.44	113.47
1	D	150	8RE	OH1-CB-CG	3.75	117.86	108.81
1	A	205	KCX	OQ1-CX-NZ	-3.73	119.17	124.96
1	D	205	KCX	OQ1-CX-NZ	-3.72	119.19	124.96
1	H	174	HLU	OH-CB-CG	3.67	117.55	109.89
1	F	174	HLU	CD1-CG-CB	3.63	117.12	111.20
1	G	205	KCX	OQ1-CX-NZ	-3.62	119.35	124.96
1	G	150	8RE	OH1-CB-CG	3.55	117.39	108.81
1	H	150	8RE	OH1-CB-CG	3.50	117.27	108.81
1	A	150	8RE	CB-CA-N	-3.40	91.31	113.84
1	C	150	8RE	OH1-CB-CG	3.36	116.92	108.81
1	B	150	8RE	CB-CA-N	-3.35	91.60	113.84
1	E	174	HLU	CD1-CG-CB	3.35	116.65	111.20
1	C	150	8RE	CB-CA-N	-3.27	92.18	113.84
1	E	150	8RE	CB-CA-N	-3.26	92.26	113.84
1	F	150	8RE	CB-CA-N	-3.24	92.37	113.84
1	B	198	LYO	CE-CD-CG	-3.20	106.73	113.47
1	A	150	8RE	OH1-CB-CG	3.19	116.51	108.81
1	G	150	8RE	CB-CA-N	-3.16	92.90	113.84
1	H	150	8RE	CB-CA-N	-3.14	93.02	113.84
1	C	48	HYP	CB-CG-CD	3.13	107.10	103.27
1	D	150	8RE	CB-CA-N	-3.05	93.62	113.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	HLU	CD1-CG-CB	3.05	116.17	111.20
1	G	174	HLU	CD1-CG-CB	2.97	116.04	111.20
1	H	48	HYP	CB-CG-CD	2.93	106.86	103.27
1	B	150	8RE	OH1-CB-CG	2.90	115.81	108.81
1	D	155	HYP	CB-CG-CD	2.83	106.74	103.27
1	B	48	HYP	CB-CG-CD	2.70	106.57	103.27
1	H	174	HLU	CG-CB-CA	2.62	119.43	113.69
1	G	48	HYP	CB-CG-CD	2.61	106.47	103.27
1	A	155	HYP	CB-CG-CD	2.60	106.45	103.27
1	B	174	HLU	CD1-CG-CB	2.59	115.42	111.20
1	E	174	HLU	CB-CA-N	-2.59	96.69	113.84
1	D	48	HYP	CB-CG-CD	2.58	106.43	103.27
1	B	48	HYP	OD1-CG-CB	-2.58	103.65	110.03
1	A	174	HLU	CB-CA-N	-2.58	96.75	113.84
1	F	174	HLU	CB-CA-N	-2.57	96.78	113.84
1	A	48	HYP	OD1-CG-CB	-2.56	103.71	110.03
1	A	48	HYP	CB-CG-CD	2.53	106.36	103.27
1	D	48	HYP	OD1-CG-CB	-2.50	103.86	110.03
1	B	174	HLU	CB-CA-N	-2.48	97.37	113.84
1	D	174	HLU	CB-CA-N	-2.45	97.60	113.84
1	D	174	HLU	CD1-CG-CB	2.42	115.14	111.20
1	C	174	HLU	CG-CB-CA	2.41	118.97	113.69
1	G	174	HLU	CB-CA-N	-2.39	97.97	113.84
1	H	174	HLU	CB-CA-N	-2.37	98.12	113.84
1	C	174	HLU	CD1-CG-CB	2.34	115.02	111.20
1	C	174	HLU	CB-CA-N	-2.31	98.52	113.84
1	H	48	HYP	OD1-CG-CB	-2.31	104.33	110.03
1	G	155	HYP	CB-CG-CD	2.25	106.03	103.27
1	E	174	HLU	CG-CB-CA	2.24	118.61	113.69
1	D	174	HLU	CG-CB-CA	2.24	118.60	113.69
1	H	205	KCX	OQ1-CX-NZ	-2.23	121.49	124.96
1	D	155	HYP	OD1-CG-CD	-2.23	105.47	110.35
1	B	155	HYP	CB-CG-CD	2.23	106.00	103.27
1	F	174	HLU	CD2-CG-CD1	2.22	116.81	110.59
1	G	48	HYP	OD1-CG-CB	-2.22	104.55	110.03
1	H	155	HYP	CB-CG-CD	2.21	105.98	103.27
1	G	174	HLU	CG-CB-CA	2.18	118.47	113.69
1	F	48	HYP	CB-CG-CD	2.18	105.94	103.27
1	G	155	HYP	OD1-CG-CD	-2.17	105.59	110.35
1	F	205	KCX	OQ1-CX-NZ	-2.17	121.60	124.96
1	C	155	HYP	CB-CG-CD	2.15	105.90	103.27
1	C	205	KCX	OQ1-CX-NZ	-2.09	121.71	124.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	174	HLU	CG-CB-CA	2.09	118.27	113.69
1	B	174	HLU	CG-CB-CA	2.06	118.21	113.69
1	A	174	HLU	CG-CB-CA	2.04	118.16	113.69
1	C	48	HYP	OD1-CG-CB	-2.03	105.02	110.03
1	F	150	8RE	O-C-CA	-2.03	119.47	124.78
1	F	174	HLU	CD2-CG-CB	2.01	114.48	111.20
1	E	48	HYP	CB-CG-CD	2.01	105.73	103.27
1	H	155	HYP	OD1-CG-CD	-2.00	105.97	110.35

