Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 05:09 PM JST

PDB ID	:	7W8N
Title	:	Microbial Hormone-sensitive lipase E53 wild type
Authors	:	Yang, X.; Li, Z.; Xu, X.; Li, J.
Deposited on	:	2021-12-08
Resolution	:	1.75 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:

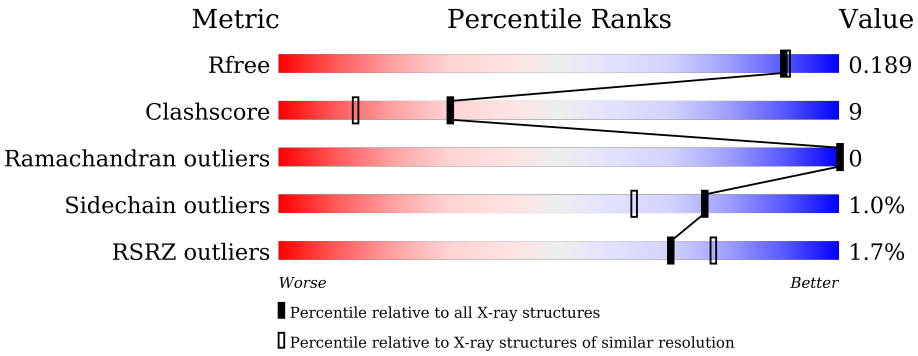
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	314	89% 8%
1	B	314	89% 8%
1	D	314	4% 88% 10%
2	C	314	2% 92% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	NPO	B	620	-	-	X	X
12	NPO	B	621	-	-	-	X
3	GOL	C	809	-	-	X	-
3	GOL	C	813	-	-	X	-
5	6NA	D	412	-	-	-	X
5	6NA	D	418	-	-	X	-
6	DMS	A	407	-	-	-	X
6	DMS	C	819	-	-	X	-
7	CCN	A	409	-	-	X	-
7	CCN	A	418	-	-	X	-
7	CCN	B	618	-	-	X	-
7	CCN	C	807	-	-	-	X
7	CCN	C	811	-	-	X	-
7	CCN	D	411	-	-	-	X
7	CCN	D	415	-	-	X	-
8	D8F	B	623	-	-	X	-
8	D8F	C	817	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 20536 atoms, of which 9530 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 Lipase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	H	N	O	S	0	0	0
			4534	1444	2257	391	430	12			
1	B	309	Total	C	H	N	O	S	0	0	0
			4559	1450	2270	391	436	12			
1	D	309	Total	C	H	N	O	S	0	0	0
			4559	1450	2270	391	436	12			

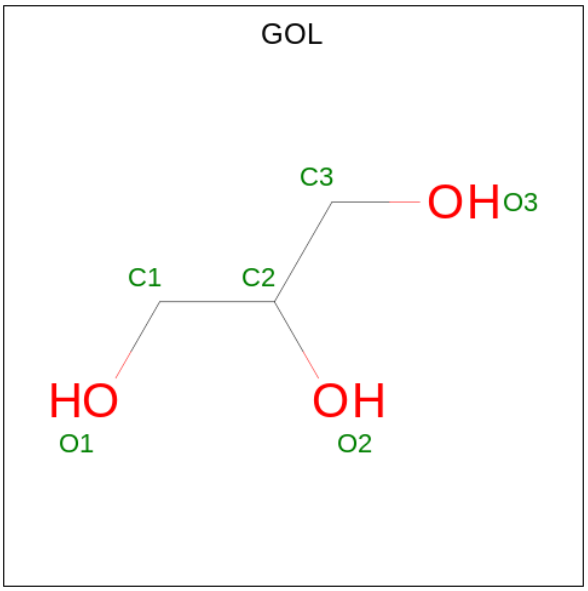
- Molecule 2 is a protein called Lipase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	309	Total	C	H	N	O	S	0	0	0
			4545	1446	2264	391	432	12			

There is a discrepancy between the modelled and reference sequences:

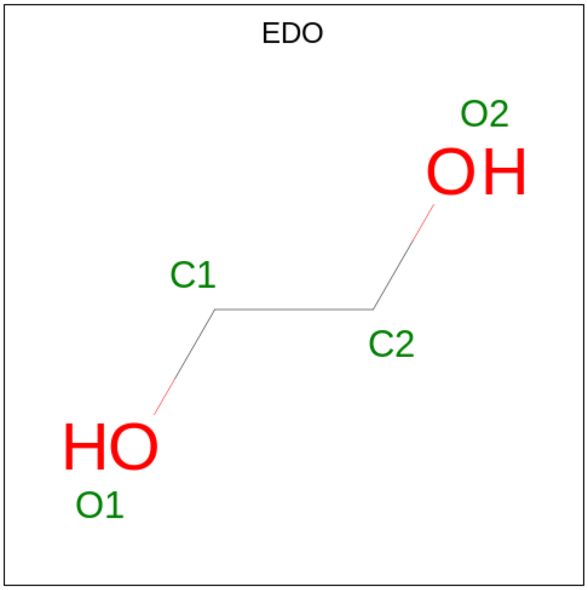
Chain	Residue	Modelled	Actual	Comment	Reference
C	204	ALA	GLU	conflict	UNP A0A074MDU6

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			9	3	3	3		
3	B	1	Total	C	H	O	0	0
			9	3	3	3		
3	C	1	Total	C	H	O	0	0
			8	3	2	3		
3	C	1	Total	C	H	O	0	0
			8	3	2	3		
3	C	1	Total	C	H	O	0	0
			9	3	3	3		
3	C	1	Total	C	H	O	0	0
			9	3	3	3		
3	C	1	Total	C	H	O	0	0
			9	3	3	3		
3	D	1	Total	C	H	O	0	0
			9	3	3	3		
3	D	1	Total	C	H	O	0	0
			8	3	2	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



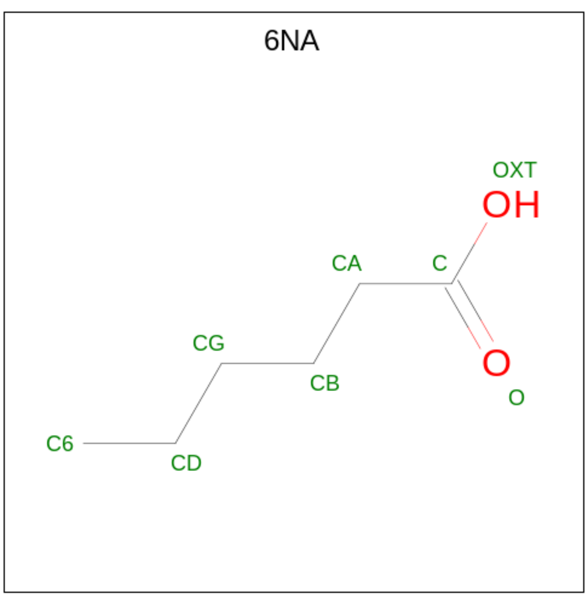
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0

Continued on next page...

Continued from previous page...

