Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 10:22 am BST

PDB ID	:	8BAI
Title	:	The surface-exposed lipo-protein of BtuG2 in complex with cyanocobalamin.
Authors	:	Whittaker, J.; Martinez Felices, J.M.; Guskov, A.; Slotboom, D.J.
Deposited on	:	2022-10-11
Resolution	:	1.69 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 (i) 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 (i)) were used in the production of this report:

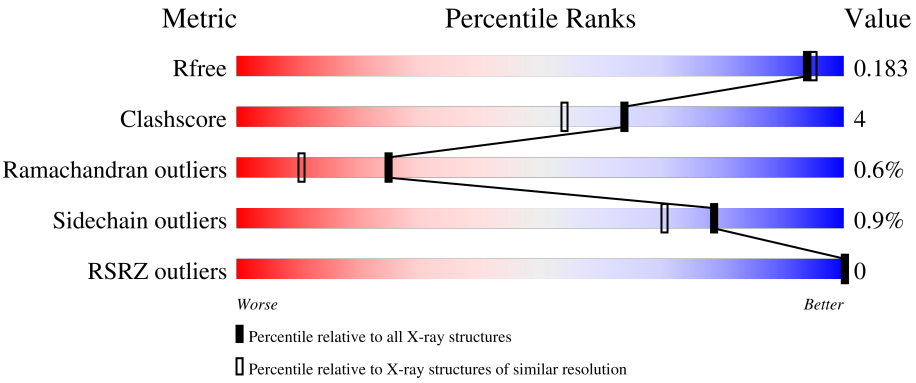
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	94% 5%
1	B	321	94% 5%
1	C	321	96%
1	D	321	95%

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
2	GOL	B	401	-	-	X	-
3	CNC	A	408	X	-	-	-
3	CNC	B	408	X	-	-	-
3	CNC	C	406	X	-	-	-
3	CNC	D	406	X	-	-	-
5	PEG	B	409	-	-	X	-
5	PEG	C	404	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11812 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.

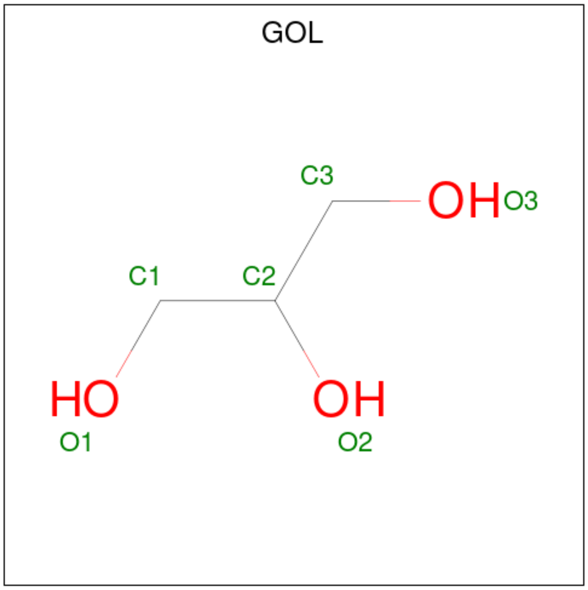
- Molecule 1 is a protein called Surface layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	1	0
			2630	1700	418	501	11			
1	B	320	Total	C	N	O	S	0	1	0
			2626	1698	417	500	11			
1	C	320	Total	C	N	O	S	0	0	0
			2621	1693	417	500	11			
1	D	321	Total	C	N	O	S	0	1	0
			2631	1701	418	501	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	LEU	-	expression tag	UNP Q8A6D0
B	322	LEU	-	expression tag	UNP Q8A6D0
C	322	LEU	-	expression tag	UNP Q8A6D0
D	322	LEU	-	expression tag	UNP Q8A6D0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0

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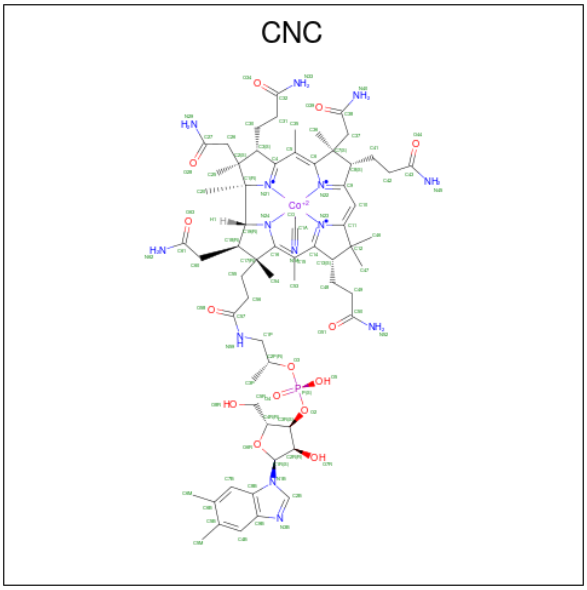
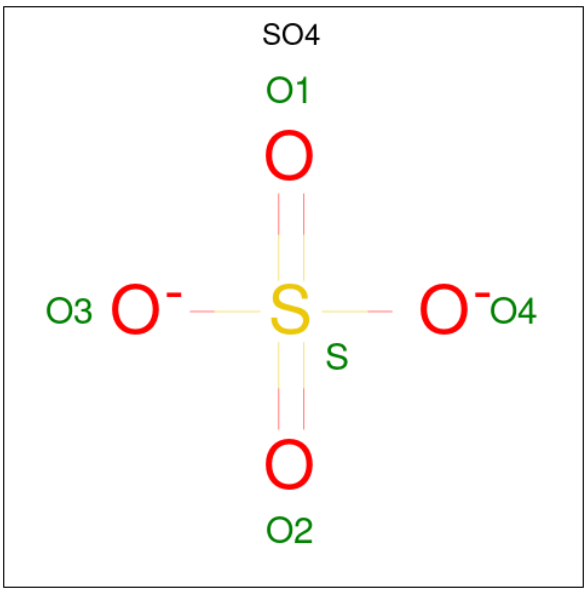
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).



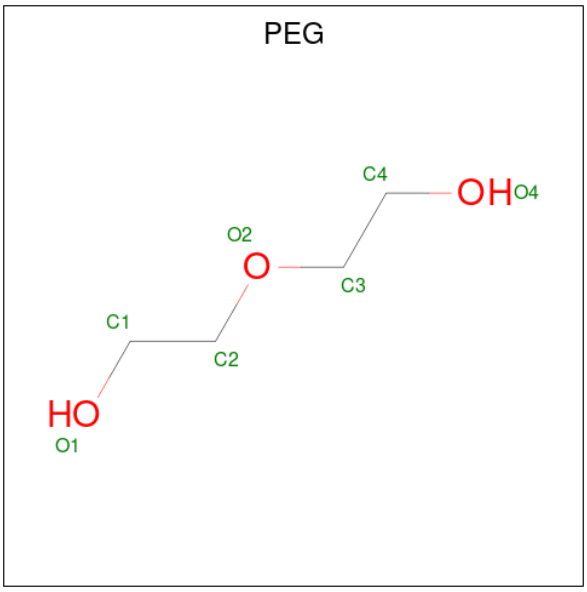
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Co N O P 93 63 1 14 14 1	0	0
3	B	1	Total C Co N O P 93 63 1 14 14 1	0	0
3	C	1	Total C Co N O P 93 63 1 14 14 1	0	0
3	D	1	Total C Co N O P 93 63 1 14 14 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 7 4 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	2	Total Na 2 2	0	0

- Molecule 7 is water.

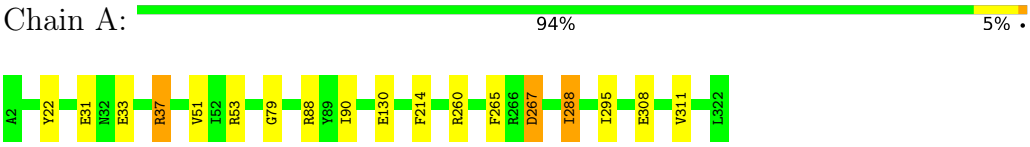
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	195	Total O 195 195	0	0
7	B	198	Total O 198 198	0	0
7	C	199	Total O 199 199	0	0
7	D	188	Total O 188 188	0	0

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.