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	174	HLU	N-CA-CB-CG
1	A	174	HLU	N-CA-CB-OH
1	A	174	HLU	C-CA-CB-CG
1	A	174	HLU	CA-CB-CG-CD1
1	A	174	HLU	CA-CB-CG-CD2
1	A	174	HLU	OH-CB-CG-CD1
1	A	174	HLU	OH-CB-CG-CD2
1	A	346	M3L	O-C-CA-CB
1	H	174	HLU	N-CA-CB-CG
1	H	174	HLU	N-CA-CB-OH
1	H	174	HLU	C-CA-CB-CG
1	H	174	HLU	CA-CB-CG-CD1
1	H	174	HLU	CA-CB-CG-CD2
1	H	174	HLU	OH-CB-CG-CD1
1	H	174	HLU	OH-CB-CG-CD2
1	H	346	M3L	O-C-CA-CB
1	F	174	HLU	N-CA-CB-CG
1	F	174	HLU	N-CA-CB-OH
1	F	174	HLU	C-CA-CB-CG
1	F	174	HLU	CA-CB-CG-CD1
1	F	174	HLU	CA-CB-CG-CD2
1	F	174	HLU	OH-CB-CG-CD1
1	F	174	HLU	OH-CB-CG-CD2
1	F	346	M3L	O-C-CA-CB
1	D	174	HLU	N-CA-CB-CG
1	D	174	HLU	N-CA-CB-OH
1	D	174	HLU	C-CA-CB-CG
1	D	174	HLU	CA-CB-CG-CD1
1	D	174	HLU	CA-CB-CG-CD2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	174	HLU	OH-CB-CG-CD1
1	D	174	HLU	OH-CB-CG-CD2
1	B	174	HLU	N-CA-CB-CG
1	B	174	HLU	N-CA-CB-OH
1	B	174	HLU	C-CA-CB-CG
1	B	174	HLU	CA-CB-CG-CD1
1	B	174	HLU	CA-CB-CG-CD2
1	B	174	HLU	OH-CB-CG-CD1
1	B	174	HLU	OH-CB-CG-CD2
1	B	346	M3L	O-C-CA-CB
1	C	174	HLU	N-CA-CB-CG
1	C	174	HLU	N-CA-CB-OH
1	C	174	HLU	C-CA-CB-CG
1	C	174	HLU	CA-CB-CG-CD2
1	C	174	HLU	OH-CB-CG-CD1
1	C	174	HLU	OH-CB-CG-CD2
1	E	174	HLU	N-CA-CB-CG
1	E	174	HLU	N-CA-CB-OH
1	E	174	HLU	C-CA-CB-CG
1	E	174	HLU	CA-CB-CG-CD1
1	E	174	HLU	CA-CB-CG-CD2
1	E	174	HLU	OH-CB-CG-CD1
1	E	174	HLU	OH-CB-CG-CD2
1	G	174	HLU	N-CA-CB-CG
1	G	174	HLU	N-CA-CB-OH
1	G	174	HLU	C-CA-CB-CG
1	G	174	HLU	CA-CB-CG-CD1
1	G	174	HLU	CA-CB-CG-CD2
1	G	174	HLU	OH-CB-CG-CD1
1	G	174	HLU	OH-CB-CG-CD2
1	G	346	M3L	O-C-CA-CB
1	A	150	8RE	O-C-CA-CB
1	A	150	8RE	C-CA-CB-CG
1	A	150	8RE	N-CA-CB-OH1
1	A	150	8RE	N-CA-CB-CG
1	A	150	8RE	CA-CB-CG-CD
1	A	150	8RE	OH1-CB-CG-OH2
1	A	150	8RE	OH1-CB-CG-CD
1	H	150	8RE	O-C-CA-CB
1	H	150	8RE	C-CA-CB-CG
1	H	150	8RE	N-CA-CB-OH1
1	H	150	8RE	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	H	150	8RE	CA-CB-CG-CD
1	H	150	8RE	OH1-CB-CG-OH2
1	H	150	8RE	OH1-CB-CG-CD
1	F	150	8RE	O-C-CA-CB
1	F	150	8RE	C-CA-CB-CG
1	F	150	8RE	N-CA-CB-OH1
1	F	150	8RE	N-CA-CB-CG
1	F	150	8RE	CA-CB-CG-CD
1	F	150	8RE	OH1-CB-CG-OH2
1	F	150	8RE	OH1-CB-CG-CD
1	D	150	8RE	O-C-CA-CB
1	D	150	8RE	C-CA-CB-CG
1	D	150	8RE	N-CA-CB-OH1
1	D	150	8RE	N-CA-CB-CG
1	D	150	8RE	CA-CB-CG-CD
1	D	150	8RE	OH1-CB-CG-OH2
1	D	150	8RE	OH1-CB-CG-CD
1	B	150	8RE	O-C-CA-CB
1	B	150	8RE	C-CA-CB-CG
1	B	150	8RE	N-CA-CB-OH1
1	B	150	8RE	N-CA-CB-CG
1	B	150	8RE	CA-CB-CG-CD
1	B	150	8RE	OH1-CB-CG-OH2
1	B	150	8RE	OH1-CB-CG-CD
1	C	150	8RE	O-C-CA-CB
1	C	150	8RE	C-CA-CB-CG
1	C	150	8RE	N-CA-CB-OH1
1	C	150	8RE	N-CA-CB-CG
1	C	150	8RE	CA-CB-CG-CD
1	C	150	8RE	OH1-CB-CG-OH2
1	C	150	8RE	OH1-CB-CG-CD
1	E	150	8RE	O-C-CA-CB
1	E	150	8RE	C-CA-CB-CG
1	E	150	8RE	N-CA-CB-OH1
1	E	150	8RE	N-CA-CB-CG
1	E	150	8RE	CA-CB-CG-CD
1	E	150	8RE	OH1-CB-CG-OH2
1	E	150	8RE	OH1-CB-CG-CD
1	G	150	8RE	O-C-CA-CB
1	G	150	8RE	C-CA-CB-CG
1	G	150	8RE	N-CA-CB-OH1
1	G	150	8RE	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	150	8RE	CA-CB-CG-CD
1	G	150	8RE	OH1-CB-CG-OH2
1	G	150	8RE	OH1-CB-CG-CD
1	A	198	LYO	CE-CD-CG-OG
1	H	198	LYO	CG-CD-CE-NZ
1	F	198	LYO	CG-CD-CE-NZ
1	D	198	LYO	CG-CD-CE-NZ
1	B	198	LYO	CE-CD-CG-OG
1	C	198	LYO	CG-CD-CE-NZ
1	E	198	LYO	CG-CD-CE-NZ
1	A	150	8RE	CA-CB-CG-OH2
1	F	150	8RE	CA-CB-CG-OH2
1	B	150	8RE	CA-CB-CG-OH2
1	E	150	8RE	CA-CB-CG-OH2
1	A	174	HLU	C-CA-CB-OH
1	H	174	HLU	C-CA-CB-OH
1	F	174	HLU	C-CA-CB-OH
1	D	174	HLU	C-CA-CB-OH
1	B	174	HLU	C-CA-CB-OH
1	C	174	HLU	C-CA-CB-OH
1	E	174	HLU	C-CA-CB-OH
1	G	174	HLU	C-CA-CB-OH
1	A	150	8RE	C-CA-CB-OH1
1	H	150	8RE	C-CA-CB-OH1
1	F	150	8RE	C-CA-CB-OH1
1	D	150	8RE	C-CA-CB-OH1
1	B	150	8RE	C-CA-CB-OH1
1	C	150	8RE	C-CA-CB-OH1
1	E	150	8RE	C-CA-CB-OH1
1	G	150	8RE	C-CA-CB-OH1
1	H	150	8RE	CA-CB-CG-OH2
1	D	150	8RE	CA-CB-CG-OH2
1	C	150	8RE	CA-CB-CG-OH2
1	G	150	8RE	CA-CB-CG-OH2
1	C	174	HLU	CA-CB-CG-CD1
1	G	346	M3L	CE-CD-CG-CB
1	D	346	M3L	CE-CD-CG-CB
1	B	198	LYO	CE-CD-CG-CB
1	E	346	M3L	CE-CD-CG-CB
1	A	346	M3L	CE-CD-CG-CB
1	F	346	M3L	CE-CD-CG-CB
1	B	346	M3L	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	C	346	M3L	CE-CD-CG-CB
1	A	198	LYO	CE-CD-CG-CB
1	G	198	LYO	CG-CD-CE-NZ
1	H	346	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	205	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 10 are monoatomic - leaving 27 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	$\#\|Z\| > 2$
5	EDO	A	503	-	3,3,3	0.52	0	2,2,2	0.30	0
5	EDO	N	201	-	3,3,3	0.44	0	2,2,2	0.22	0
4	CAP	G	502	3	17,20,20	0.67	0	22,31,31	0.88	0
4	CAP	H	502	3	17,20,20	0.69	0	22,31,31	0.94	0
4	CAP	F	502	3	17,20,20	0.72	0	22,31,31	0.83	0
4	CAP	E	502	3	17,20,20	0.70	0	22,31,31	0.85	0
5	EDO	M	203	-	3,3,3	0.51	0	2,2,2	0.31	0
5	EDO	I	203	-	3,3,3	0.47	0	2,2,2	0.18	0
5	EDO	K	203	-	3,3,3	0.39	0	2,2,2	0.63	0
5	EDO	K	204	-	3,3,3	0.51	0	2,2,2	0.29	0
5	EDO	K	201	-	3,3,3	0.39	0	2,2,2	0.37	0
4	CAP	A	502	3	17,20,20	0.76	0	22,31,31	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CAP	B	502	3	17,20,20	0.76	0	22,31,31	0.93	1 (4%)
5	EDO	I	204	-	3,3,3	0.43	0	2,2,2	0.41	0
5	EDO	K	202	-	3,3,3	0.39	0	2,2,2	0.34	0
5	EDO	L	201	-	3,3,3	0.44	0	2,2,2	0.56	0
5	EDO	I	202	-	3,3,3	0.51	0	2,2,2	0.26	0
5	EDO	O	203	-	3,3,3	0.41	0	2,2,2	0.30	0
5	EDO	P	201	-	3,3,3	0.45	0	2,2,2	0.26	0
4	CAP	D	502	3	17,20,20	0.72	0	22,31,31	0.97	0
5	EDO	M	202	-	3,3,3	0.47	0	2,2,2	0.28	0
4	CAP	C	502	3	17,20,20	0.71	0	22,31,31	0.97	0
5	EDO	M	201	-	3,3,3	0.53	0	2,2,2	0.18	0
5	EDO	J	202	-	3,3,3	0.38	0	2,2,2	0.25	0
5	EDO	O	202	-	3,3,3	0.53	0	2,2,2	0.18	0
5	EDO	J	201	-	3,3,3	0.45	0	2,2,2	0.52	0
5	EDO	O	201	-	3,3,3	0.56	0	2,2,2	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	N	201	-	-	0/1/1/1	-
4	CAP	G	502	3	-	9/29/29/29	-
4	CAP	H	502	3	-	8/29/29/29	-
4	CAP	F	502	3	-	8/29/29/29	-
4	CAP	E	502	3	-	8/29/29/29	-
5	EDO	M	203	-	-	0/1/1/1	-
5	EDO	I	203	-	-	0/1/1/1	-
5	EDO	K	203	-	-	1/1/1/1	-
5	EDO	K	204	-	-	0/1/1/1	-
5	EDO	K	201	-	-	0/1/1/1	-
4	CAP	A	502	3	-	7/29/29/29	-
4	CAP	B	502	3	-	9/29/29/29	-
5	EDO	I	204	-	-	0/1/1/1	-
5	EDO	K	202	-	-	0/1/1/1	-
5	EDO	L	201	-	-	0/1/1/1	-
5	EDO	I	202	-	-	0/1/1/1	-
5	EDO	O	203	-	-	0/1/1/1	-
5	EDO	P	201	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	D	502	3	-	8/29/29/29	-
5	EDO	M	202	-	-	0/1/1/1	-
4	CAP	C	502	3	-	8/29/29/29	-
5	EDO	M	201	-	-	0/1/1/1	-
5	EDO	J	202	-	-	0/1/1/1	-
5	EDO	O	202	-	-	0/1/1/1	-
5	EDO	J	201	-	-	0/1/1/1	-
5	EDO	O	201	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	502	CAP	O6P-P2-O5P	2.00	115.28	107.64

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	CAP	O7-C-C2-C1
4	A	502	CAP	O6-C-C2-C3
4	A	502	CAP	O7-C-C2-O2
4	A	502	CAP	C2-C3-C4-O4
4	A	502	CAP	O3-C3-C4-O4
4	H	502	CAP	O6-C-C2-C1
4	H	502	CAP	O6-C-C2-O2
4	H	502	CAP	C2-C3-C4-O4
4	H	502	CAP	O3-C3-C4-O4
4	F	502	CAP	O6-C-C2-C1
4	F	502	CAP	O6-C-C2-O2
4	F	502	CAP	O3-C3-C4-O4
4	D	502	CAP	O1-C1-C2-O2
4	D	502	CAP	O7-C-C2-C1
4	D	502	CAP	O6-C-C2-C3
4	D	502	CAP	O7-C-C2-O2
4	D	502	CAP	O3-C3-C4-O4
4	B	502	CAP	O7-C-C2-C1
4	B	502	CAP	O6-C-C2-C3
4	B	502	CAP	O6-C-C2-O2
4	B	502	CAP	O7-C-C2-O2
4	B	502	CAP	C2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	502	CAP	O3-C3-C4-O4
4	C	502	CAP	O6-C-C2-C1
4	C	502	CAP	O6-C-C2-O2
4	C	502	CAP	C2-C3-C4-O4
4	C	502	CAP	O3-C3-C4-O4
4	E	502	CAP	O6-C-C2-C1
4	E	502	CAP	O7-C-C2-C1
4	E	502	CAP	O6-C-C2-O2
4	E	502	CAP	O7-C-C2-O2
4	E	502	CAP	C2-C3-C4-O4
4	E	502	CAP	O3-C3-C4-O4
4	G	502	CAP	O7-C-C2-C1
4	G	502	CAP	O6-C-C2-C3
4	G	502	CAP	O6-C-C2-O2
4	G	502	CAP	O7-C-C2-O2
4	G	502	CAP	O3-C3-C4-O4
4	H	502	CAP	O7-C-C2-C1
4	F	502	CAP	O7-C-C2-C1
4	C	502	CAP	O7-C-C2-C1
4	A	502	CAP	O2-C2-C3-C4
4	H	502	CAP	O2-C2-C3-C4
4	F	502	CAP	O2-C2-C3-C4
4	D	502	CAP	O2-C2-C3-C4
4	B	502	CAP	O2-C2-C3-C4
4	C	502	CAP	O2-C2-C3-C4
4	E	502	CAP	O2-C2-C3-C4
4	G	502	CAP	O2-C2-C3-C4
4	F	502	CAP	C2-C3-C4-O4
4	D	502	CAP	C2-C3-C4-O4
4	G	502	CAP	C2-C3-C4-O4
4	H	502	CAP	O7-C-C2-O2
4	F	502	CAP	O7-C-C2-O2
4	C	502	CAP	O7-C-C2-O2
5	K	203	EDO	O1-C1-C2-O2
4	A	502	CAP	O6-C-C2-O2
4	G	502	CAP	O1-C1-C2-O2
4	H	502	CAP	O7-C-C2-C3
4	F	502	CAP	O7-C-C2-C3
4	B	502	CAP	O7-C-C2-C3
4	C	502	CAP	O7-C-C2-C3
4	E	502	CAP	O7-C-C2-C3
4	B	502	CAP	O6-C-C2-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	502	CAP	O6-C-C2-C1
4	D	502	CAP	O6-C-C2-O2