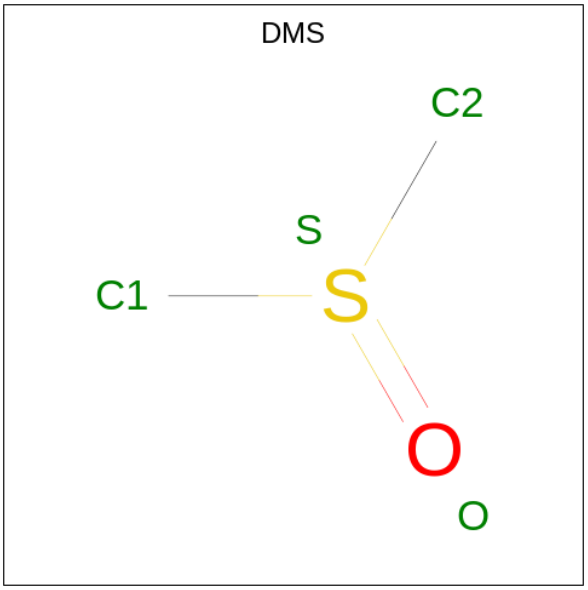
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 5 is HEXANOIC ACID (three-letter code: 6NA) (formula: $C_6H_{12}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 19 6 11 2	0	0
5	A	1	Total C H O 19 6 11 2	0	0
5	C	1	Total C H O 19 6 11 2	0	0
5	D	1	Total C H O 19 6 11 2	0	0
5	D	1	Total C H O 19 6 11 2	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



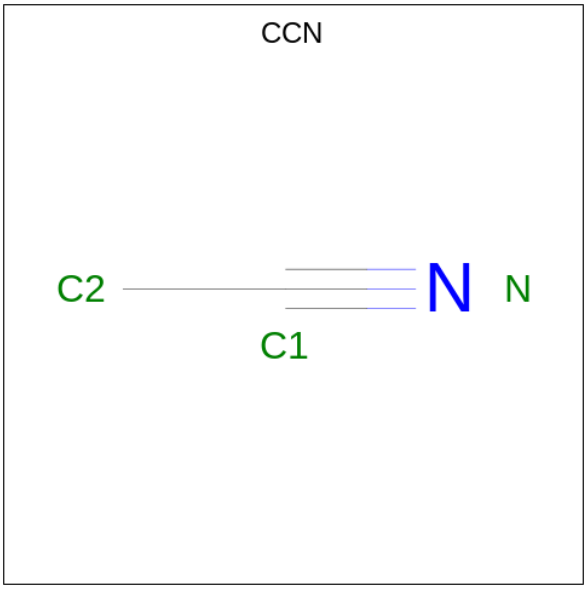
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O S 10 2 6 1 1	0	0
6	A	1	Total C H O S 10 2 6 1 1	0	0
6	A	1	Total C H O S 10 2 6 1 1	0	0
6	A	1	Total C H O S 10 2 6 1 1	0	0
6	B	1	Total C H O S 10 2 6 1 1	0	0
6	B	1	Total C H O S 10 2 6 1 1	0	0
6	B	1	Total C H O S 10 2 6 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is ACETONITRILE (three-letter code: CCN) (formula: C_2H_3N).



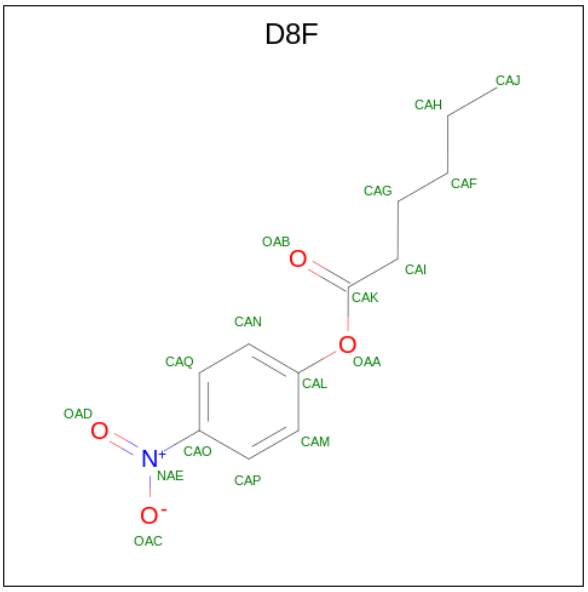
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	N	0	0
			6	2	3	1		
7	A	1	Total	C	H	N	0	0
			6	2	3	1		
7	A	1	Total	C	H	N	0	0
			6	2	3	1		
7	A	1	Total	C	H	N	0	0
			6	2	3	1		
7	A	1	Total	C	H	N	0	0
			6	2	3	1		

Continued on next page...

Continued from previous page...

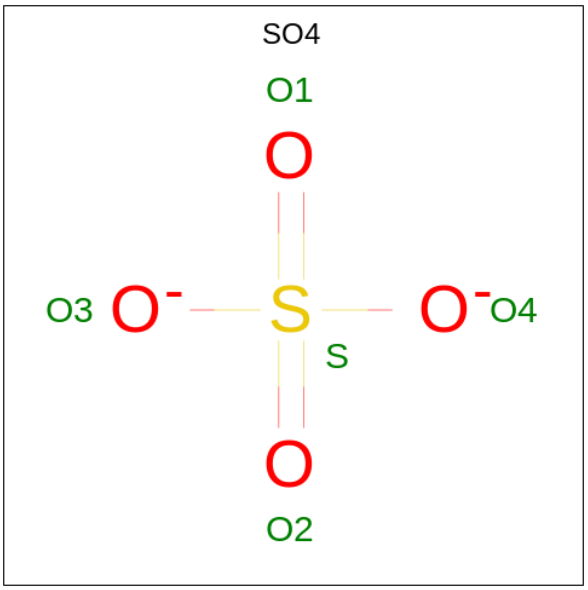
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 6	C 2	H 3	N 1	0	0
7	B	1	Total 6	C 2	H 3	N 1	0	0
7	B	1	Total 6	C 2	H 3	N 1	0	0
7	B	1	Total 6	C 2	H 3	N 1	0	0
7	B	1	Total 6	C 2	H 3	N 1	0	0
7	B	1	Total 6	C 2	H 3	N 1	0	0
7	B	1	Total 6	C 2	H 3	N 1	0	0
7	C	1	Total 6	C 2	H 3	N 1	0	0
7	C	1	Total 6	C 2	H 3	N 1	0	0
7	C	1	Total 6	C 2	H 3	N 1	0	0
7	C	1	Total 6	C 2	H 3	N 1	0	0
7	D	1	Total 6	C 2	H 3	N 1	0	0
7	D	1	Total 6	C 2	H 3	N 1	0	0
7	D	1	Total 6	C 2	H 3	N 1	0	0
7	D	1	Total 6	C 2	H 3	N 1	0	0
7	D	1	Total 6	C 2	H 3	N 1	0	0
7	D	1	Total 6	C 2	H 3	N 1	0	0
7	D	1	Total 6	C 2	H 3	N 1	0	0
7	D	1	Total 6	C 2	H 3	N 1	0	0

- Molecule 8 is (4-nitrophenyl) hexanoate (three-letter code: D8F) (formula: $C_{12}H_{15}NO_4$) (labeled as "Ligand of Interest" by depositor).