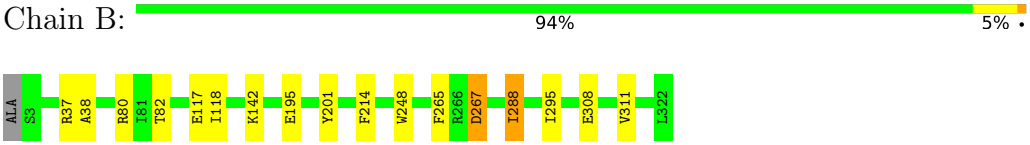
• Molecule 1: Surface layer protein

Chain A:



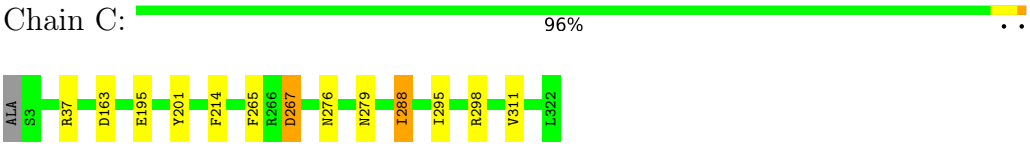
• Molecule 1: Surface layer protein

Chain B:



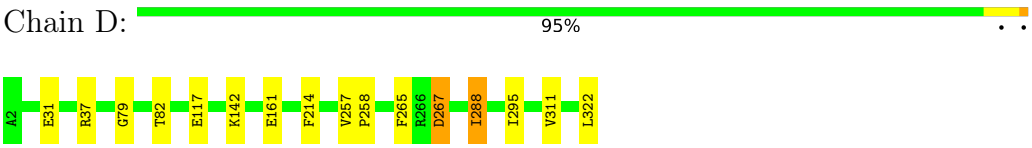
• Molecule 1: Surface layer protein

Chain C:



• Molecule 1: Surface layer protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.24Å 79.94Å 101.05Å 89.97° 89.89° 82.28°	Depositor
Resolution (Å)	42.63 – 1.69 42.59 – 1.69	Depositor EDS
% Data completeness (in resolution range)	96.3 (42.63-1.69) 83.6 (42.59-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.45 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.157 , 0.180 0.157 , 0.183	Depositor DCC
R_{free} test set	1812 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.460 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11812	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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: CNC, PEG, SO4, GOL, NA

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	0.52	0/2706	0.87	0/3684
1	B	0.53	0/2702	0.88	0/3678
1	C	0.52	0/2694	0.87	0/3667
1	D	0.52	0/2707	0.88	0/3685
All	All	0.52	0/10809	0.87	0/14714

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	2630	0	2515	17	0
1	B	2626	0	2512	20	0
1	C	2621	0	2501	10	0
1	D	2631	0	2517	15	0
2	A	42	0	56	5	0
2	B	36	0	48	10	0
2	C	18	0	24	3	0
2	D	30	0	40	0	0
3	A	93	0	87	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	93	0	87	4	0
3	C	93	0	87	6	0
3	D	93	0	87	7	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	B	7	0	10	9	0
5	C	7	0	10	5	0
6	D	2	0	0	0	0
7	A	195	0	0	4	0
7	B	198	0	0	2	0
7	C	199	0	0	3	0
7	D	188	0	0	2	0
All	All	11812	0	10581	90	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 4.

All (90) 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)
1:B:37:ARG:HH11	2:B:401:GOL:C1	1.53	1.22
1:B:37:ARG:HH11	2:B:401:GOL:H12	1.06	1.14
1:D:37:ARG:HB2	1:D:37:ARG:HH11	1.19	1.03
1:B:37:ARG:NH1	2:B:401:GOL:C1	2.29	0.94
3:D:406:CNC:H362	3:D:406:CNC:H351	1.51	0.90
1:B:37:ARG:NH1	2:B:401:GOL:H12	1.86	0.89
3:C:406:CNC:H362	3:C:406:CNC:H351	1.54	0.88
1:D:37:ARG:HH11	1:D:37:ARG:CB	1.86	0.88
1:D:37:ARG:HB2	1:D:37:ARG:NH1	1.89	0.88
3:C:406:CNC:H552	3:C:406:CNC:H531	1.57	0.86
1:B:118:ILE:H	5:B:409:PEG:H21	1.41	0.85
1:A:37:ARG:HH11	1:A:37:ARG:HB3	1.41	0.85
1:A:37:ARG:HB3	1:A:37:ARG:NH1	1.92	0.84
1:B:37:ARG:HH11	2:B:401:GOL:H11	1.43	0.83
3:B:408:CNC:H362	3:B:408:CNC:H351	1.64	0.80
1:A:260:ARG:HH12	1:B:80:ARG:HH22	1.28	0.79
1:B:37:ARG:NH1	2:B:401:GOL:H11	2.00	0.77
3:D:406:CNC:H552	3:D:406:CNC:H531	1.69	0.74
3:A:408:CNC:H351	3:A:408:CNC:H362	1.71	0.72
3:B:408:CNC:H552	3:B:408:CNC:H531	1.72	0.71
1:A:130:GLU:HG3	7:A:603:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:407:GOL:H11	7:A:530:HOH:O	1.95	0.67
1:A:88:ARG:HH12	3:A:408:CNC:H292	1.42	0.66
1:A:37:ARG:HH11	1:A:37:ARG:CB	2.08	0.66
3:D:406:CNC:H351	3:D:406:CNC:C36	2.26	0.66
1:C:288:ILE:HD11	1:C:295:ILE:HG22	1.79	0.65
2:A:403:GOL:H11	7:A:653:HOH:O	1.97	0.65
1:B:288:ILE:HD11	1:B:295:ILE:HG22	1.80	0.64
1:A:288:ILE:HD11	1:A:295:ILE:HG22	1.80	0.64
1:C:163:ASP:HB2	2:C:402:GOL:H32	1.79	0.64
1:D:142:LYS:HE3	1:D:161:GLU:HG3	1.78	0.64
1:D:288:ILE:HD11	1:D:295:ILE:HG22	1.81	0.62
1:D:142:LYS:NZ	7:D:501:HOH:O	2.33	0.61
1:B:308:GLU:O	2:B:406:GOL:H2	2.00	0.61
1:B:118:ILE:H	5:B:409:PEG:C2	2.14	0.59
1:A:31:GLU:OE2	1:A:37:ARG:HD3	2.02	0.59
5:B:409:PEG:H12	1:D:82:THR:OG1	2.03	0.59
1:B:117:GLU:HG2	5:B:409:PEG:C1	2.33	0.58
3:C:406:CNC:H531	3:C:406:CNC:C55	2.25	0.58
1:C:298:ARG:NH2	5:C:404:PEG:H42	2.20	0.57
1:B:117:GLU:HA	5:B:409:PEG:H11	1.88	0.56
3:A:408:CNC:H601	3:A:408:CNC:H262	1.88	0.55
1:C:279:ASN:ND2	5:C:404:PEG:H32	2.20	0.55
1:D:142:LYS:HE3	1:D:161:GLU:CG	2.36	0.55
1:B:142:LYS:NZ	7:B:504:HOH:O	2.39	0.55
2:C:401:GOL:H32	7:C:526:HOH:O	2.05	0.55
3:A:408:CNC:H552	3:A:408:CNC:H531	1.89	0.55
1:A:308:GLU:OE1	1:D:161:GLU:HG3	2.06	0.54
3:D:406:CNC:H531	3:D:406:CNC:C55	2.33	0.54
5:B:409:PEG:H42	1:D:117:GLU:HA	1.90	0.54
3:B:408:CNC:H531	3:B:408:CNC:C55	2.38	0.53
1:A:308:GLU:O	2:A:403:GOL:H2	2.09	0.52
3:A:408:CNC:H3	3:A:408:CNC:H291	1.75	0.51
1:C:195:GLU:HG2	1:C:201:TYR:CE2	2.45	0.51
1:C:279:ASN:HD22	5:C:404:PEG:H32	1.76	0.51
1:C:37:ARG:HB2	7:C:551:HOH:O	2.11	0.50
3:D:406:CNC:O28	3:D:406:CNC:H3	2.11	0.50
3:C:406:CNC:H351	3:C:406:CNC:C36	2.32	0.49
1:D:79:GLY:HA2	7:D:610:HOH:O	2.13	0.48
1:B:195:GLU:HG2	1:B:201:TYR:CE2	2.49	0.48
2:B:406:GOL:C1	7:B:652:HOH:O	2.61	0.48
1:A:51[B]:VAL:HG21	1:A:90:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:HG2	5:B:409:PEG:H11	1.94	0.48
3:A:408:CNC:H3	3:A:408:CNC:N29	2.29	0.47
1:A:79:GLY:HA2	7:A:523:HOH:O	2.15	0.47
1:A:22:TYR:CZ	2:A:402:GOL:H11	2.50	0.47
1:C:265:PHE:CZ	1:C:267:ASP:HA	2.50	0.47
1:A:33:GLU:O	1:A:37:ARG:HG3	2.14	0.46
1:D:265:PHE:CZ	1:D:267:ASP:HA	2.51	0.46
1:A:265:PHE:CZ	1:A:267:ASP:HA	2.51	0.46
3:C:406:CNC:H533	3:C:406:CNC:H482	1.97	0.45
1:B:265:PHE:CZ	1:B:267:ASP:HA	2.52	0.45
1:B:248:TRP:CD1	2:B:402:GOL:H32	2.52	0.45
5:B:409:PEG:H22	1:D:82:THR:O	2.17	0.45
3:C:406:CNC:O28	3:C:406:CNC:H3	2.17	0.44
1:A:88:ARG:NH1	3:A:408:CNC:H292	2.14	0.44
1:A:53:ARG:HD3	2:A:405:GOL:H31	2.00	0.44
3:A:408:CNC:H462	3:A:408:CNC:H10	1.76	0.43
3:A:408:CNC:H541	3:A:408:CNC:H602	1.81	0.43
1:B:38:ALA:HA	2:B:401:GOL:H2	2.01	0.43
1:C:276:ASN:HD21	5:C:404:PEG:H21	1.84	0.43
3:A:408:CNC:H301	3:A:408:CNC:H253	1.84	0.42
3:D:406:CNC:H461	3:D:406:CNC:H491	2.01	0.42
2:C:401:GOL:H31	7:C:622:HOH:O	2.20	0.42
1:D:31:GLU:OE1	1:D:37:ARG:HD2	2.19	0.41
3:B:408:CNC:O28	3:B:408:CNC:H3	2.20	0.41
1:C:276:ASN:ND2	5:C:404:PEG:H21	2.35	0.41
1:B:82:THR:OG1	5:B:409:PEG:H41	2.20	0.41
3:D:406:CNC:H601	3:D:406:CNC:H262	2.03	0.40
1:D:257:VAL:HB	1:D:258:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	320/321 (100%)	302 (94%)	16 (5%)	2 (1%)	25 11
1	B	319/321 (99%)	301 (94%)	16 (5%)	2 (1%)	25 11
1	C	318/321 (99%)	300 (94%)	16 (5%)	2 (1%)	25 11
1	D	320/321 (100%)	302 (94%)	16 (5%)	2 (1%)	25 11
All	All	1277/1284 (100%)	1205 (94%)	64 (5%)	8 (1%)	25 11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	VAL
1	B	311	VAL
1	C	311	VAL
1	D	311	VAL
1	A	288	ILE
1	B	288	ILE
1	C	288	ILE
1	D	288	ILE