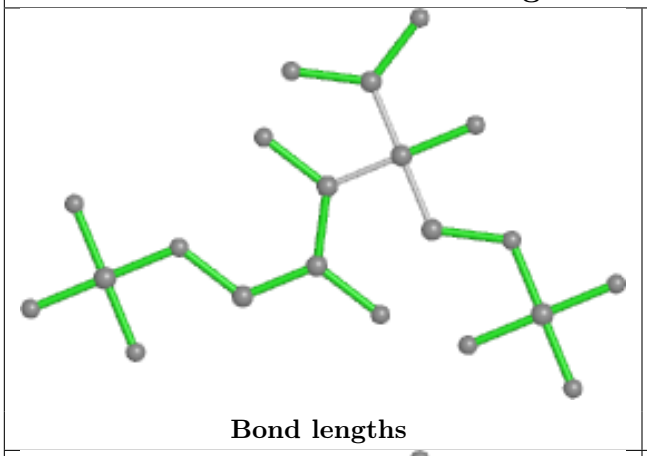
There are no ring outliers.

2 monomers are involved in 3 short contacts:

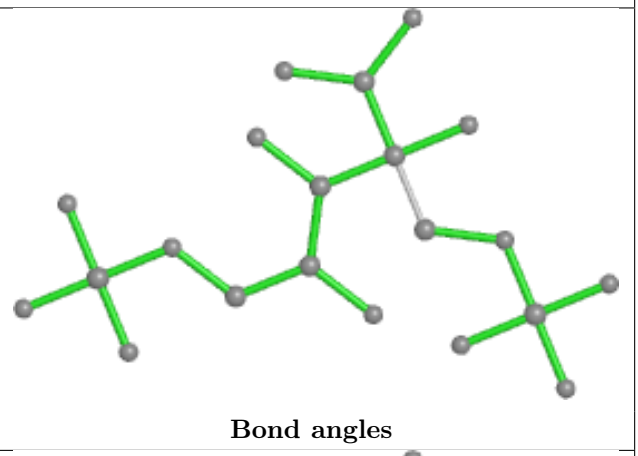
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	203	EDO	2	0
5	I	204	EDO	1	0

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.