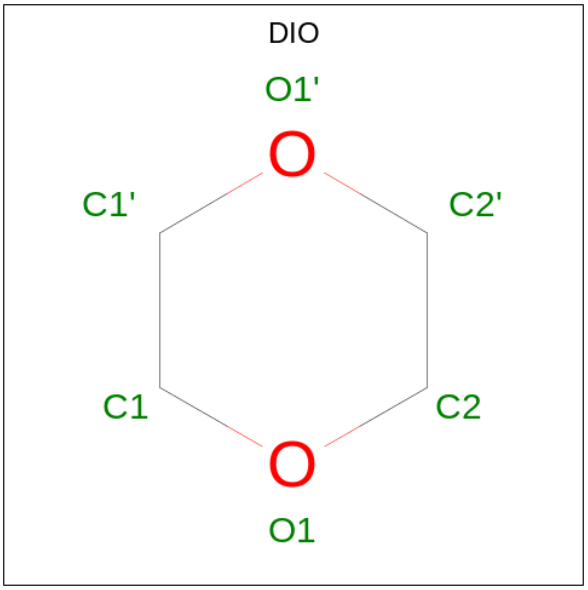
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			32	12	15	1	4		
8	B	1	Total	C	H	N	O	0	0
			32	12	15	1	4		
8	C	1	Total	C	H	N	O	0	0
			32	12	15	1	4		
8	D	1	Total	C	H	N	O	0	0
			32	12	15	1	4		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



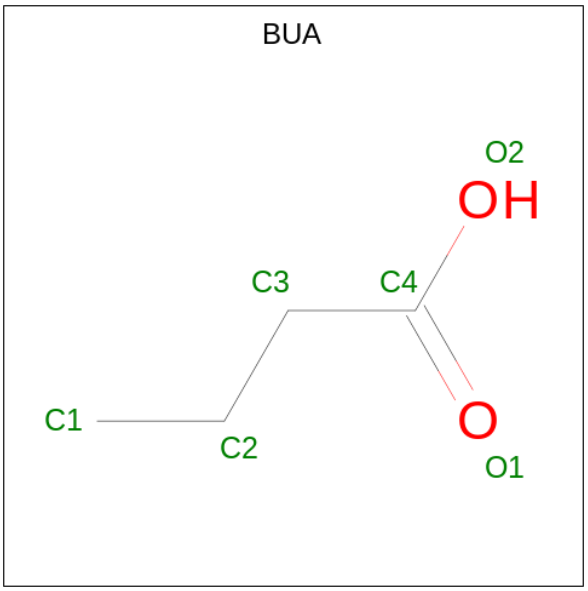
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0

- Molecule 10 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



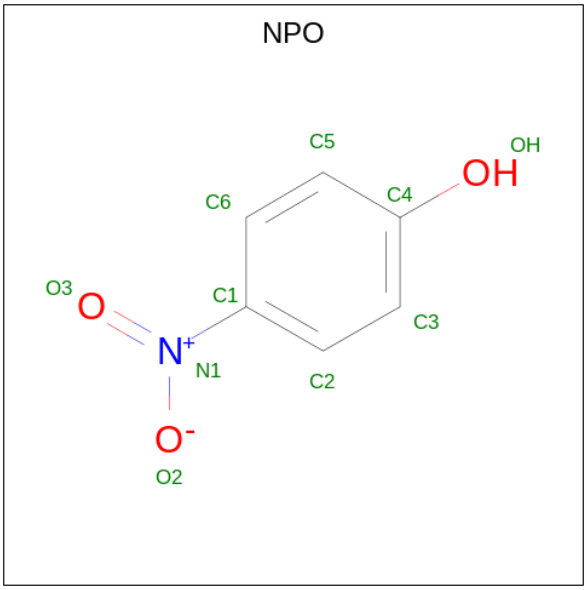
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C H O 14 4 8 2	0	0

- Molecule 11 is butanoic acid (three-letter code: BUA) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C H O 13 4 7 2	0	0

- Molecule 12 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C H N O 15 6 5 1 3	0	0
12	B	1	Total C H N O 15 6 5 1 3	0	0
12	D	1	Total C H N O 15 6 5 1 3	0	0

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total Na 1 1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	399	Total O 399 399	0	0
14	B	323	Total O 323 323	0	0

Continued on next page...

Continued from previous page...

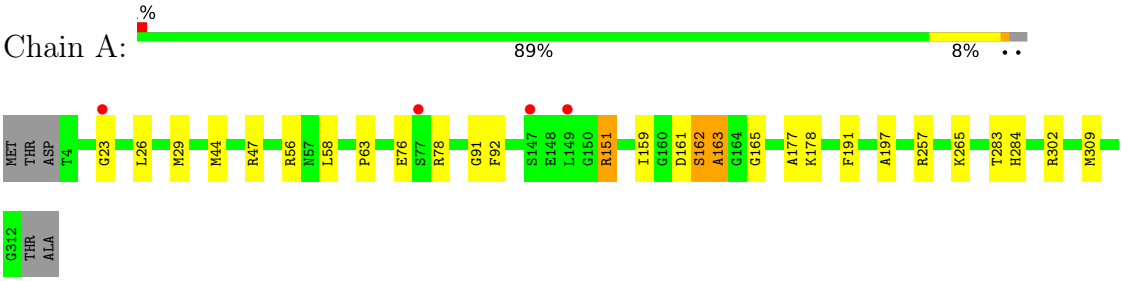
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	397	Total O 397 397	0	0
14	D	312	Total O 312 312	0	0

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.

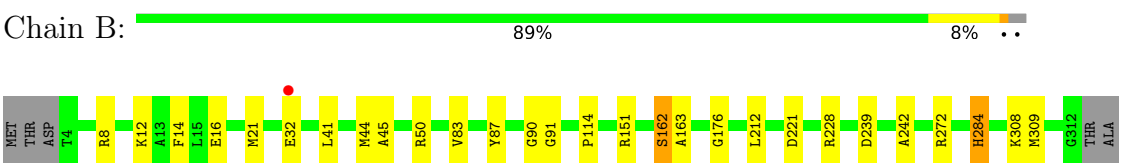
• Molecule 1: Lipase

Chain A:



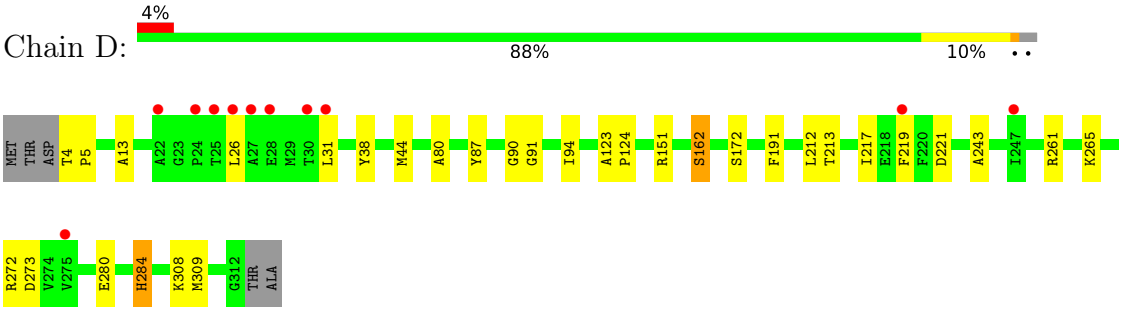
• Molecule 1: Lipase

Chain B:



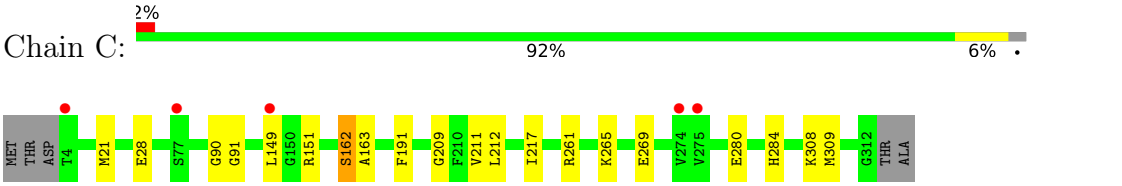
• Molecule 1: Lipase

Chain D:



• Molecule 2: Lipase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	70.58Å 129.84Å 221.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 1.75 48.71 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.71-1.75) 99.9 (48.71-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0257, PHENIX 1.18	Depositor
R, R_{free}	0.164 , 0.179 0.179 , 0.189	Depositor DCC
R_{free} test set	10276 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20536	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.07% 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: EDO, BUA, DMS, D8F, SO4, NA, NPO, 6NA, GOL, CCN, DIO

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	1/2328 (0.0%)	0.73	2/3178 (0.1%)
1	B	0.48	1/2340 (0.0%)	0.64	1/3193 (0.0%)
1	D	0.48	1/2340 (0.0%)	0.66	1/3193 (0.0%)
2	C	0.58	2/2332 (0.1%)	0.73	2/3183 (0.1%)
All	All	0.52	5/9340 (0.1%)	0.69	6/12747 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	284	HIS	CE1-NE2	-6.39	1.18	1.32
2	C	284	HIS	ND1-CE1	-5.96	1.19	1.34
1	B	284	HIS	ND1-CE1	-5.58	1.20	1.34
2	C	284	HIS	CG-ND1	-5.24	1.27	1.38
1	A	162	SER	CA-CB	-5.12	1.45	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	ALA	CB-CA-C	-6.86	99.81	110.10
1	A	162	SER	CB-CA-C	6.02	121.53	110.10
1	D	162	SER	CB-CA-C	6.01	121.52	110.10
1	B	162	SER	CB-CA-C	5.94	121.39	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	162	SER	CB-CA-C	5.79	121.10	110.10
2	C	211	VAL	N-CA-C	5.25	125.19	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2277	2257	2257	37	0
1	B	2289	2270	2269	37	1
1	D	2289	2270	2269	43	0
2	C	2281	2264	2264	33	0
3	A	6	3	8	0	0
3	B	6	3	8	0	0
3	C	30	13	37	12	0
3	D	12	5	15	2	0
4	A	16	24	24	4	0
4	B	28	42	42	2	0
4	C	32	48	48	2	0
4	D	24	36	36	2	0
5	A	16	22	22	2	0
5	C	8	11	11	0	0
5	D	16	22	22	15	0
6	A	16	24	24	6	0
6	B	20	30	30	2	0
6	C	4	6	6	4	0
6	D	12	18	18	3	0
7	A	18	18	18	5	0
7	B	18	18	18	6	0
7	C	12	12	12	5	0
7	D	24	24	24	8	0
8	A	17	15	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	17	15	0	10	0
8	C	17	15	0	9	0
8	D	17	15	0	5	0
9	A	10	0	0	0	0
10	B	6	8	8	0	0
11	B	6	7	7	2	0
12	B	20	10	10	10	1
12	D	10	5	5	3	0
13	C	1	0	0	0	0
14	A	399	0	0	13	0
14	B	323	0	0	9	0
14	C	397	0	0	10	0
14	D	312	0	0	15	0
All	All	11006	9530	9512	175	1

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 9.