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	285/284 (100%)	282 (99%)	3 (1%)	73 63
1	B	285/284 (100%)	283 (99%)	2 (1%)	84 77
1	C	284/284 (100%)	282 (99%)	2 (1%)	84 77
1	D	285/284 (100%)	282 (99%)	3 (1%)	73 63
All	All	1139/1136 (100%)	1129 (99%)	10 (1%)	78 70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	214	PHE
1	A	267	ASP

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Mol	Chain	Res	Type
1	B	214	PHE
1	B	267	ASP
1	C	214	PHE
1	C	267	ASP
1	D	214	PHE
1	D	267	ASP
1	D	322	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
2	GOL	B	402	-	5,5,5	0.11	0	5,5,5	0.64	0
2	GOL	C	402	-	5,5,5	0.21	0	5,5,5	0.58	0
2	GOL	D	405	-	5,5,5	0.11	0	5,5,5	0.38	0
2	GOL	D	403	-	5,5,5	0.11	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CNC	C	406	-	90,103,103	1.22	10 (11%)	139,171,171	1.66	28 (20%)
2	GOL	A	405	-	5,5,5	0.09	0	5,5,5	0.18	0
2	GOL	D	402	-	5,5,5	0.06	0	5,5,5	0.33	0
3	CNC	B	408	-	90,103,103	1.29	7 (7%)	139,171,171	1.61	25 (17%)
2	GOL	B	406	-	5,5,5	0.16	0	5,5,5	0.48	0
3	CNC	A	408	-	90,103,103	1.49	5 (5%)	139,171,171	1.60	16 (11%)
4	SO4	B	407	-	4,4,4	0.34	0	6,6,6	0.13	0
2	GOL	B	405	-	5,5,5	0.14	0	5,5,5	0.31	0
3	CNC	D	406	-	90,103,103	1.28	11 (12%)	139,171,171	1.50	19 (13%)
2	GOL	A	401	-	5,5,5	0.14	0	5,5,5	0.35	0
4	SO4	C	405	-	4,4,4	0.35	0	6,6,6	0.11	0
2	GOL	A	407	-	5,5,5	0.25	0	5,5,5	0.56	0
2	GOL	A	402	-	5,5,5	0.14	0	5,5,5	0.34	0
2	GOL	A	404	-	5,5,5	0.09	0	5,5,5	0.27	0
5	PEG	C	404	-	6,6,6	0.37	0	5,5,5	0.42	0
2	GOL	B	404	-	5,5,5	0.11	0	5,5,5	0.26	0
2	GOL	A	403	-	5,5,5	0.14	0	5,5,5	0.51	0
2	GOL	C	401	-	5,5,5	0.18	0	5,5,5	0.48	0
2	GOL	C	403	-	5,5,5	0.16	0	5,5,5	0.61	0
2	GOL	B	401	-	5,5,5	0.34	0	5,5,5	0.78	0
2	GOL	D	404	-	5,5,5	0.11	0	5,5,5	0.42	0
2	GOL	A	406	-	5,5,5	0.57	0	5,5,5	0.95	0
5	PEG	B	409	-	6,6,6	1.55	1 (16%)	5,5,5	0.98	0
2	GOL	B	403	-	5,5,5	0.06	0	5,5,5	1.15	1 (20%)
2	GOL	D	401	-	5,5,5	0.16	0	5,5,5	0.52	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
2	GOL	B	402	-	-	4/4/4/4	-
2	GOL	C	402	-	-	4/4/4/4	-
2	GOL	D	405	-	-	2/4/4/4	-
2	GOL	D	403	-	-	0/4/4/4	-
3	CNC	C	406	-	1/1/36/38	1/52/235/235	0/3/11/11
3	CNC	B	408	-	1/1/36/38	1/52/235/235	0/3/11/11
2	GOL	A	405	-	-	2/4/4/4	-
2	GOL	D	402	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CNC	A	408	-	2/2/36/38	4/52/235/235	0/3/11/11
2	GOL	B	406	-	-	2/4/4/4	-
2	GOL	B	405	-	-	0/4/4/4	-
3	CNC	D	406	-	1/1/36/38	2/52/235/235	0/3/11/11
2	GOL	A	401	-	-	3/4/4/4	-
2	GOL	A	407	-	-	4/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	A	404	-	-	1/4/4/4	-
5	PEG	C	404	-	-	2/4/4/4	-
2	GOL	B	404	-	-	3/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-
2	GOL	C	403	-	-	4/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	D	404	-	-	2/4/4/4	-
2	GOL	A	406	-	-	0/4/4/4	-
5	PEG	B	409	-	-	4/4/4/4	-
2	GOL	B	403	-	-	2/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	408	CNC	C19-N24	-10.61	1.27	1.49
3	D	406	CNC	C19-N24	-5.73	1.37	1.49
3	B	408	CNC	C19-N24	-5.40	1.37	1.49
3	C	406	CNC	C19-N24	-4.46	1.39	1.49
3	D	406	CNC	C6B-C5B	3.66	1.50	1.40
5	B	409	PEG	O4-C4	3.54	1.60	1.42
3	C	406	CNC	C6B-C5B	3.44	1.49	1.40
3	B	408	CNC	C6B-C5B	3.44	1.49	1.40
3	A	408	CNC	C8B-C9B	3.35	1.47	1.40
3	B	408	CNC	C35-C5	3.25	1.57	1.50
3	B	408	CNC	C10-C9	3.01	1.47	1.39
3	A	408	CNC	C6B-C5B	2.95	1.48	1.40
3	D	406	CNC	C53-C15	2.94	1.57	1.50
3	C	406	CNC	C25-C2	2.68	1.59	1.54
3	B	408	CNC	C25-C2	2.61	1.59	1.54
3	D	406	CNC	C30-C3	2.42	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	408	CNC	C10-C11	-2.36	1.30	1.37
3	D	406	CNC	O6R-C1R	2.35	1.44	1.41
3	C	406	CNC	C10-C9	2.30	1.45	1.39
3	D	406	CNC	C60-C18	2.24	1.59	1.54
3	C	406	CNC	C35-C5	2.24	1.55	1.50
3	D	406	CNC	C6M-C6B	2.20	1.55	1.51
3	B	408	CNC	C18-C19	-2.19	1.49	1.54
3	A	408	CNC	C4B-C9B	-2.17	1.38	1.41
3	B	408	CNC	O7R-C2R	2.14	1.48	1.43
3	D	406	CNC	C25-C2	2.12	1.58	1.54
3	C	406	CNC	C18-C19	-2.12	1.50	1.54
3	C	406	CNC	C20-C1	2.12	1.57	1.53
3	C	406	CNC	O7R-C2R	2.10	1.47	1.43
3	D	406	CNC	C18-C19	-2.10	1.50	1.54
3	C	406	CNC	C17-C18	2.08	1.58	1.54
3	D	406	CNC	C8B-C9B	2.07	1.44	1.40
3	D	406	CNC	C56-C57	2.05	1.55	1.51
3	C	406	CNC	C56-C57	2.04	1.55	1.51