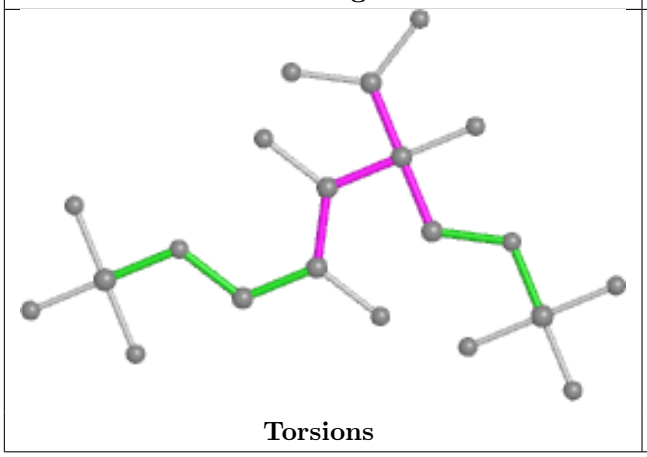
Ligand CAP G 502



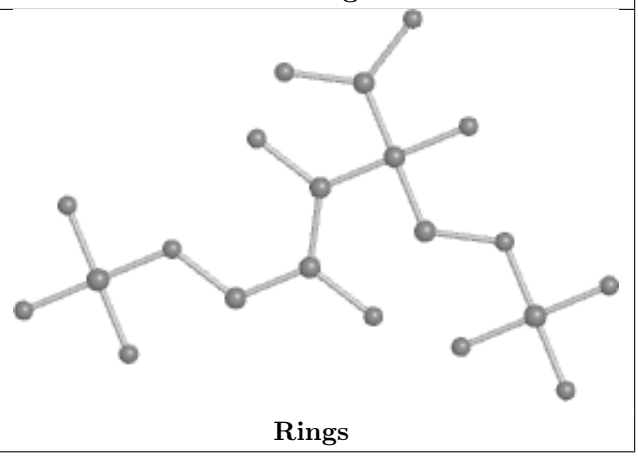
Bond lengths



Bond angles

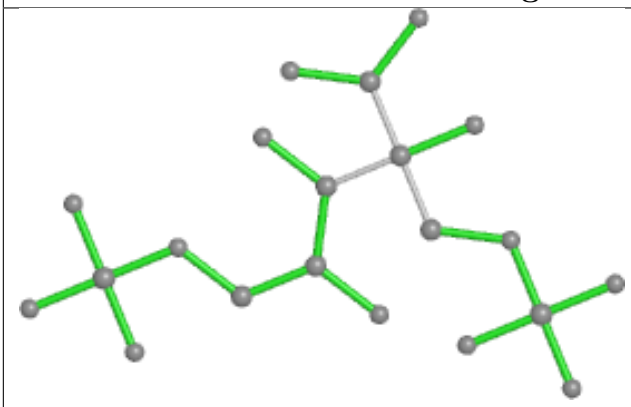


Torsions

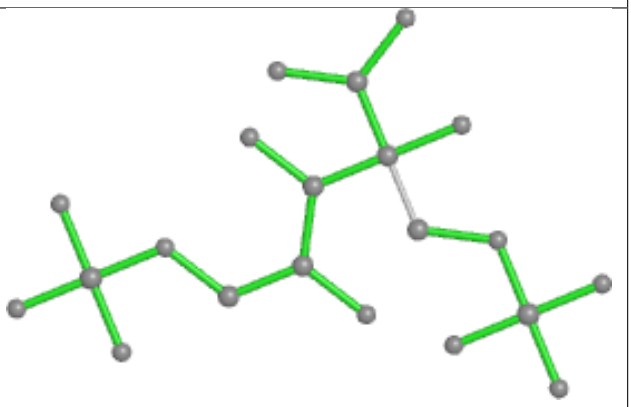


Rings

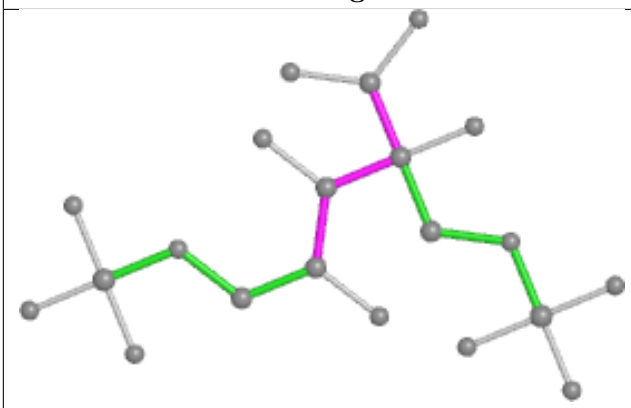
Ligand CAP H 502



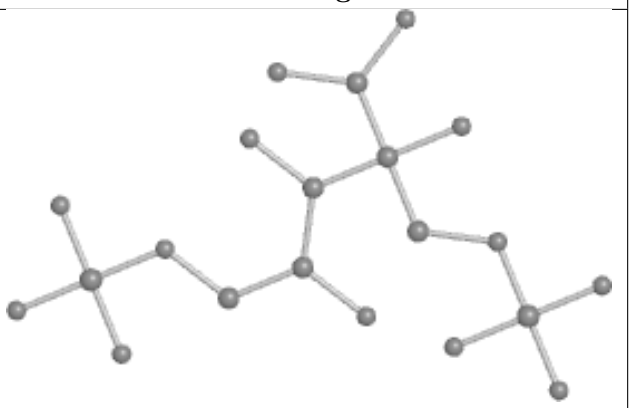
Bond lengths



Bond angles

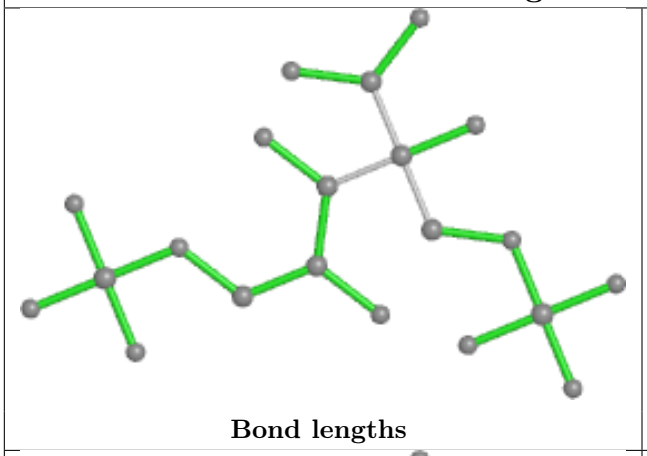


Torsions

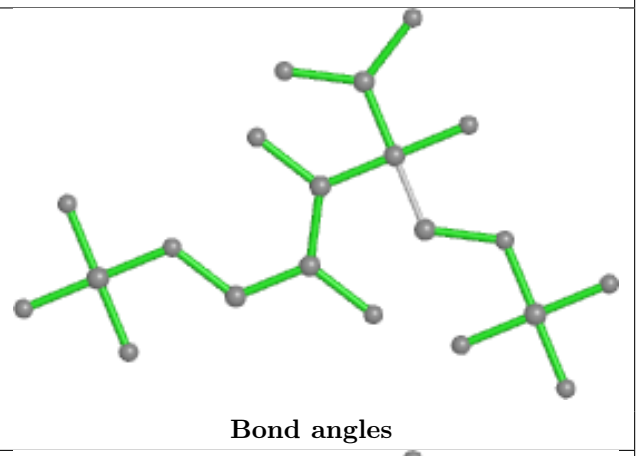


Rings

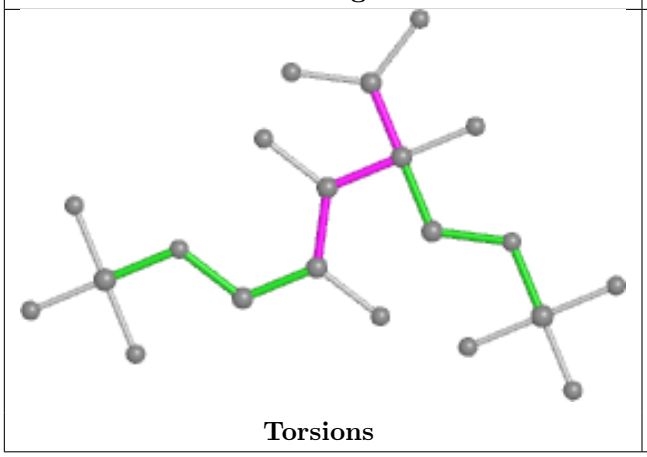
Ligand CAP F 502



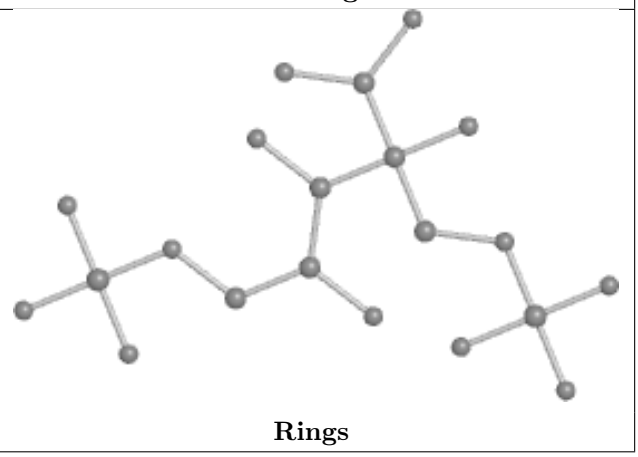
Bond lengths



Bond angles

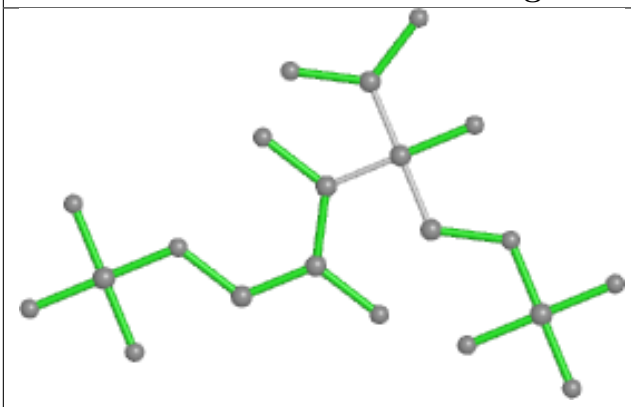


Torsions

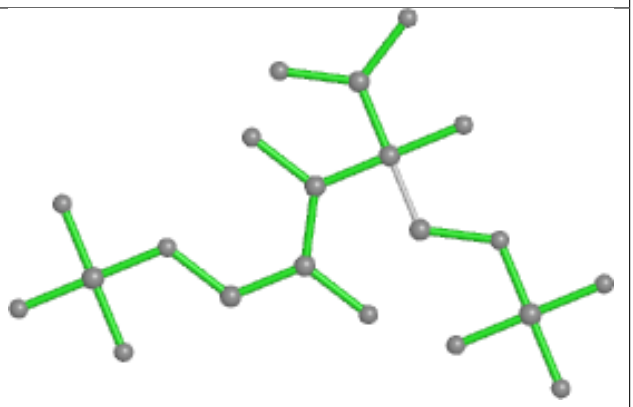


Rings

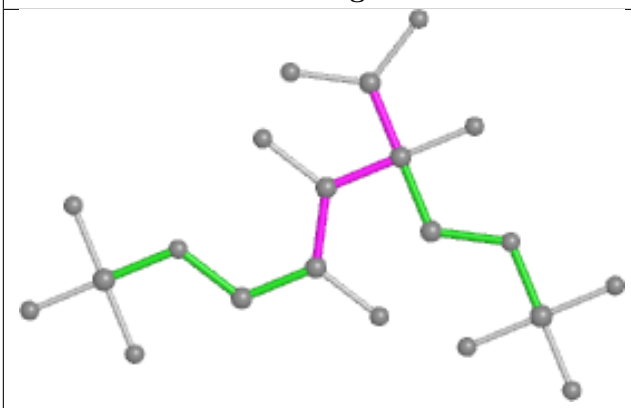
Ligand CAP E 502



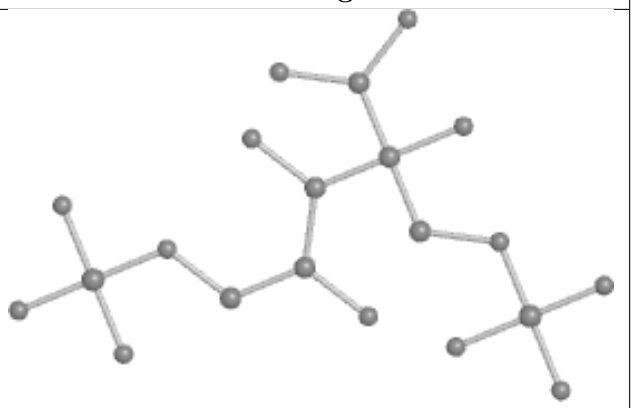
Bond lengths



Bond angles

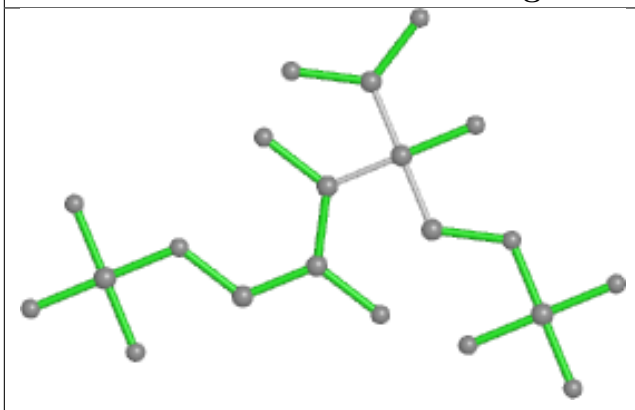


Torsions

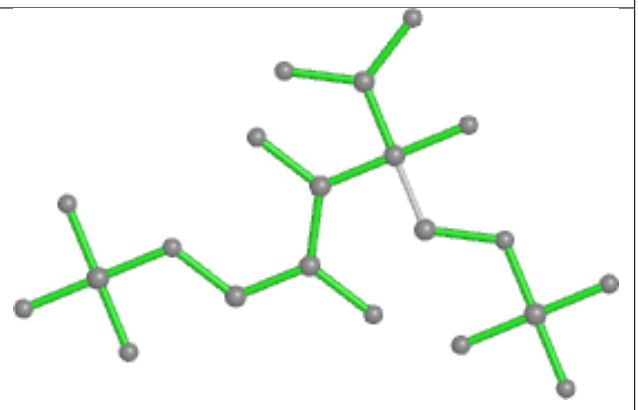


Rings

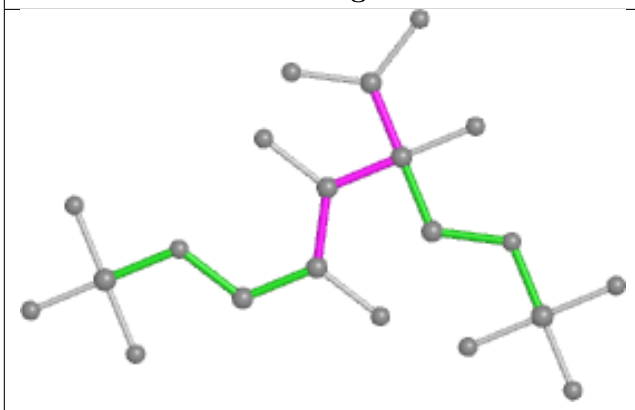
Ligand CAP A 502



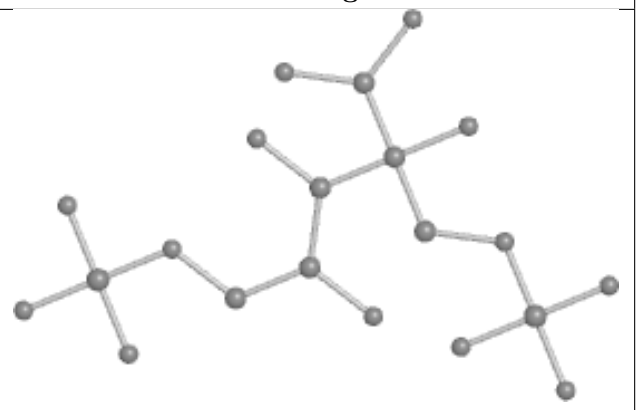
Bond lengths



Bond angles

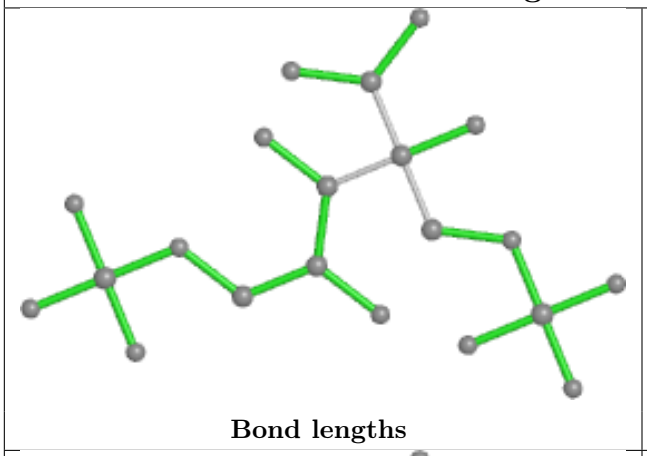


Torsions

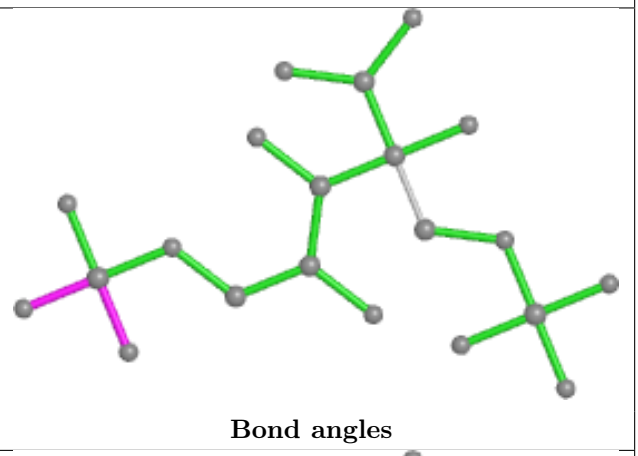


Rings

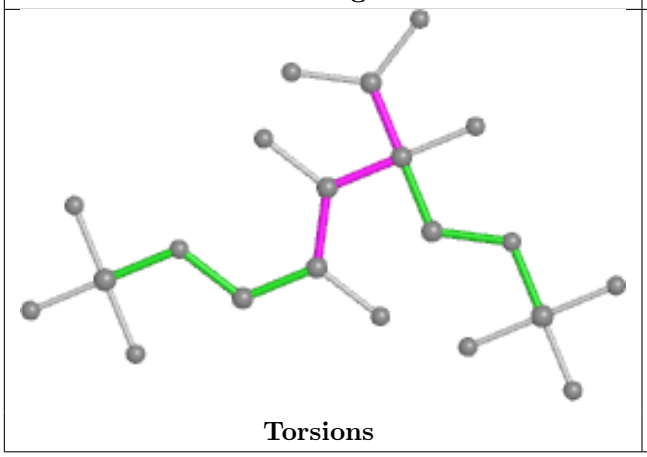
Ligand CAP B 502



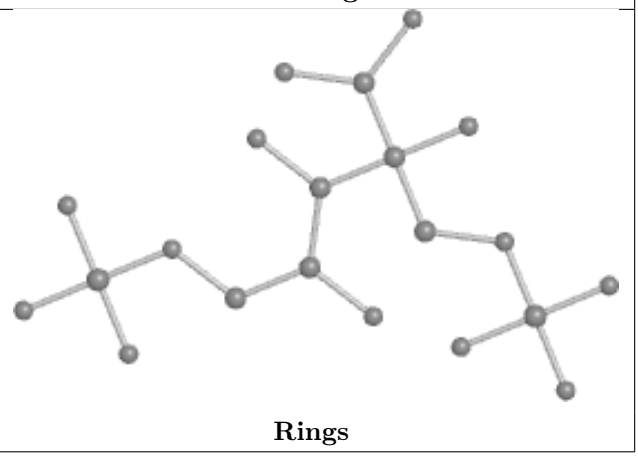
Bond lengths



Bond angles

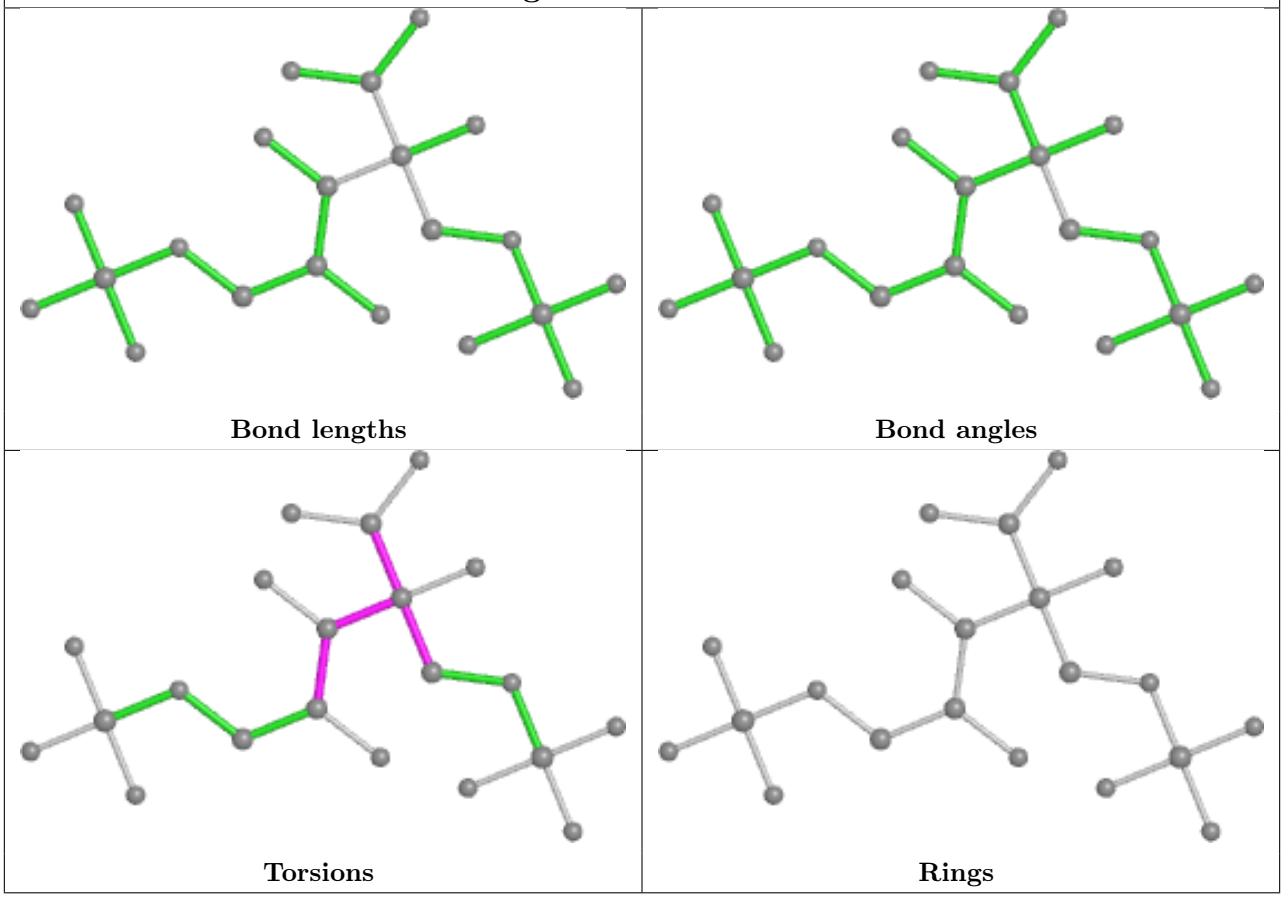


Torsions

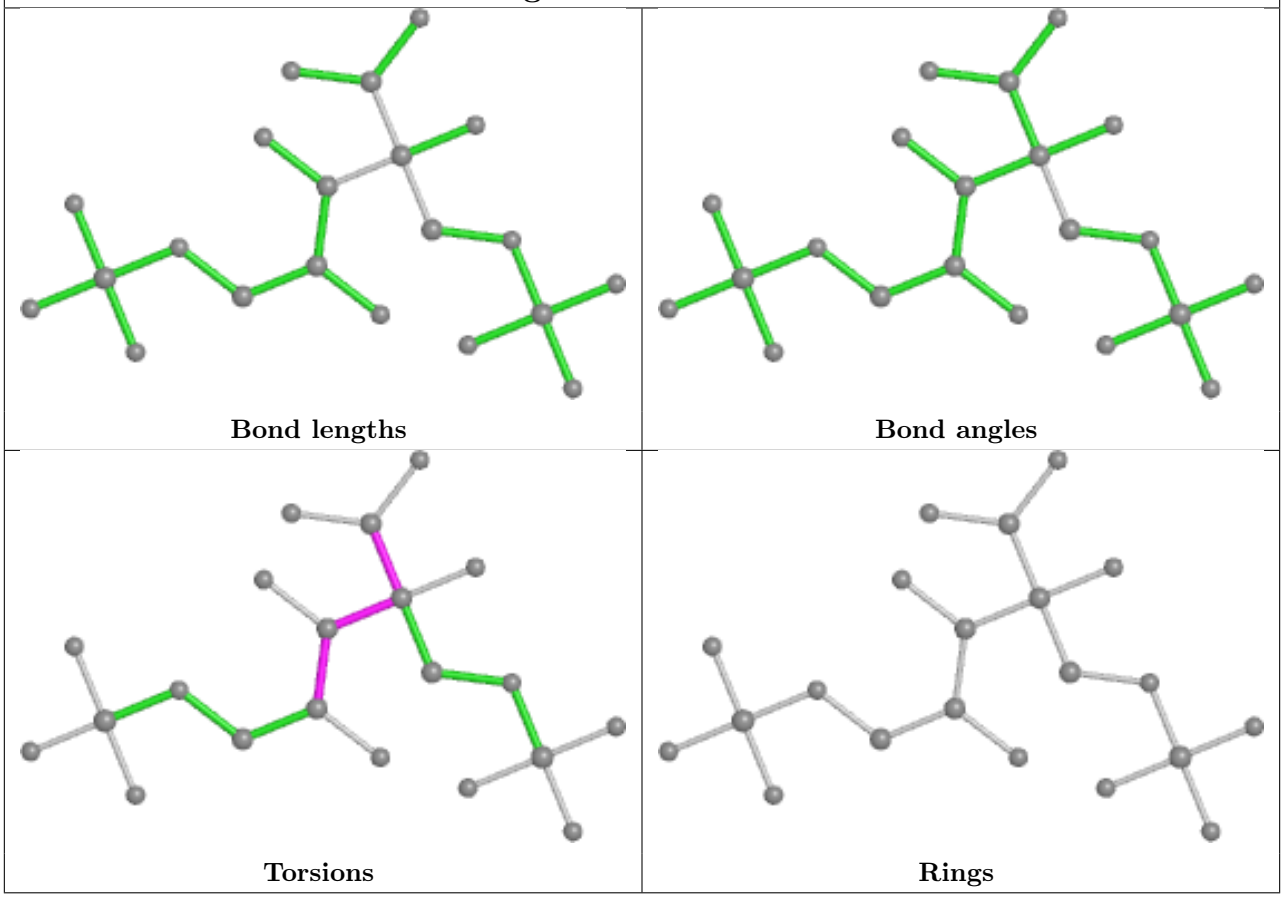


Rings

Ligand CAP D 502



Ligand CAP C 502



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	473/490 (96%)	-0.68	1 (0%) 95 95	10, 16, 31, 56	0
1	B	473/490 (96%)	-0.70	1 (0%) 95 95	10, 16, 30, 57	0
1	C	473/490 (96%)	-0.79	0 100 100	9, 14, 27, 41	0
1	D	473/490 (96%)	-0.81	0 100 100	9, 14, 27, 43	0
1	E	473/490 (96%)	-0.78	0 100 100	8, 14, 28, 41	0
1	F	473/490 (96%)	-0.77	0 100 100	8, 14, 28, 44	0