All (175) 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:162:SER:OG	8:B:623:D8F:CAN	2.20	0.89
1:A:177:ALA:O	1:A:178:LYS:HE2	1.75	0.87
6:A:414:DMS:O	14:A:501:HOH:O	1.92	0.85
1:B:162:SER:OG	8:B:623:D8F:CAQ	2.29	0.81
6:D:401:DMS:S	5:D:418:6NA:H6C3	2.22	0.79
1:D:162:SER:HB2	1:D:284:HIS:CE1	2.20	0.75
1:B:45:ALA:HB2	12:B:620:NPO:H5	1.69	0.73
1:D:162:SER:HB2	1:D:284:HIS:NE2	2.03	0.73
6:C:819:DMS:H11	14:C:1194:HOH:O	1.89	0.72
12:B:620:NPO:O2	14:B:701:HOH:O	2.06	0.71
3:C:809:GOL:H11	14:D:1611:HOH:O	1.90	0.71
1:D:80:ALA:O	7:D:408:CCN:H23	1.91	0.70
2:C:91:GLY:H	8:C:817:D8F:CAN	2.04	0.70
1:B:45:ALA:HB2	12:B:620:NPO:C5	2.21	0.70
2:C:21:MET:CE	3:C:813:GOL:H12	2.22	0.69
2:C:280:GLU:HG3	5:D:418:6NA:C6	2.24	0.68
1:B:162:SER:OG	8:B:623:D8F:CAL	2.41	0.68
1:A:91:GLY:H	8:A:416:D8F:CAN	2.06	0.68
4:A:405:EDO:O1	14:A:502:HOH:O	2.11	0.66
1:B:221:ASP:OD1	1:B:228:ARG:NH2	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:280:GLU:OE1	14:C:901:HOH:O	2.15	0.65
1:D:280:GLU:OE1	14:D:1501:HOH:O	2.14	0.65
11:B:615:BUA:H12	14:B:1005:HOH:O	1.97	0.65
2:C:280:GLU:CG	5:D:418:6NA:H6C1	2.27	0.65
1:D:162:SER:OG	8:D:423:D8F:CAN	2.45	0.64
1:A:162:SER:O	1:A:165:GLY:N	2.30	0.64
7:A:418:CCN:H21	14:B:822:HOH:O	1.99	0.63
2:C:261:ARG:HH22	3:C:809:GOL:H12	1.65	0.61
1:B:91:GLY:H	8:B:623:D8F:CAN	2.13	0.61
1:B:45:ALA:HA	12:B:620:NPO:H6	1.84	0.60
1:A:56:ARG:NH1	1:A:58:LEU:HD21	2.17	0.59
1:A:177:ALA:O	1:A:178:LYS:CE	2.49	0.59
1:A:309:MET:CE	1:B:309:MET:HE3	2.32	0.58
1:A:309:MET:SD	14:B:925:HOH:O	2.57	0.58
2:C:280:GLU:CG	5:D:418:6NA:C6	2.81	0.58
4:A:412:EDO:O1	14:A:503:HOH:O	2.17	0.58
1:D:31:LEU:HD13	5:D:412:6NA:HGC2	1.86	0.58
1:A:257:ARG:HH12	5:A:403:6NA:HBC1	1.69	0.58
1:A:92:PHE:CE1	1:A:163:ALA:HB1	2.39	0.58
1:A:162:SER:OG	8:A:416:D8F:CAN	2.52	0.58
1:D:272:ARG:NE	5:D:418:6NA:O	2.37	0.56
4:C:805:EDO:HO1	3:C:809:GOL:HO2	1.52	0.56
1:A:151:ARG:O	14:A:504:HOH:O	2.17	0.56
2:C:162:SER:OG	8:C:817:D8F:CAN	2.53	0.56
2:C:309:MET:CE	1:D:309:MET:HE3	2.36	0.56
1:B:50:ARG:NH1	14:B:705:HOH:O	2.37	0.56
1:D:261:ARG:HH22	4:D:414:EDO:C1	2.19	0.55
1:A:47:ARG:HH22	6:A:414:DMS:C2	2.20	0.54
3:D:402:GOL:H12	14:D:1555:HOH:O	2.07	0.54
1:D:162:SER:OG	8:D:423:D8F:CAQ	2.55	0.54
1:D:243:ALA:O	5:D:418:6NA:O	2.25	0.54
1:D:44:MET:CE	12:D:421:NPO:O2	2.55	0.54
7:C:811:CCN:H21	14:C:1215:HOH:O	2.08	0.54
2:C:162:SER:OG	8:C:817:D8F:CAL	2.55	0.53
1:D:162:SER:CB	1:D:284:HIS:CE1	2.89	0.53
1:A:63:PRO:O	14:A:505:HOH:O	2.19	0.53
2:C:21:MET:HE1	3:C:813:GOL:C3	2.39	0.53
1:D:219:PHE:CZ	5:D:412:6NA:H6C3	2.44	0.53
1:D:162:SER:OG	8:D:423:D8F:CAL	2.58	0.52
1:B:162:SER:OG	8:B:623:D8F:CAO	2.57	0.52
1:B:176:GLY:HA3	7:B:618:CCN:H23	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HE	4:A:404:EDO:C2	2.22	0.52
1:B:242:ALA:HB3	7:B:618:CCN:H22	1.91	0.52
1:D:44:MET:HB2	7:D:415:CCN:C1	2.40	0.52
6:C:819:DMS:O	14:C:902:HOH:O	2.18	0.52
1:D:162:SER:CB	1:D:284:HIS:NE2	2.73	0.51
6:C:819:DMS:H22	14:C:1194:HOH:O	2.11	0.51
1:A:76:GLU:CB	14:A:855:HOH:O	2.57	0.51
1:B:14:PHE:CE1	12:B:620:NPO:C3	2.93	0.51
1:D:44:MET:HE2	12:D:421:NPO:O2	2.11	0.51
1:B:14:PHE:CE1	12:B:620:NPO:C2	2.93	0.51
1:B:41:LEU:CD1	12:B:620:NPO:OH	2.59	0.50
1:B:8:ARG:HB3	4:B:605:EDO:H22	1.93	0.50
14:C:1182:HOH:O	7:D:404:CCN:H23	2.10	0.50
6:D:401:DMS:O	5:D:418:6NA:H6C3	2.11	0.50
1:D:272:ARG:HB3	5:D:418:6NA:O	2.11	0.50
1:A:309:MET:HE2	1:B:309:MET:HE3	1.93	0.49
1:D:91:GLY:H	8:D:423:D8F:CAN	2.25	0.49
2:C:91:GLY:N	8:C:817:D8F:CAN	2.75	0.49
2:C:269:GLU:OE1	1:D:265:LYS:NZ	2.44	0.49
3:C:809:GOL:H32	14:D:1556:HOH:O	2.12	0.49
6:C:819:DMS:H12	14:D:1735:HOH:O	2.11	0.49
1:A:162:SER:HB2	1:A:284:HIS:CE1	2.47	0.49
1:B:162:SER:OG	8:B:623:D8F:CAM	2.60	0.49
2:C:21:MET:HE1	3:C:813:GOL:H31	1.93	0.49
2:C:149:LEU:HD23	14:C:928:HOH:O	2.13	0.49
1:A:309:MET:HE3	1:B:309:MET:HE3	1.94	0.48
1:D:44:MET:HB2	7:D:415:CCN:H22	1.94	0.48