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	408	CNC	C18-C19-N24	7.07	113.11	101.88
3	A	408	CNC	C20-C1-C19	-6.26	97.68	110.23
3	C	406	CNC	C18-C19-N24	6.11	111.58	101.88
3	A	408	CNC	C1-C19-N24	5.98	115.80	106.33
3	D	406	CNC	C18-C19-N24	5.57	110.73	101.88
3	B	408	CNC	C20-C1-C19	-5.48	99.24	110.23
3	D	406	CNC	C20-C1-C19	-5.46	99.28	110.23
3	C	406	CNC	C2-C1-C19	5.38	127.95	118.72
3	A	408	CNC	C1-C19-C18	5.23	129.54	121.81
3	A	408	CNC	C2-C1-C19	5.12	127.50	118.72
3	B	408	CNC	C1-C19-C18	5.08	129.32	121.81
3	A	408	CNC	C12-C11-C10	-4.93	119.04	123.54
3	C	406	CNC	C20-C1-C19	-4.49	101.23	110.23
3	C	406	CNC	C2P-C1P-N59	-4.32	106.56	112.93
3	D	406	CNC	C2-C1-C19	4.24	126.00	118.72
3	B	408	CNC	C18-C19-N24	4.20	108.56	101.88
3	D	406	CNC	C1-C19-C18	4.00	127.72	121.81
3	B	408	CNC	C2P-C1P-N59	-3.87	107.22	112.93
3	C	406	CNC	C1-C19-N24	3.81	112.37	106.33
3	D	406	CNC	C1-C19-N24	3.80	112.35	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	406	CNC	C2-C1-N21	3.71	106.94	101.77
3	B	408	CNC	C49-C48-C13	3.57	125.04	114.73
3	B	408	CNC	C8-C9-N22	3.51	117.75	110.77
3	A	408	CNC	C12-C11-N23	3.44	115.20	111.48
3	B	408	CNC	C1-C19-N24	3.43	111.77	106.33
3	B	408	CNC	C2-C1-C19	3.33	124.44	118.72
3	B	408	CNC	C13-C14-N23	3.25	116.38	109.39
3	C	406	CNC	C12-C11-C10	-3.22	120.60	123.54
3	B	408	CNC	C36-C7-C37	3.12	115.95	110.80
3	C	406	CNC	C8-C9-N22	3.06	116.86	110.77
3	C	406	CNC	C1-C19-C18	3.02	126.27	121.81
3	B	408	CNC	O6R-C1R-C2R	-2.99	102.56	106.93
3	B	408	CNC	C60-C18-C19	2.98	121.18	114.09
3	B	408	CNC	C35-C5-C6	2.95	127.13	122.43
3	B	408	CNC	C9-C10-C11	-2.91	121.58	125.88
3	C	406	CNC	C7B-C6B-C5B	-2.88	115.06	119.91
3	C	406	CNC	C6M-C6B-C7B	2.78	127.01	120.34
3	C	406	CNC	C48-C13-C14	-2.77	103.18	109.63
3	D	406	CNC	C8-C9-N22	2.77	116.29	110.77
3	A	408	CNC	C9-C10-C11	-2.67	121.94	125.88
3	D	406	CNC	C49-C48-C13	-2.66	107.06	114.73
3	D	406	CNC	C55-C56-C57	-2.66	105.43	111.23
3	B	408	CNC	C5B-C4B-C9B	-2.62	117.51	121.22
3	C	406	CNC	C7-C6-N22	2.62	112.72	107.94
3	B	408	CNC	C2-C1-N21	2.61	105.40	101.77
3	C	406	CNC	O58-C57-C56	-2.58	117.31	122.02
3	B	408	CNC	C12-C13-C14	-2.57	98.46	101.86
3	C	406	CNC	C56-C55-C17	-2.55	110.59	115.52
3	C	406	CNC	O6R-C1R-C2R	-2.55	103.20	106.93
3	D	406	CNC	C30-C3-C4	-2.53	103.74	109.63
3	B	408	CNC	C7-C8-C9	-2.52	97.68	100.90
3	B	408	CNC	C12-C11-C10	-2.48	121.28	123.54
3	D	406	CNC	C2P-C1P-N59	-2.45	109.33	112.93
3	C	406	CNC	C60-C18-C19	2.44	119.90	114.09
3	D	406	CNC	O8R-C5R-C4R	-2.42	103.00	111.29
3	D	406	CNC	C47-C12-C46	-2.40	105.29	109.35
3	C	406	CNC	C7-C6-C5	-2.36	124.35	128.07
3	A	408	CNC	C26-C2-C1	2.33	113.64	110.01
3	D	406	CNC	C60-C18-C19	2.33	119.64	114.09
3	A	408	CNC	C8-C9-N22	2.32	115.39	110.77
3	C	406	CNC	C10-C9-N22	-2.31	123.08	125.73
3	B	408	CNC	O8R-C5R-C4R	-2.31	103.37	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	406	CNC	O58-C57-N59	2.30	127.36	123.01
3	D	406	CNC	C12-C11-C10	-2.29	121.45	123.54
3	C	406	CNC	C2-C1-N21	2.28	104.95	101.77
3	C	406	CNC	C12-C11-N23	2.27	113.94	111.48
3	B	408	CNC	C8-C9-C10	-2.26	118.43	123.32
3	A	408	CNC	C13-C12-C11	-2.25	97.84	100.90
3	C	406	CNC	C54-C17-C18	-2.25	109.66	112.98
3	A	408	CNC	C60-C18-C19	2.25	119.45	114.09
3	B	408	CNC	C6M-C6B-C7B	2.22	125.64	120.34
3	A	408	CNC	C20-C1-N21	2.16	113.81	110.27
3	A	408	CNC	C37-C7-C8	2.16	114.16	108.39
3	B	408	CNC	C48-C13-C14	-2.13	104.66	109.63
3	C	406	CNC	C3-C4-C5	-2.12	120.24	123.81
3	C	406	CNC	C7-C8-C9	-2.12	98.20	100.90
3	D	406	CNC	C7-C8-C9	-2.11	98.20	100.90
3	C	406	CNC	O8R-C5R-C4R	-2.10	104.08	111.29
3	A	408	CNC	C2P-C1P-N59	-2.09	109.85	112.93
3	C	406	CNC	C13-C14-N23	2.09	113.88	109.39
2	B	403	GOL	O2-C2-C3	2.09	118.32	109.12
3	D	406	CNC	C25-C2-C1	2.07	116.90	113.78
3	C	406	CNC	C19-N24-C16	-2.06	108.64	111.96
3	B	408	CNC	C15-C14-N23	-2.05	122.61	126.68
3	A	408	CNC	C17-C18-C19	-2.04	100.20	102.66
3	D	406	CNC	C31-C30-C3	-2.04	108.85	114.73
3	C	406	CNC	C15-C16-N24	-2.02	120.33	122.38
3	B	408	CNC	C54-C17-C55	-2.02	105.92	109.25
3	D	406	CNC	C7-C6-N22	2.01	111.60	107.94

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	408	CNC	N24
3	A	408	CNC	C19
3	B	408	CNC	N24
3	C	406	CNC	N24
3	D	406	CNC	N24

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	403	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-C3
2	B	402	GOL	C1-C2-C3-O3
2	B	403	GOL	O1-C1-C2-C3
2	B	406	GOL	C1-C2-C3-O3
2	C	402	GOL	O1-C1-C2-O2
2	C	402	GOL	C1-C2-C3-O3
2	C	402	GOL	O2-C2-C3-O3
2	D	402	GOL	C1-C2-C3-O3
2	D	404	GOL	C1-C2-C3-O3
2	D	405	GOL	O1-C1-C2-O2
5	C	404	PEG	C1-C2-O2-C3
3	D	406	CNC	C13-C48-C49-C50
5	B	409	PEG	O2-C3-C4-O4
2	A	403	GOL	O1-C1-C2-O2
2	D	404	GOL	O2-C2-C3-O3
2	A	404	GOL	O1-C1-C2-C3
2	A	405	GOL	O1-C1-C2-C3
2	A	407	GOL	O1-C1-C2-C3
2	A	407	GOL	C1-C2-C3-O3
2	B	402	GOL	O1-C1-C2-C3
2	C	401	GOL	O1-C1-C2-C3
2	C	402	GOL	O1-C1-C2-C3
2	C	403	GOL	O1-C1-C2-C3
2	C	403	GOL	C1-C2-C3-O3
2	D	401	GOL	C1-C2-C3-O3
2	D	402	GOL	O1-C1-C2-C3
2	D	405	GOL	O1-C1-C2-C3
5	C	404	PEG	O2-C3-C4-O4
2	A	407	GOL	O1-C1-C2-O2
2	B	402	GOL	O2-C2-C3-O3
2	B	406	GOL	O2-C2-C3-O3
2	C	403	GOL	O2-C2-C3-O3
2	D	402	GOL	O2-C2-C3-O3
3	B	408	CNC	C13-C48-C49-C50
2	A	405	GOL	O1-C1-C2-O2
2	B	401	GOL	O1-C1-C2-O2
2	B	403	GOL	O2-C2-C3-O3
3	A	408	CNC	C13-C48-C49-C50
5	B	409	PEG	C1-C2-O2-C3
3	A	408	CNC	C30-C31-C32-O34
2	B	402	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	404	GOL	O1-C1-C2-O2
2	B	404	GOL	O2-C2-C3-O3
2	C	403	GOL	O1-C1-C2-O2
2	D	401	GOL	O2-C2-C3-O3
2	D	402	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-C3
5	B	409	PEG	O1-C1-C2-O2
3	A	408	CNC	C30-C31-C32-N33
5	B	409	PEG	C4-C3-O2-C2
2	C	401	GOL	C1-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
3	C	406	CNC	C7-C37-C38-O39
2	C	401	GOL	O1-C1-C2-O2
3	A	408	CNC	C2-C26-C27-O28
2	A	407	GOL	O2-C2-C3-O3
2	B	404	GOL	C1-C2-C3-O3
3	D	406	CNC	C17-C18-C60-C61

There are no ring outliers.