1	G	473/490 (96%)	-0.81	0 100 100	9, 14, 27, 41	0
1	H	473/490 (96%)	-0.81	0 100 100	9, 14, 27, 43	0
2	I	139/139 (100%)	-0.58	2 (1%) 75 77	11, 19, 31, 49	0
2	J	139/139 (100%)	-0.69	0 100 100	12, 18, 29, 49	0
2	K	139/139 (100%)	-0.66	1 (0%) 87 88	11, 18, 30, 46	0
2	L	139/139 (100%)	-0.61	0 100 100	10, 18, 30, 58	0
2	M	139/139 (100%)	-0.72	0 100 100	10, 18, 30, 50	0
2	N	139/139 (100%)	-0.64	2 (1%) 75 77	11, 18, 29, 49	0
2	O	139/139 (100%)	-0.65	1 (0%) 87 88	12, 19, 30, 48	0
2	P	139/139 (100%)	-0.69	1 (0%) 87 88	10, 19, 29, 49	0
All	All	4896/5032 (97%)	-0.74	9 (0%) 95 95	8, 16, 29, 58	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	57	ASP	2.8
2	N	57	ASP	2.6
2	I	57	ASP	2.4
2	P	57	ASP	2.2
2	I	58	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	57	ASP	2.1
1	A	484	GLU	2.1
2	N	58	ILE	2.1
1	B	483	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	HYP	B	48	8/9	0.92	0.09	18,19,24,30	0
1	HYP	A	48	8/9	0.93	0.08	18,20,24,29	0
1	HLU	E	174	9/10	0.93	0.10	12,15,18,19	0
1	HLU	A	174	9/10	0.94	0.09	14,17,20,21	0
1	HYP	D	48	8/9	0.95	0.09	13,15,20,28	0
1	HLU	H	174	9/10	0.95	0.08	13,15,19,22	0
1	HYP	C	48	8/9	0.95	0.09	12,16,21,25	0
1	HYP	E	48	8/9	0.95	0.09	14,16,22,28	0
1	HYP	F	48	8/9	0.95	0.08	14,16,22,27	0
1	HYP	G	48	8/9	0.95	0.09	12,14,19,29	0
1	8RE	A	150	11/12	0.95	0.09	10,12,19,19	0
1	HLU	F	174	9/10	0.96	0.09	10,14,17,20	0
1	HLU	C	174	9/10	0.96	0.07	12,14,18,20	0
1	M3L	C	346	12/13	0.96	0.09	13,16,25,25	0
1	HYP	H	48	8/9	0.96	0.07	11,16,18,22	0
1	HYP	H	155	8/9	0.96	0.08	8,11,13,14	0
1	HYP	B	155	8/9	0.96	0.07	12,12,15,15	0
1	HLU	G	174	9/10	0.96	0.09	9,13,17,20	0
1	KCX	G	205	12/13	0.96	0.08	9,10,12,13	0
1	HLU	B	174	9/10	0.96	0.07	13,18,20,22	0
1	8RE	H	150	11/12	0.96	0.09	7,11,15,17	0
1	8RE	F	150	11/12	0.96	0.07	8,10,16,17	0
1	8RE	D	150	11/12	0.96	0.07	8,12,17,17	0
1	8RE	B	150	11/12	0.96	0.08	10,11,19,20	0