1:A:162:SER:OG	8:A:416:D8F:CAL	2.61	0.48
1:B:12:LYS:O	1:B:16:GLU:HG2	2.13	0.48
3:C:809:GOL:C3	14:D:1556:HOH:O	2.60	0.48
1:D:308:LYS:NZ	14:D:1506:HOH:O	2.46	0.48
1:A:26:LEU:HA	1:A:29:MET:HE3	1.96	0.48
1:A:151:ARG:C	14:A:504:HOH:O	2.52	0.48
2:C:261:ARG:HH22	3:C:809:GOL:C1	2.27	0.48
1:B:44:MET:SD	12:B:621:NPO:H3	2.54	0.48
1:A:162:SER:OG	8:A:416:D8F:CAQ	2.62	0.47
1:B:163:ALA:H	8:B:623:D8F:CAQ	2.28	0.47
1:A:76:GLU:O	6:A:406:DMS:C1	2.63	0.47
1:B:41:LEU:HD12	12:B:620:NPO:OH	2.14	0.47
1:D:280:GLU:OE2	14:D:1502:HOH:O	2.20	0.47
7:D:419:CCN:H21	14:D:1686:HOH:O	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:HG22	1:B:114:PRO:HG2	1.97	0.46
2:C:28:GLU:HG3	7:C:808:CCN:H23	1.98	0.46
1:D:273:ASP:HB2	5:D:418:6NA:HAC2	1.96	0.46
1:A:159:ILE:HB	14:A:832:HOH:O	2.16	0.46
7:B:618:CCN:C2	14:B:794:HOH:O	2.64	0.46
2:C:261:ARG:HH12	3:C:809:GOL:H32	1.81	0.46
2:C:309:MET:CE	1:D:309:MET:CE	2.93	0.46
1:B:90:GLY:H	8:B:623:D8F:CAN	2.29	0.46
1:B:272:ARG:HH12	6:B:612:DMS:C1	2.28	0.46
2:C:309:MET:HE2	1:D:309:MET:HE3	1.96	0.46
1:D:4:THR:CB	1:D:5:PRO:CD	2.94	0.46
7:A:409:CCN:H21	14:A:538:HOH:O	2.15	0.45
2:C:309:MET:SD	14:D:1721:HOH:O	2.61	0.45
5:D:418:6NA:HDC2	5:D:418:6NA:HAC1	1.80	0.45
1:D:172:SER:HB2	14:D:1632:HOH:O	2.16	0.45
6:D:401:DMS:H21	14:D:1595:HOH:O	2.14	0.45
2:C:309:MET:HE3	1:D:309:MET:CE	2.46	0.45
4:B:624:EDO:C1	14:B:838:HOH:O	2.64	0.45
1:A:197:ALA:H	6:A:415:DMS:C1	2.29	0.45
1:A:91:GLY:N	8:A:416:D8F:CAN	2.75	0.45
7:A:418:CCN:H23	6:B:612:DMS:O	2.17	0.45
1:B:308:LYS:O	11:B:615:BUA:H13	2.17	0.45
1:D:123:ALA:HB1	1:D:124:PRO:HA	1.99	0.45
2:C:90:GLY:H	8:C:817:D8F:CAN	2.30	0.44
1:D:212:LEU:HD11	1:D:217:ILE:HG13	1.98	0.44
1:A:309:MET:HE3	1:B:309:MET:CE	2.47	0.44
7:A:409:CCN:C2	14:A:538:HOH:O	2.65	0.44
2:C:308:LYS:HE3	14:C:1158:HOH:O	2.17	0.44
2:C:309:MET:HE3	1:D:309:MET:HE3	1.98	0.44
7:B:618:CCN:H21	14:B:794:HOH:O	2.16	0.44
1:B:91:GLY:N	8:B:623:D8F:CAN	2.81	0.44
1:D:212:LEU:HD11	1:D:217:ILE:CG1	2.47	0.43
1:B:212:LEU:HB2	1:B:284:HIS:CD2	2.53	0.43
7:D:411:CCN:H23	14:D:1783:HOH:O	2.18	0.43
1:A:47:ARG:HH22	6:A:414:DMS:H21	1.82	0.43
7:A:408:CCN:H21	14:A:661:HOH:O	2.18	0.43
1:D:221:ASP:HB2	3:D:410:GOL:H32	1.99	0.43
1:D:273:ASP:H	5:D:418:6NA:CA	2.32	0.43
2:C:212:LEU:HD11	2:C:217:ILE:HG13	2.01	0.43
7:C:811:CCN:H22	14:C:1169:HOH:O	2.18	0.43
1:A:162:SER:O	1:A:163:ALA:C	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:607:CCN:H22	14:B:1006:HOH:O	2.18	0.43
1:A:44:MET:HB2	3:C:813:GOL:H31	2.00	0.42
1:D:261:ARG:HH22	4:D:414:EDO:H11	1.83	0.42
1:D:38:TYR:CG	1:D:94:ILE:HD12	2.54	0.42
1:D:44:MET:HB2	7:D:415:CCN:C2	2.49	0.42
5:D:418:6NA:HDC2	14:D:1603:HOH:O	2.19	0.42
1:B:44:MET:HG2	12:B:621:NPO:C2	2.50	0.42
7:D:420:CCN:H21	14:D:1665:HOH:O	2.19	0.42
2:C:162:SER:OG	8:C:817:D8F:CAM	2.68	0.42
2:C:265:LYS:HE3	4:C:818:EDO:H12	2.02	0.42
1:A:161:ASP:HB2	1:A:191:PHE:CE1	2.55	0.41
1:B:239:ASP:HB3	7:B:614:CCN:H23	2.02	0.41
2:C:163:ALA:H	8:C:817:D8F:CAQ	2.32	0.41
2:C:21:MET:HE2	3:C:813:GOL:H12	1.99	0.41
2:C:209:GLY:H	7:C:811:CCN:H23	1.85	0.41
1:A:91:GLY:HA2	8:A:416:D8F:CAQ	2.51	0.41
1:A:309:MET:CE	1:B:309:MET:CE	2.96	0.41
1:B:221:ASP:CG	1:B:228:ARG:NH2	2.74	0.41
8:C:817:D8F:OAB	14:C:903:HOH:O	2.22	0.41
1:A:92:PHE:CZ	1:A:163:ALA:HB1	2.55	0.41
1:A:265:LYS:HZ1	5:A:417:6NA:HBC1	1.84	0.41
1:D:13:ALA:HB1	12:D:421:NPO:OH	2.20	0.41
1:D:213:THR:O	1:D:217:ILE:HG13	2.21	0.41
1:B:32:GLU:HA	1:B:32:GLU:OE2	2.21	0.40
1:A:23:GLY:HA3	14:A:664:HOH:O	2.20	0.40
1:B:162:SER:CB	8:B:623:D8F:CAN	2.99	0.40
2:C:269:GLU:OE2	7:C:821:CCN:H22	2.21	0.40
4:A:405:EDO:H12	14:A:776:HOH:O	2.20	0.40
2:C:163:ALA:H	8:C:817:D8F:CAN	2.35	0.40
1:D:26:LEU:O	5:D:412:6NA:H6C1	2.21	0.40
1:D:90:GLY:H	8:D:423:D8F:CAN	2.33	0.40
1:A:76:GLU:O	6:A:406:DMS:H13	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:MET:SD	12:B:621:NPO:OH[2_754]	2.14	0.06