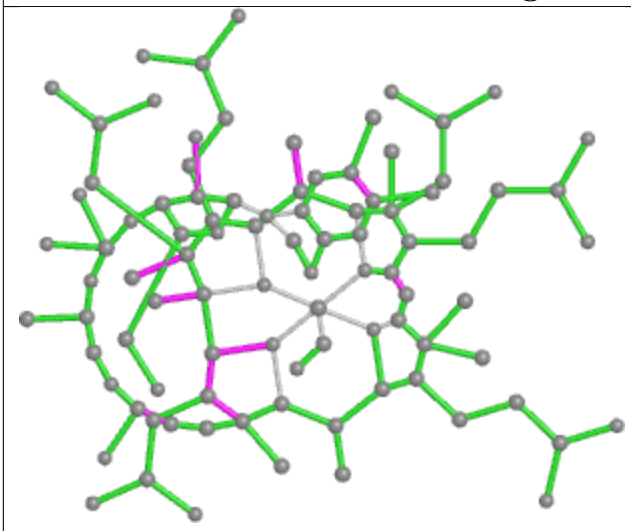
15 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	GOL	1	0
2	C	402	GOL	1	0
3	C	406	CNC	6	0
2	A	405	GOL	1	0
3	B	408	CNC	4	0
2	B	406	GOL	2	0
3	A	408	CNC	10	0
3	D	406	CNC	7	0
2	A	407	GOL	1	0
2	A	402	GOL	1	0
5	C	404	PEG	5	0
2	A	403	GOL	2	0
2	C	401	GOL	2	0
2	B	401	GOL	7	0
5	B	409	PEG	9	0

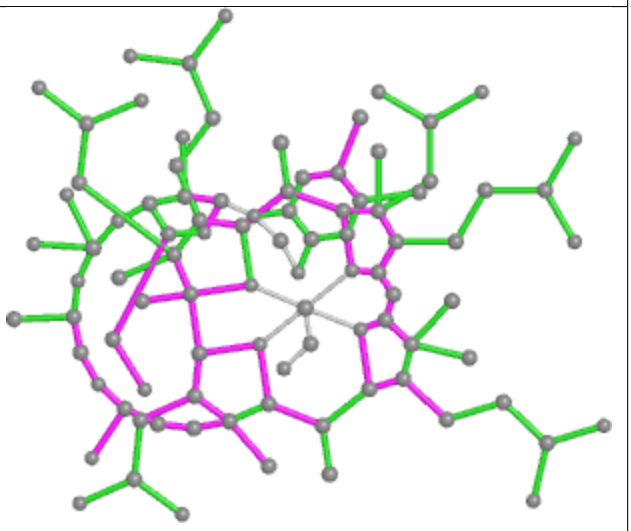
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