1	8RE	C	150	11/12	0.96	0.08	8,10,17,18	0
1	LYO	H	198	10/11	0.96	0.08	10,14,22,27	0
1	LYO	C	198	10/11	0.96	0.07	10,15,24,28	0
1	M3L	A	346	12/13	0.97	0.08	15,22,27,30	0
1	HYP	C	155	8/9	0.97	0.07	8,11,13,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	HYP	D	155	8/9	0.97	0.06	10,12,13,18	0
1	HLU	D	174	9/10	0.97	0.10	10,13,18,20	0
1	HYP	A	155	8/9	0.97	0.07	11,12,16,16	0
1	HYP	F	155	8/9	0.97	0.07	8,10,13,15	0
1	CSO	A	109	7/8	0.97	0.07	12,15,17,25	0
1	8RE	E	150	11/12	0.97	0.07	9,11,15,17	0
1	8RE	G	150	11/12	0.97	0.08	7,12,17,19	0
1	LYO	A	198	10/11	0.97	0.07	12,18,25,28	0
1	HYP	G	155	8/9	0.97	0.06	10,11,13,17	0
1	LYO	F	198	10/11	0.97	0.08	10,15,23,26	0
1	KCX	B	205	12/13	0.97	0.06	13,14,15,18	0
1	M3L	G	346	12/13	0.98	0.06	11,18,23,24	0
1	KCX	D	205	12/13	0.98	0.06	8,10,12,13	0
1	M3L	D	346	12/13	0.98	0.07	10,17,22,23	0
1	KCX	F	205	12/13	0.98	0.06	11,12,13,14	0
1	CSO	B	109	7/8	0.98	0.06	13,14,16,25	0
1	CSO	E	109	7/8	0.98	0.06	9,12,14,21	0
1	HYP	E	155	8/9	0.98	0.06	9,10,14,15	0
1	M3L	F	346	12/13	0.98	0.08	12,18,27,27	0
1	M3L	E	346	12/13	0.98	0.06	12,17,25,25	0
1	KCX	A	205	12/13	0.98	0.05	12,14,16,17	0
1	KCX	H	205	12/13	0.98	0.06	10,12,14,14	0
1	M3L	B	346	12/13	0.98	0.06	15,22,29,30	0
1	LYO	D	198	10/11	0.98	0.07	9,16,24,26	0
1	LYO	B	198	10/11	0.98	0.07	12,16,25,27	0
1	M3L	H	346	12/13	0.98	0.07	12,16,22,24	0
1	LYO	E	198	10/11	0.98	0.06	11,16,21,21	0
1	LYO	G	198	10/11	0.98	0.07	10,16,24,25	0
1	CSO	G	109	7/8	0.99	0.06	10,12,15,22	0
1	CSO	D	109	7/8	0.99	0.05	11,11,15,21	0
1	CSO	F	109	7/8	0.99	0.06	10,12,13,20	0
1	KCX	C	205	12/13	0.99	0.06	10,11,13,14	0
1	KCX	E	205	12/13	0.99	0.05	11,11,14,14	0
1	CSO	H	109	7/8	0.99	0.06	10,12,13,19	0
1	CSO	C	109	7/8	0.99	0.05	11,12,13,19	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

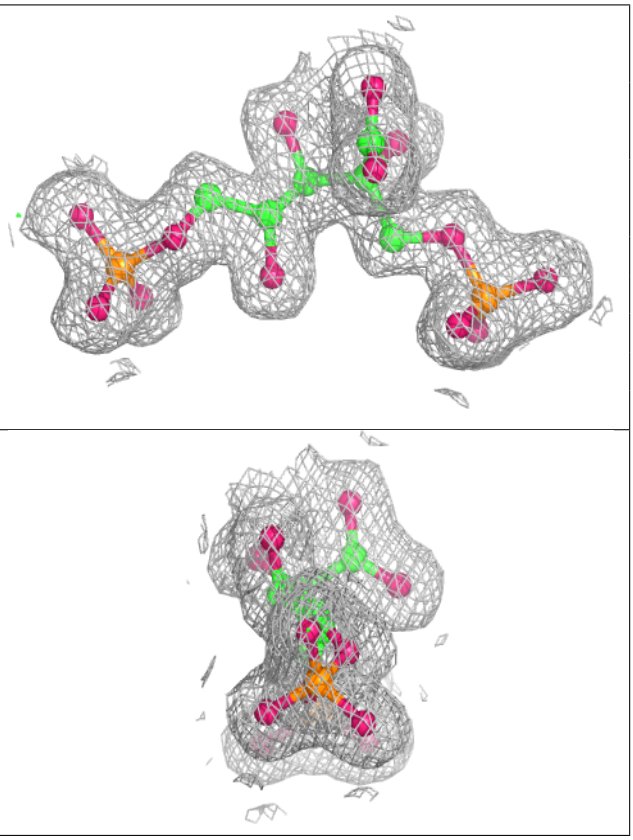
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