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	307/314 (98%)	300 (98%)	7 (2%)	0	100	100
1	B	307/314 (98%)	301 (98%)	6 (2%)	0	100	100
1	D	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
2	C	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
All	All	1228/1256 (98%)	1199 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	232/240 (97%)	230 (99%)	2 (1%)	78	67
1	B	235/240 (98%)	233 (99%)	2 (1%)	78	67
1	D	235/240 (98%)	232 (99%)	3 (1%)	69	54
2	C	233/239 (98%)	231 (99%)	2 (1%)	78	67
All	All	935/959 (98%)	926 (99%)	9 (1%)	76	63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	151	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	87	TYR
1	B	151	ARG
2	C	151	ARG
2	C	191	PHE
1	D	87	TYR
1	D	151	ARG
1	D	191	PHE

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 88 ligands modelled in this entry, 1 is monoatomic - leaving 87 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	$\#\|Z\| > 2$
8	D8F	B	623	-	16,17,17	3.38	7 (43%)	19,21,21	1.53	3 (15%)
4	EDO	C	804	-	3,3,3	0.41	0	2,2,2	0.72	0
9	SO4	A	419	-	4,4,4	0.12	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	B	601	-	3,3,3	0.51	0	2,2,2	0.15	0
4	EDO	A	404	-	3,3,3	0.55	0	2,2,2	0.07	0
3	GOL	D	402	-	5,5,5	0.92	0	5,5,5	1.46	1 (20%)
7	CCN	C	811	-	2,2,2	0.91	0	1,1,1	0.36	0
7	CCN	D	415	-	2,2,2	0.94	0	1,1,1	0.44	0
6	DMS	D	409	-	3,3,3	0.72	0	3,3,3	0.60	0
7	CCN	B	614	-	2,2,2	0.93	0	1,1,1	0.16	0
4	EDO	D	422	-	3,3,3	0.48	0	2,2,2	0.30	0
3	GOL	C	802	-	5,5,5	1.36	0	5,5,5	1.37	0
3	GOL	A	401	-	5,5,5	1.25	1 (20%)	5,5,5	0.79	0
7	CCN	D	416	-	2,2,2	0.94	0	1,1,1	0.48	0
4	EDO	B	605	-	3,3,3	0.43	0	2,2,2	0.45	0
4	EDO	B	603	-	3,3,3	0.35	0	2,2,2	0.80	0
6	DMS	D	401	-	3,3,3	0.70	0	3,3,3	0.97	0
3	GOL	D	410	-	5,5,5	0.84	0	5,5,5	1.25	1 (20%)
3	GOL	C	809	-	5,5,5	1.26	0	5,5,5	1.21	1 (20%)
7	CCN	A	408	-	2,2,2	0.87	0	1,1,1	0.29	0
4	EDO	B	602	-	3,3,3	0.23	0	2,2,2	0.92	0
4	EDO	D	403	-	3,3,3	0.53	0	2,2,2	0.29	0
7	CCN	C	808	-	2,2,2	0.85	0	1,1,1	0.35	0
6	DMS	A	414	-	3,3,3	0.68	0	3,3,3	0.81	0
12	NPO	D	421	-	9,10,10	1.26	1 (11%)	11,13,13	0.77	0
6	DMS	A	415	-	3,3,3	0.75	0	3,3,3	0.84	0
7	CCN	B	613	-	2,2,2	0.88	0	1,1,1	0.49	0
7	CCN	A	413	-	2,2,2	0.88	0	1,1,1	0.28	0
7	CCN	B	607	-	2,2,2	0.93	0	1,1,1	0.26	0
3	GOL	C	813	-	5,5,5	1.29	0	5,5,5	0.73	0
7	CCN	B	609	-	2,2,2	0.94	0	1,1,1	0.38	0
7	CCN	C	821	-	2,2,2	1.03	0	1,1,1	0.39	0
7	CCN	A	418	-	2,2,2	0.96	0	1,1,1	0.27	0
4	EDO	D	406	-	3,3,3	0.39	0	2,2,2	0.60	0
4	EDO	A	412	-	3,3,3	0.56	0	2,2,2	0.12	0
9	SO4	A	420	-	4,4,4	0.16	0	6,6,6	0.13	0
7	CCN	A	409	-	2,2,2	0.90	0	1,1,1	0.38	0
11	BUA	B	615	-	5,5,5	1.10	0	5,5,5	1.29	1 (20%)
6	DMS	B	616	-	3,3,3	0.73	0	3,3,3	0.75	0
6	DMS	B	611	-	3,3,3	0.69	0	3,3,3	0.73	0
7	CCN	D	417	-	2,2,2	0.97	0	1,1,1	0.49	0
5	6NA	A	403	-	7,7,7	0.94	0	7,7,7	1.53	1 (14%)
4	EDO	D	407	-	3,3,3	0.57	0	2,2,2	0.20	0
6	DMS	B	622	-	3,3,3	0.70	0	3,3,3	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	CCN	D	420	-	2,2,2	0.91	0	1,1,1	0.20	0
4	EDO	B	624	-	3,3,3	0.37	0	2,2,2	0.25	0
6	DMS	D	413	-	3,3,3	0.71	0	3,3,3	0.80	0
4	EDO	A	402	-	3,3,3	0.32	0	2,2,2	0.57	0
6	DMS	B	612	-	3,3,3	0.67	0	3,3,3	0.96	0
4	EDO	C	812	-	3,3,3	0.62	0	2,2,2	0.20	0
7	CCN	D	419	-	2,2,2	0.98	0	1,1,1	0.28	0
6	DMS	B	617	-	3,3,3	0.67	0	3,3,3	0.67	0
4	EDO	D	405	-	3,3,3	0.48	0	2,2,2	0.23	0
7	CCN	A	411	-	2,2,2	0.90	0	1,1,1	0.42	0
7	CCN	D	408	-	2,2,2	0.89	0	1,1,1	0.07	0
4	EDO	C	806	-	3,3,3	0.46	0	2,2,2	0.65	0
5	6NA	D	418	-	7,7,7	0.87	1 (14%)	7,7,7	1.42	1 (14%)
7	CCN	D	404	-	2,2,2	0.89	0	1,1,1	0.38	0
3	GOL	C	816	-	5,5,5	0.80	0	5,5,5	1.24	0
4	EDO	B	606	-	3,3,3	0.48	0	2,2,2	0.28	0
4	EDO	C	801	-	3,3,3	0.41	0	2,2,2	0.43	0
3	GOL	C	814	-	5,5,5	0.61	0	5,5,5	1.17	0
3	GOL	B	619	-	5,5,5	0.84	0	5,5,5	1.02	0
7	CCN	C	807	-	2,2,2	0.88	0	1,1,1	0.34	0
5	6NA	C	810	-	7,7,7	1.03	0	7,7,7	1.10	0
4	EDO	B	608	-	3,3,3	0.50	0	2,2,2	0.45	0
6	DMS	C	819	-	3,3,3	0.68	0	3,3,3	0.72	0
12	NPO	B	621	-	9,10,10	1.13	1 (11%)	11,13,13	0.96	1 (9%)
6	DMS	A	407	-	3,3,3	0.68	0	3,3,3	0.61	0
4	EDO	A	405	-	3,3,3	0.52	0	2,2,2	0.09	0
5	6NA	A	417	-	7,7,7	0.97	0	7,7,7	1.44	1 (14%)
8	D8F	D	423	-	16,17,17	3.59	8 (50%)	19,21,21	1.58	3 (15%)
7	CCN	A	410	-	2,2,2	0.91	0	1,1,1	0.42	0
8	D8F	C	817	-	16,17,17	3.09	7 (43%)	19,21,21	1.59	2 (10%)
4	EDO	C	805	-	3,3,3	0.45	0	2,2,2	0.44	0
7	CCN	D	411	-	2,2,2	0.91	0	1,1,1	0.29	0
10	DIO	B	604	-	6,6,6	0.69	0	6,6,6	0.71	0
5	6NA	D	412	-	7,7,7	0.92	0	7,7,7	1.22	0
7	CCN	B	610	-	2,2,2	0.97	0	1,1,1	0.12	0
4	EDO	C	815	-	3,3,3	0.54	0	2,2,2	0.33	0
4	EDO	C	818	-	3,3,3	0.49	0	2,2,2	0.25	0
4	EDO	D	414	-	3,3,3	0.46	0	2,2,2	0.85	0
4	EDO	C	803	-	3,3,3	0.48	0	2,2,2	0.24	0
12	NPO	B	620	-	9,10,10	1.34	1 (11%)	11,13,13	4.13	2 (18%)
7	CCN	B	618	-	2,2,2	0.89	0	1,1,1	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	D8F	A	416	-	16,17,17	3.29	8 (50%)	19,21,21	1.84	3 (15%)
6	DMS	A	406	-	3,3,3	0.63	0	3,3,3	0.88	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
8	D8F	B	623	-	-	7/11/13/13	0/1/1/1
3	GOL	C	814	-	-	2/4/4/4	-
3	GOL	B	619	-	-	4/4/4/4	-
12	NPO	D	421	-	-	0/2/4/4	0/1/1/1
4	EDO	C	804	-	-	0/1/1/1	-
4	EDO	B	601	-	-	1/1/1/1	-
4	EDO	B	624	-	-	1/1/1/1	-
5	6NA	C	810	-	-	4/5/5/5	-
4	EDO	B	608	-	-	1/1/1/1	-
4	EDO	A	402	-	-	1/1/1/1	-
4	EDO	C	812	-	-	1/1/1/1	-
12	NPO	B	621	-	-	2/2/4/4	0/1/1/1
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	D	405	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
5	6NA	A	417	-	-	1/5/5/5	-
8	D8F	D	423	-	-	5/11/13/13	0/1/1/1
3	GOL	D	402	-	-	2/4/4/4	-
3	GOL	C	813	-	-	2/4/4/4	-
8	D8F	C	817	-	-	5/11/13/13	0/1/1/1
4	EDO	D	422	-	-	1/1/1/1	-
4	EDO	C	805	-	-	1/1/1/1	-
3	GOL	C	802	-	-	3/4/4/4	-
4	EDO	C	806	-	-	1/1/1/1	-
4	EDO	D	406	-	-	0/1/1/1	-
5	6NA	D	418	-	-	4/5/5/5	-
3	GOL	A	401	-	-	1/4/4/4	-
4	EDO	A	412	-	-	0/1/1/1	-
4	EDO	B	605	-	-	1/1/1/1	-
10	DIO	B	604	-	-	-	0/1/1/1
4	EDO	B	603	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BUA	B	615	-	-	1/3/3/3	-
5	6NA	D	412	-	-	3/5/5/5	-
4	EDO	C	815	-	-	1/1/1/1	-
3	GOL	C	816	-	-	1/4/4/4	-
3	GOL	D	410	-	-	4/4/4/4	-
3	GOL	C	809	-	-	4/4/4/4	-
4	EDO	B	606	-	-	1/1/1/1	-
4	EDO	C	801	-	-	0/1/1/1	-
4	EDO	C	818	-	-	1/1/1/1	-
4	EDO	C	803	-	-	0/1/1/1	-
4	EDO	B	602	-	-	0/1/1/1	-
4	EDO	D	403	-	-	1/1/1/1	-
4	EDO	D	414	-	-	1/1/1/1	-
12	NPO	B	620	-	-	0/2/4/4	0/1/1/1
5	6NA	A	403	-	-	4/5/5/5	-
4	EDO	D	407	-	-	1/1/1/1	-
8	D8F	A	416	-	-	6/11/13/13	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	423	D8F	CAP-CAM	8.00	1.53	1.38
8	B	623	D8F	CAP-CAM	7.55	1.52	1.38
8	A	416	D8F	CAP-CAM	7.39	1.52	1.38
8	D	423	D8F	CAQ-CAO	7.04	1.52	1.38
8	C	817	D8F	CAP-CAM	6.55	1.50	1.38
8	C	817	D8F	CAQ-CAO	6.47	1.51	1.38
8	A	416	D8F	CAQ-CAO	6.39	1.51	1.38
8	B	623	D8F	CAQ-CAO	6.38	1.51	1.38
8	D	423	D8F	CAN-CAL	6.35	1.51	1.38
8	B	623	D8F	CAN-CAL	5.85	1.50	1.38
8	A	416	D8F	CAN-CAL	4.66	1.48	1.38
8	C	817	D8F	CAN-CAL	4.24	1.47	1.38
8	C	817	D8F	CAP-CAO	-3.96	1.31	1.38
8	B	623	D8F	CAP-CAO	-3.90	1.31	1.38
8	A	416	D8F	CAQ-CAN	-3.88	1.31	1.38
8	D	423	D8F	CAQ-CAN	-3.86	1.31	1.38
8	A	416	D8F	CAP-CAO	-3.83	1.31	1.38
8	C	817	D8F	CAQ-CAN	-3.81	1.31	1.38
8	D	423	D8F	CAP-CAO	-3.74	1.31	1.38
8	B	623	D8F	CAQ-CAN	-3.67	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	421	NPO	O3-N1	-3.51	1.16	1.22
12	B	620	NPO	O3-N1	-3.31	1.17	1.22
8	D	423	D8F	CAM-CAL	-3.13	1.32	1.38
8	B	623	D8F	CAM-CAL	-3.08	1.32	1.38
8	A	416	D8F	CAM-CAL	-3.07	1.32	1.38
8	C	817	D8F	CAM-CAL	-2.88	1.32	1.38
12	B	621	NPO	O3-N1	-2.73	1.18	1.22
8	A	416	D8F	OAD-NAE	-2.63	1.18	1.22
8	B	623	D8F	OAA-CAK	2.23	1.42	1.35
8	D	423	D8F	OAD-NAE	-2.23	1.19	1.22
3	A	401	GOL	C1-C2	2.19	1.60	1.51
8	D	423	D8F	OAA-CAK	2.16	1.42	1.35
8	A	416	D8F	OAA-CAK	2.13	1.42	1.35
5	D	418	6NA	OXT-C	-2.11	1.23	1.30
8	C	817	D8F	OAD-NAE	-2.05	1.19	1.22