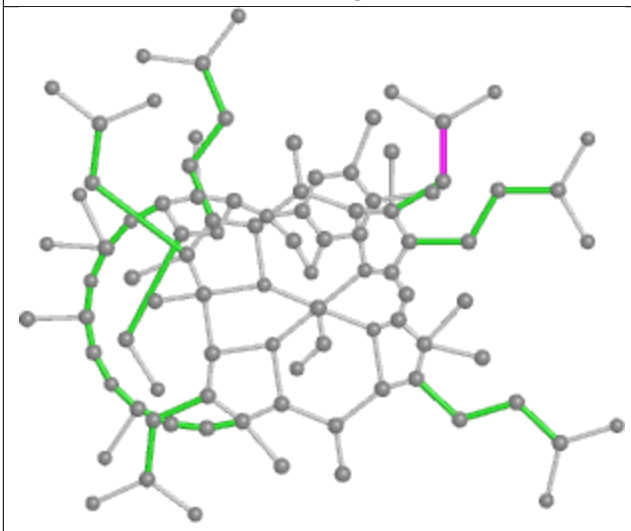
Ligand CNC C 406



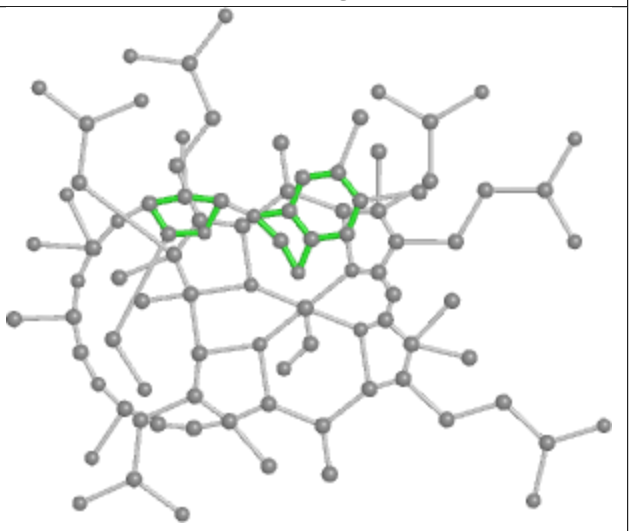
Bond lengths



Bond angles

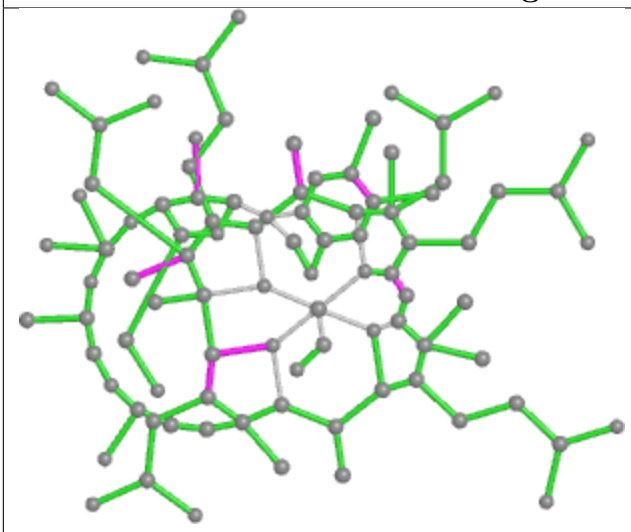


Torsions

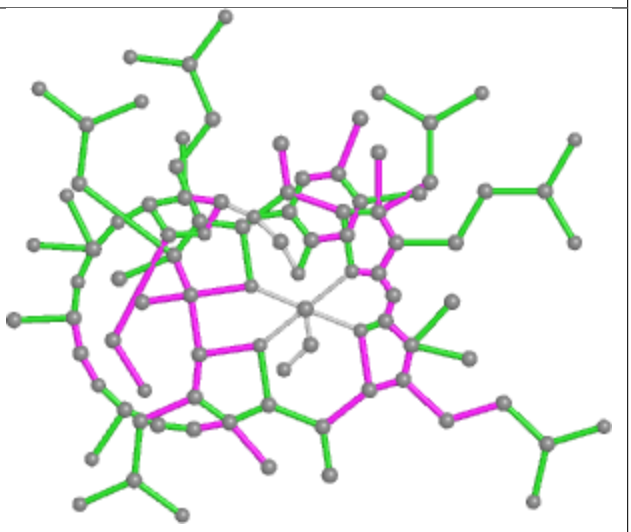


Rings

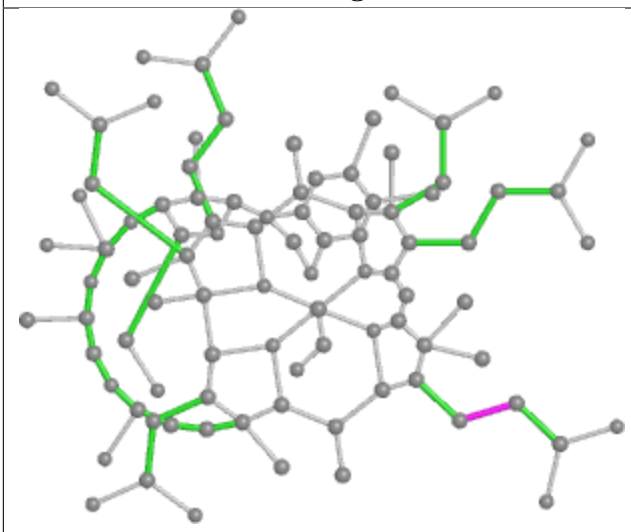
Ligand CNC B 408



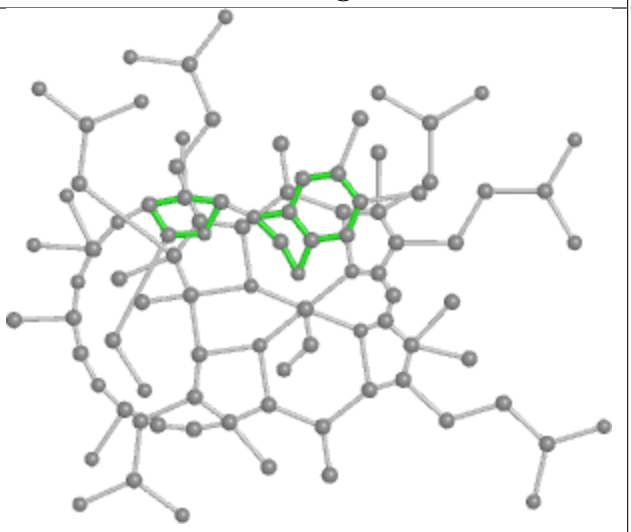
Bond lengths



Bond angles

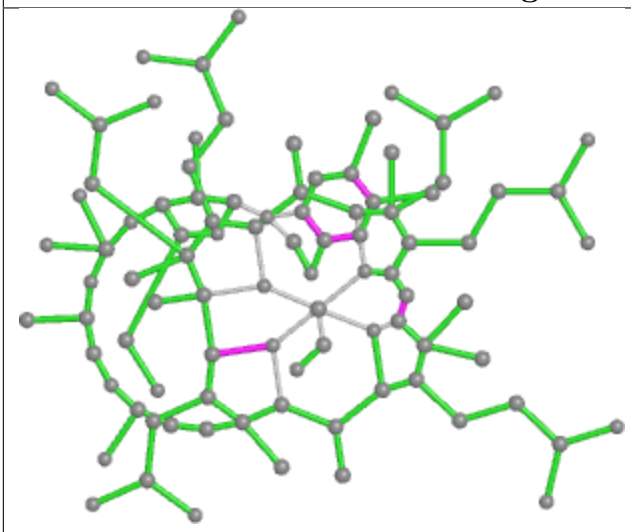


Torsions

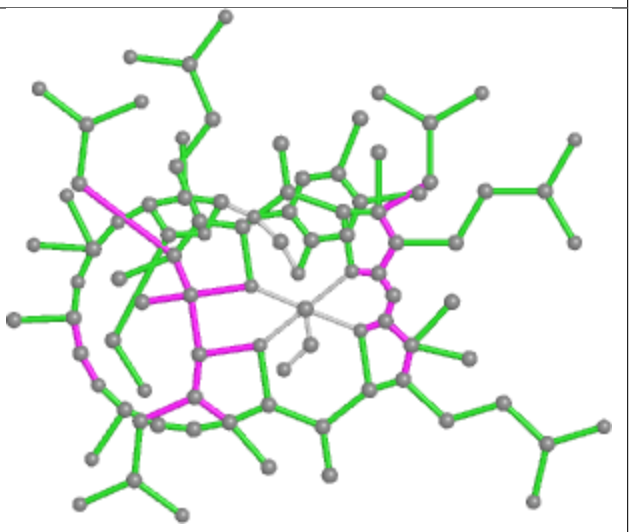


Rings

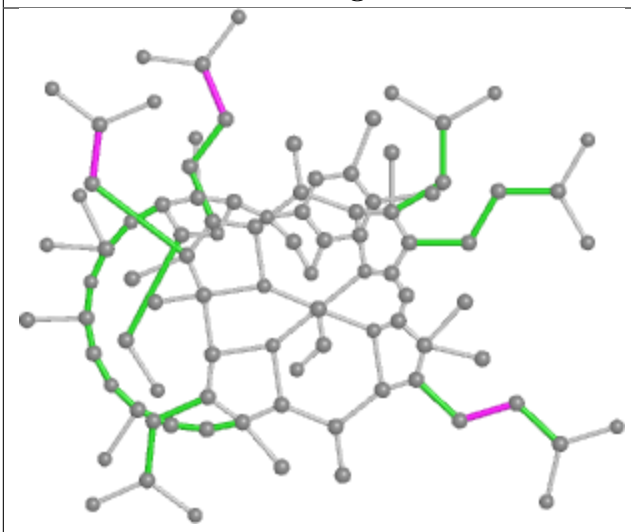
Ligand CNC A 408



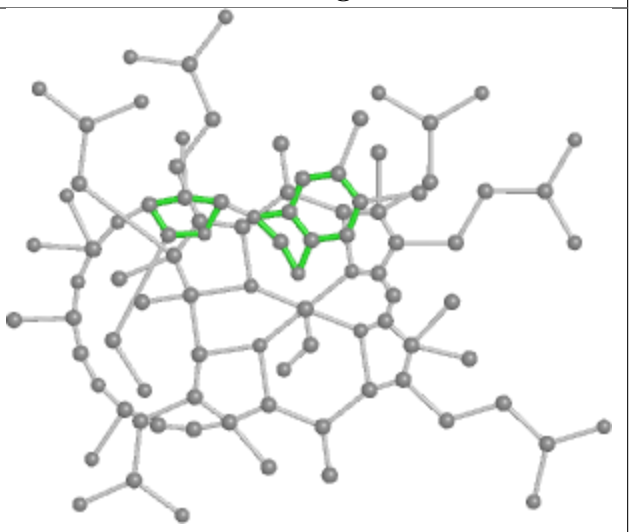
Bond lengths



Bond angles

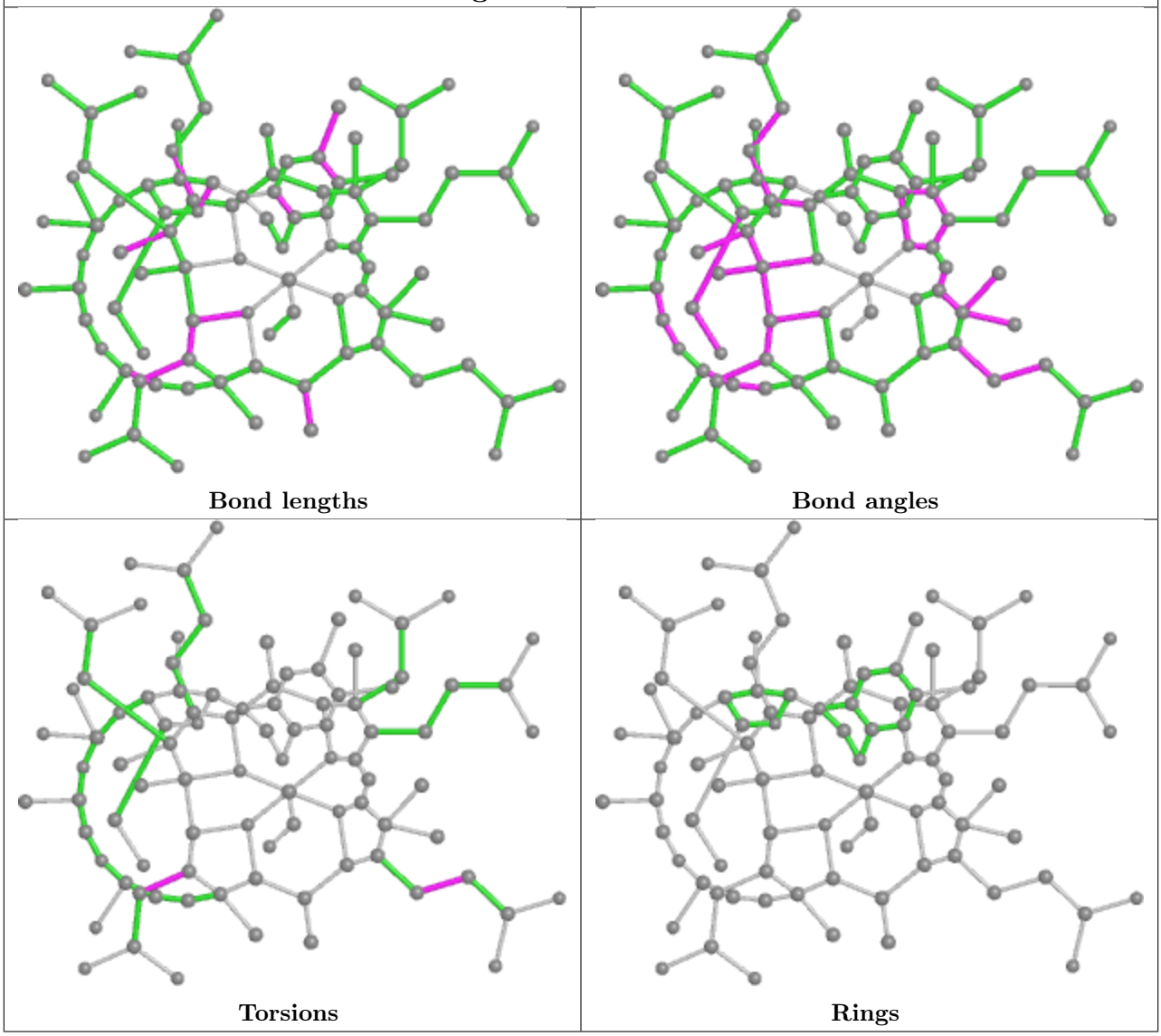


Torsions



Rings

Ligand CNC D 406



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	321/321 (100%)	-0.41	0	100	100	9, 16, 29, 36	0
1	B	320/321 (99%)	-0.36	0	100	100	9, 16, 29, 44	0
1	C	320/321 (99%)	-0.46	0	100	100	9, 16, 31, 47	0
1	D	321/321 (100%)	-0.50	0	100	100	10, 16, 31, 42	0
All	All	1282/1284 (99%)	-0.43	0	100	100	9, 16, 30, 47	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	404	6/6	0.78	0.18	39,53,56,64	0
2	GOL	C	402	6/6	0.81	0.28	32,53,59,67	0
4	SO4	B	407	5/5	0.81	0.16	69,81,86,88	0
5	PEG	C	404	7/7	0.81	0.26	33,37,42,48	0

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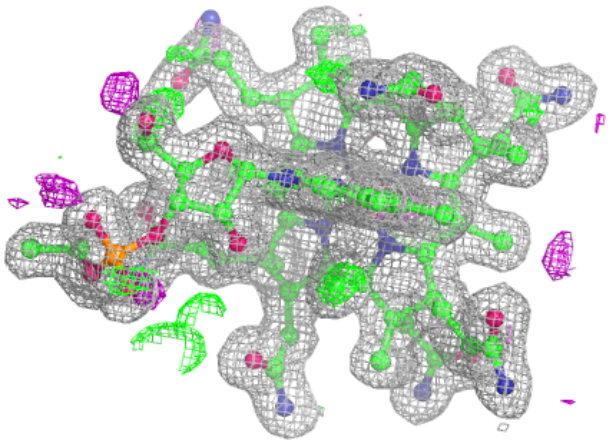