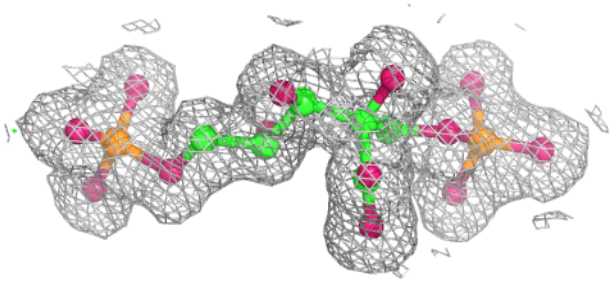
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	O	201	4/4	0.83	0.24	21,21,25,31	0
5	EDO	M	201	4/4	0.86	0.21	19,23,23,29	0
5	EDO	K	204	4/4	0.87	0.24	20,22,25,29	0
5	EDO	M	203	4/4	0.89	0.20	21,23,25,29	0
5	EDO	O	202	4/4	0.89	0.16	20,22,25,31	0
5	EDO	I	204	4/4	0.90	0.14	26,31,32,37	0
5	EDO	A	503	4/4	0.90	0.25	19,22,25,32	0
5	EDO	I	202	4/4	0.91	0.25	20,24,25,28	0
5	EDO	K	203	4/4	0.92	0.10	17,22,28,32	0
5	EDO	P	201	4/4	0.94	0.10	16,20,21,22	0
5	EDO	I	203	4/4	0.95	0.10	16,21,21,22	0
5	EDO	O	203	4/4	0.97	0.06	15,17,21,24	0
5	EDO	M	202	4/4	0.97	0.13	17,20,21,22	0
5	EDO	N	201	4/4	0.97	0.07	14,17,20,24	0
5	EDO	J	202	4/4	0.98	0.07	13,16,20,26	0
3	MG	I	201	1/1	0.98	0.17	21,21,21,21	0
3	MG	N	202	1/1	0.98	0.15	20,20,20,20	0
5	EDO	L	201	4/4	0.98	0.12	18,18,18,21	0
4	CAP	E	502	21/21	0.99	0.06	10,13,14,16	0
4	CAP	G	502	21/21	0.99	0.06	9,12,13,14	0
3	MG	H	501	1/1	0.99	0.06	13,13,13,13	0
4	CAP	A	502	21/21	0.99	0.06	13,15,17,19	0
4	CAP	H	502	21/21	0.99	0.05	10,12,13,16	0
5	EDO	J	201	4/4	0.99	0.14	11,14,20,24	0
4	CAP	F	502	21/21	0.99	0.06	10,13,14,15	0
5	EDO	K	201	4/4	0.99	0.13	15,15,20,23	0
5	EDO	K	202	4/4	0.99	0.11	15,15,18,24	0
4	CAP	D	502	21/21	0.99	0.05	9,12,13,15	0
4	CAP	B	502	21/21	0.99	0.05	13,15,16,18	0
4	CAP	C	502	21/21	0.99	0.05	10,12,13,15	0
3	MG	G	501	1/1	1.00	0.08	12,12,12,12	0
3	MG	F	501	1/1	1.00	0.04	13,13,13,13	0
3	MG	A	501	1/1	1.00	0.04	14,14,14,14	0
3	MG	D	501	1/1	1.00	0.05	13,13,13,13	0
3	MG	B	501	1/1	1.00	0.04	14,14,14,14	0
3	MG	C	501	1/1	1.00	0.04	14,14,14,14	0
3	MG	E	501	1/1	1.00	0.04	13,13,13,13	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 CAP E 502:

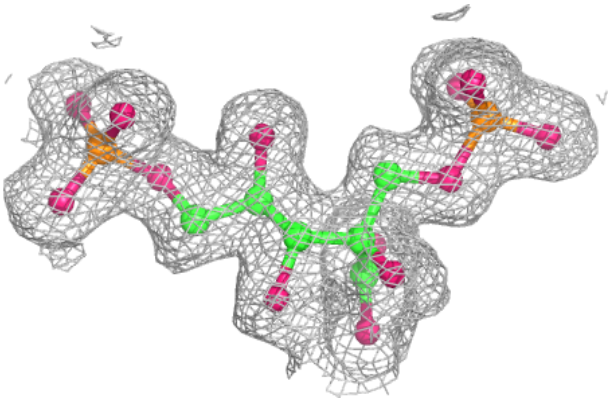
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

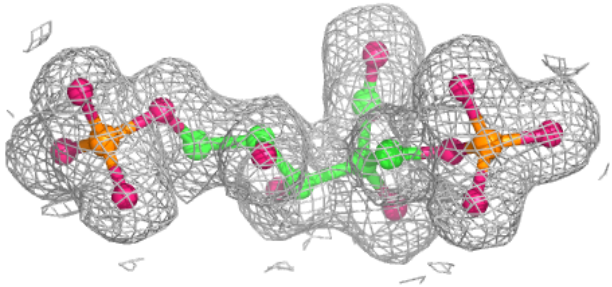


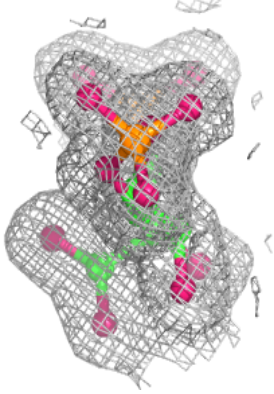


Electron density around CAP G 502:

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

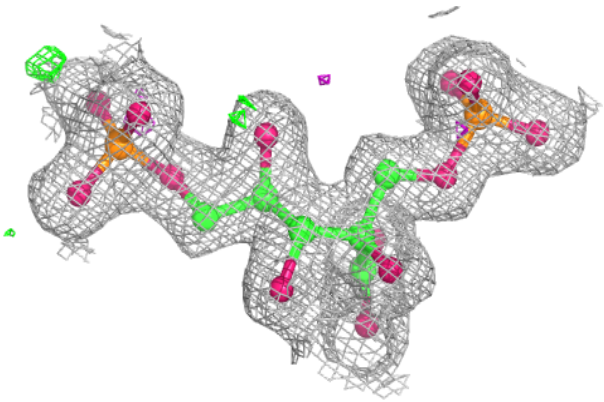


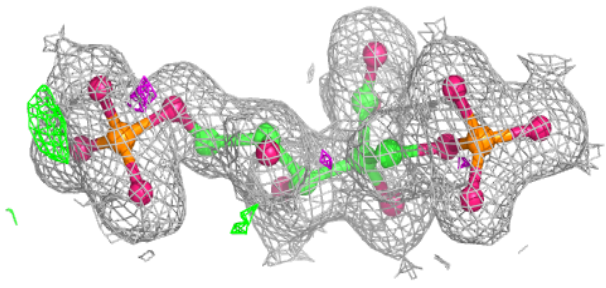


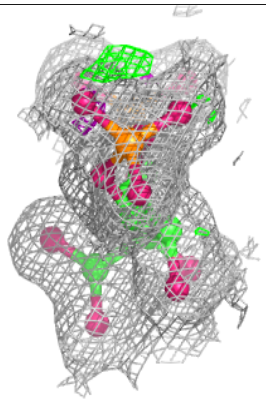


Electron density around CAP A 502:

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

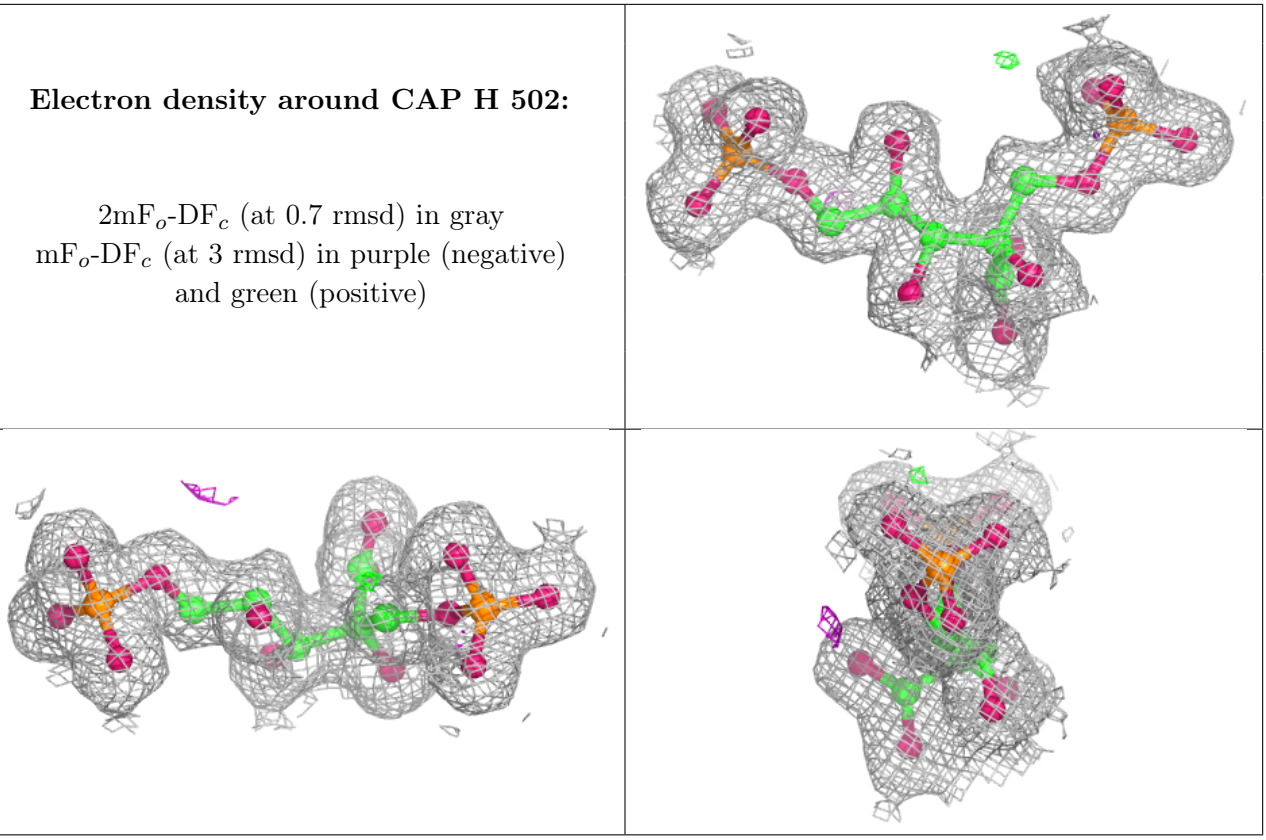






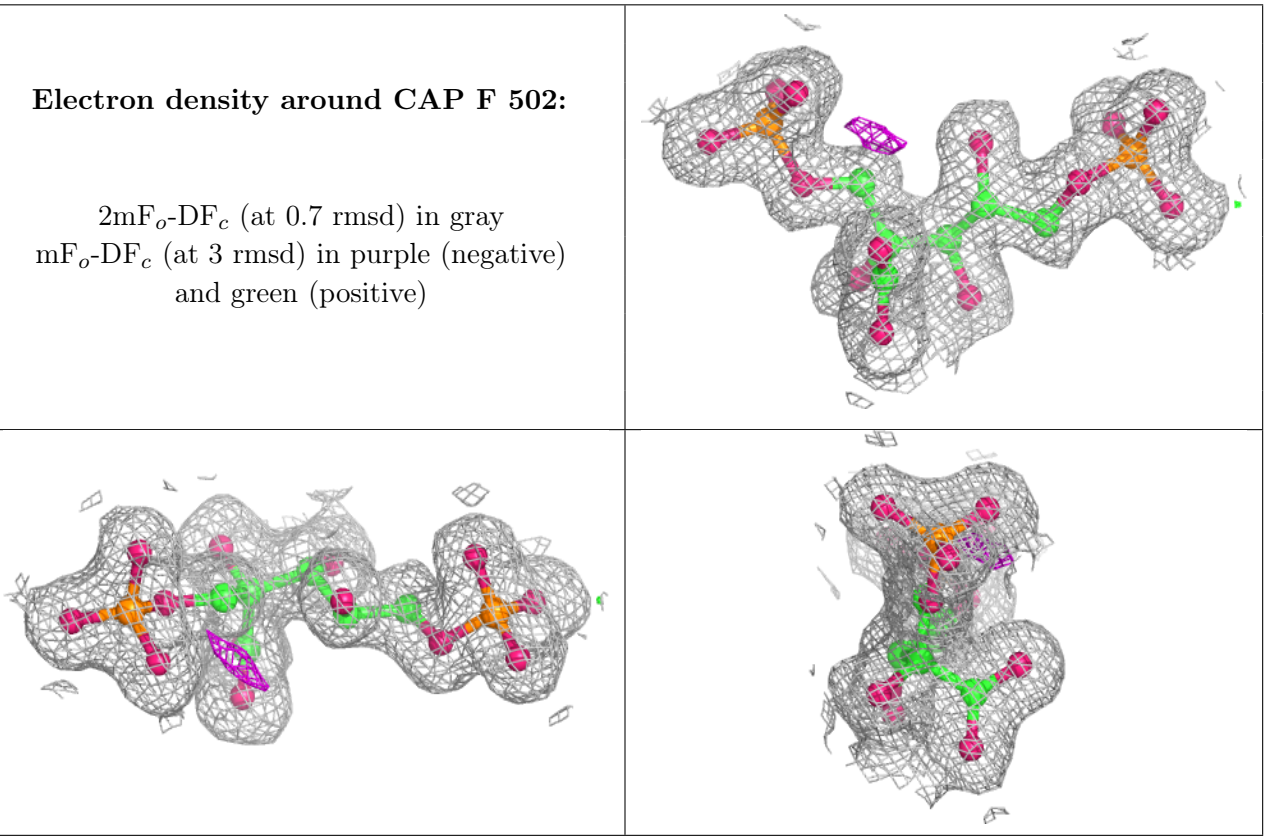
Electron density around CAP H 502:

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



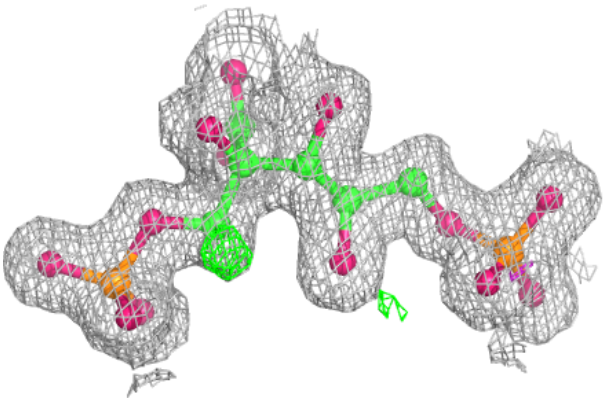
Electron density around CAP F 502:

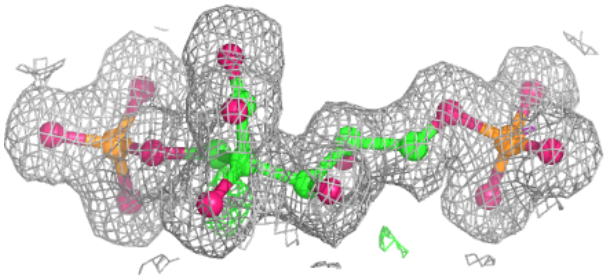
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

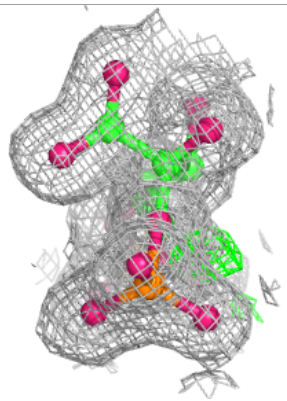


Electron density around CAP D 502:

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

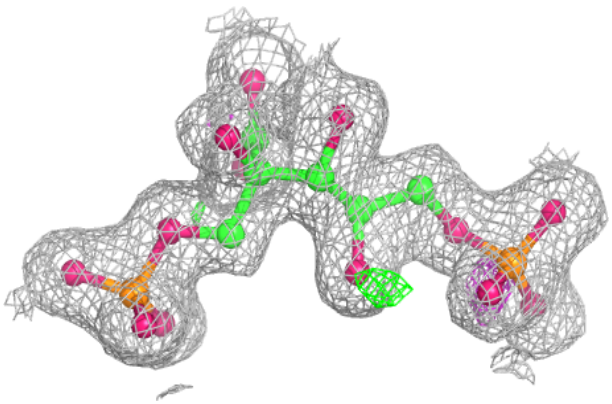


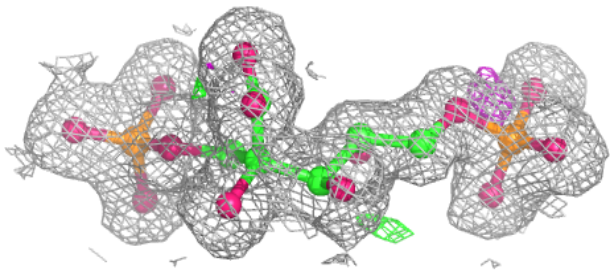


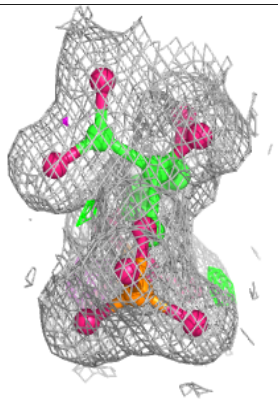


Electron density around CAP B 502:

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

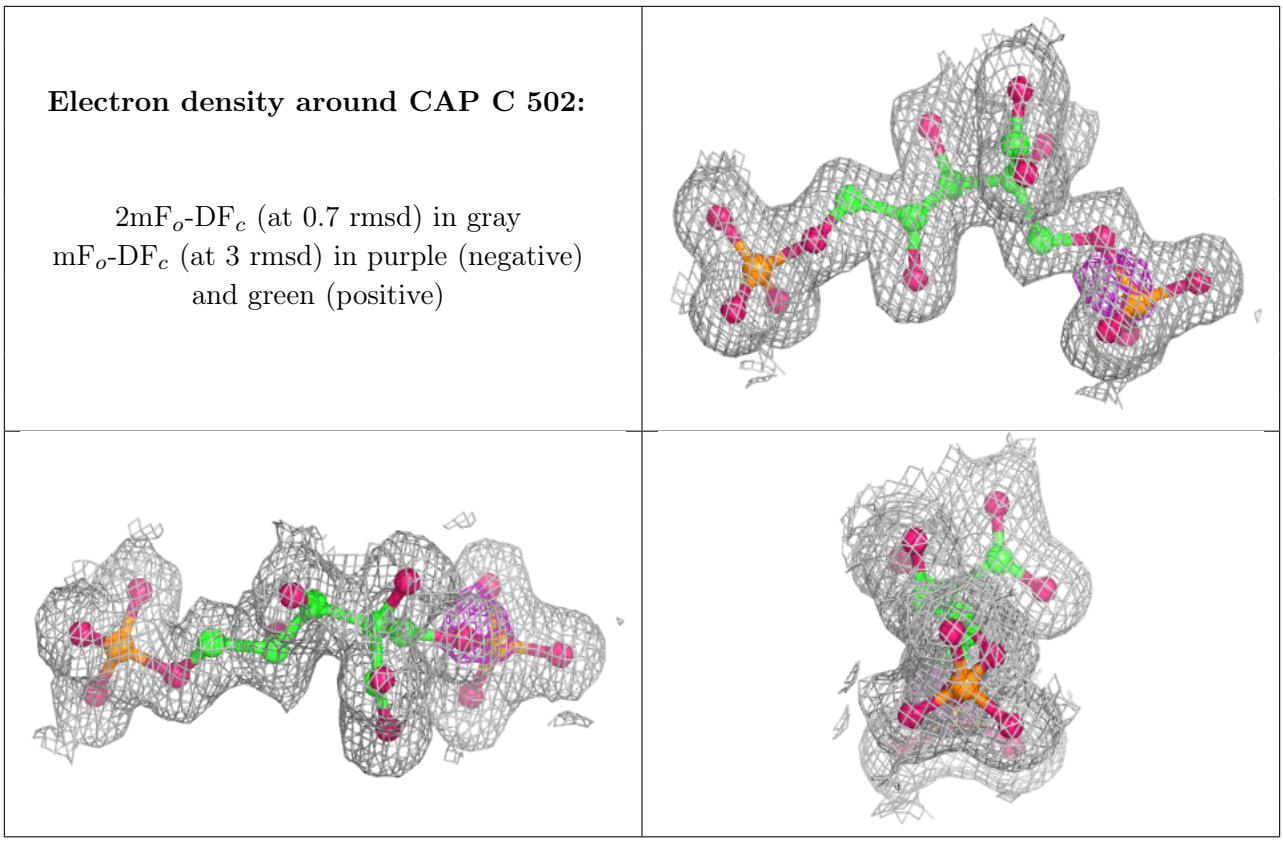






Electron density around CAP C 502:

$2mF_o$-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 (i)

There are no such residues in this entry.