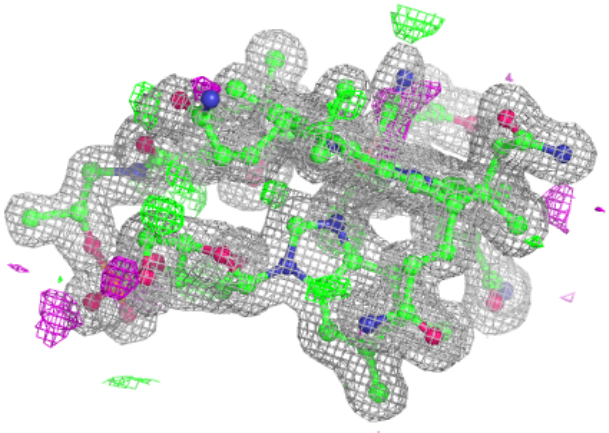
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	405	5/5	0.82	0.22	77,82,90,93	0
2	GOL	A	403	6/6	0.87	0.19	29,35,44,53	0
2	GOL	B	401	6/6	0.89	0.17	24,28,36,53	0
2	GOL	B	405	6/6	0.90	0.16	40,54,55,69	0
2	GOL	D	402	6/6	0.90	0.10	42,53,57,62	0
2	GOL	D	404	6/6	0.90	0.20	23,41,47,49	0
2	GOL	B	404	6/6	0.91	0.14	33,50,55,65	0
5	PEG	B	409	7/7	0.91	0.15	17,24,29,37	0
2	GOL	A	405	6/6	0.91	0.15	25,47,53,60	0
2	GOL	D	403	6/6	0.92	0.18	29,54,57,59	0
2	GOL	A	407	6/6	0.92	0.13	35,41,49,50	0
2	GOL	B	406	6/6	0.92	0.21	32,43,48,57	0
2	GOL	C	401	6/6	0.93	0.11	32,43,46,54	0
2	GOL	C	403	6/6	0.94	0.18	22,40,47,47	0
2	GOL	B	402	6/6	0.94	0.19	21,44,53,68	0
2	GOL	A	402	6/6	0.94	0.11	31,31,34,38	0
2	GOL	A	406	6/6	0.94	0.14	16,24,28,32	0
2	GOL	A	401	6/6	0.95	0.21	20,40,48,48	0
2	GOL	D	401	6/6	0.96	0.14	16,24,26,31	0
2	GOL	D	405	6/6	0.96	0.15	17,32,39,56	0
2	GOL	B	403	6/6	0.97	0.11	17,28,29,30	0
3	CNC	C	406	93/93	0.98	0.07	8,12,21,45	0
3	CNC	D	406	93/93	0.98	0.08	9,13,22,42	0
3	CNC	A	408	93/93	0.98	0.08	8,12,23,43	0
3	CNC	B	408	93/93	0.99	0.09	8,12,20,43	0
6	NA	D	407	1/1	0.99	0.11	31,31,31,31	0
6	NA	D	408	1/1	0.99	0.09	23,23,23,23	0

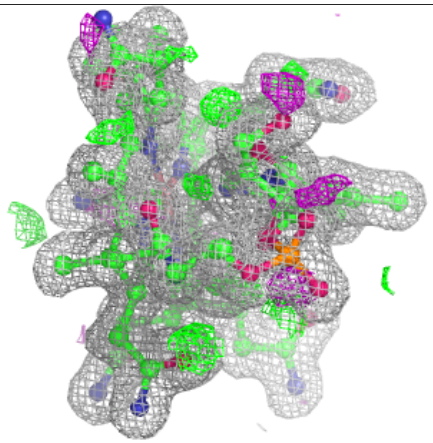
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CNC C 406:

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

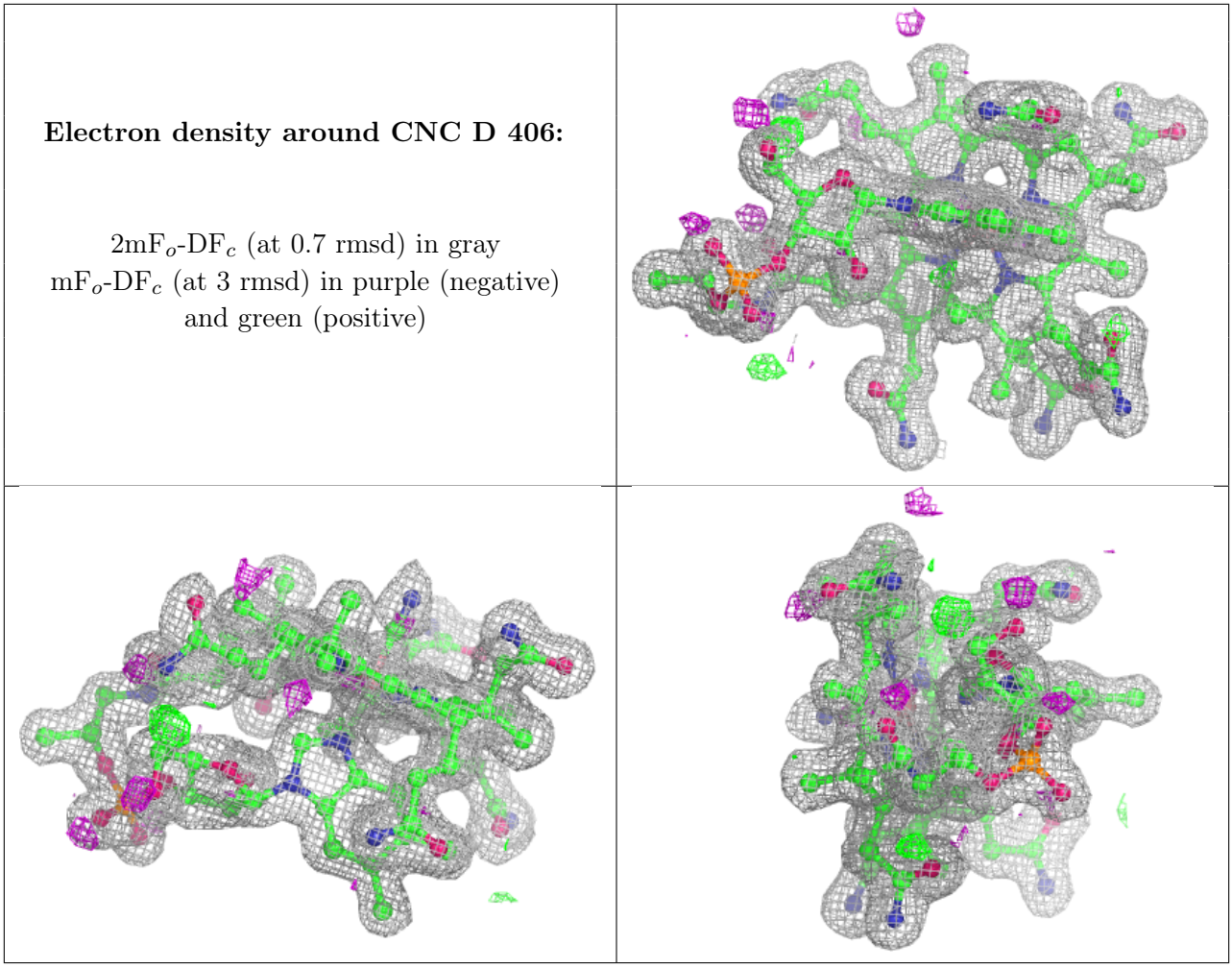






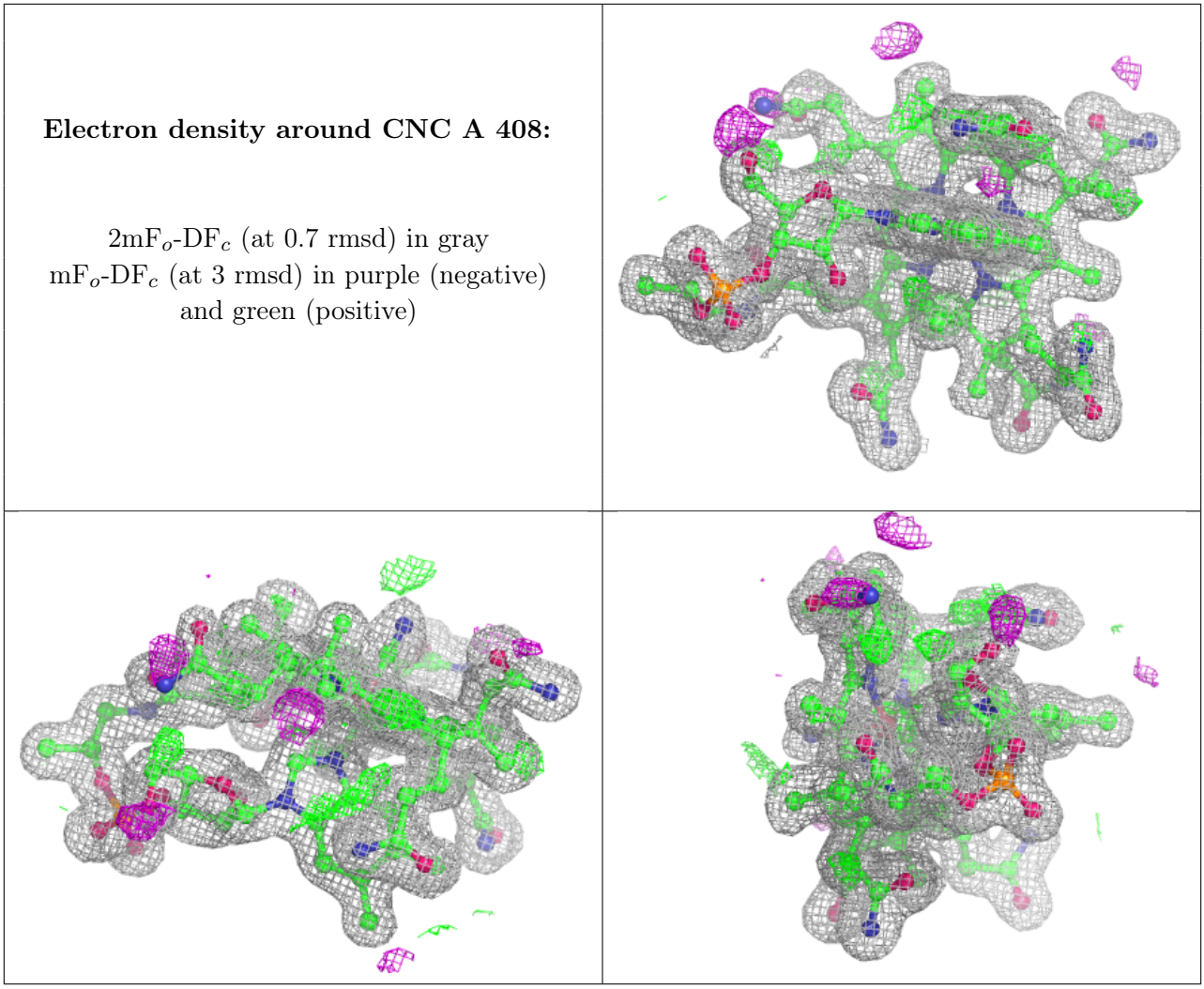
Electron density around CNC D 406:

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



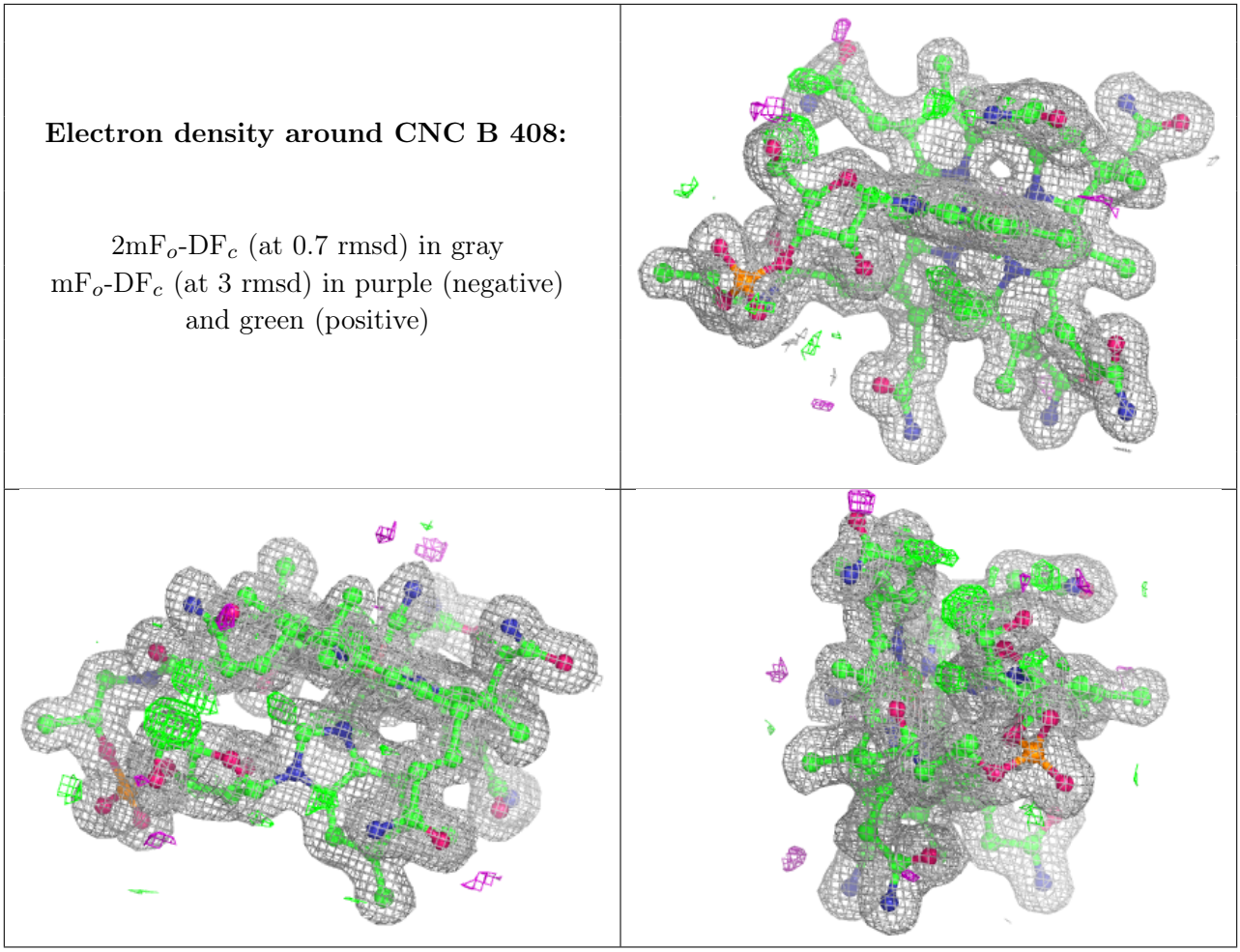
Electron density around CNC A 408:

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



Electron density around CNC B 408:

$2mF_o$-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.