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	620	NPO	C6-C1-N1	9.85	126.79	119.38
12	B	620	NPO	C2-C1-N1	-8.94	112.65	119.38
8	C	817	D8F	CAL-OAA-CAK	-4.79	106.92	119.42
8	D	423	D8F	OAA-CAK-CAI	4.40	123.39	110.67
8	A	416	D8F	OAA-CAK-CAI	4.40	123.38	110.67
8	B	623	D8F	OAA-CAK-CAI	4.21	122.84	110.67
8	A	416	D8F	CAP-CAO-NAE	3.82	122.25	119.38
8	A	416	D8F	CAL-OAA-CAK	-3.19	111.11	119.42
5	A	403	6NA	CB-CA-C	-3.10	106.66	114.47
8	C	817	D8F	OAA-CAK-CAI	3.06	119.53	110.67
5	D	418	6NA	OXT-C-CA	2.73	122.81	114.03
12	B	621	NPO	C6-C1-N1	2.70	121.41	119.38
8	B	623	D8F	CAP-CAO-NAE	2.55	121.30	119.38
5	A	417	6NA	OXT-C-CA	2.47	121.96	114.03
8	B	623	D8F	CAL-OAA-CAK	-2.33	113.34	119.42
3	D	402	GOL	C3-C2-C1	-2.21	103.10	111.70
8	D	423	D8F	CAP-CAO-NAE	2.18	121.01	119.38
3	D	410	GOL	C3-C2-C1	-2.17	103.25	111.70
8	D	423	D8F	OAA-CAK-OAB	-2.14	118.75	122.84
11	B	615	BUA	O2-C4-C3	2.08	120.71	114.03
3	C	809	GOL	C3-C2-C1	-2.06	103.69	111.70

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	619	GOL	O1-C1-C2-O2
3	B	619	GOL	O1-C1-C2-C3
3	B	619	GOL	C1-C2-C3-O3
3	C	802	GOL	C1-C2-C3-O3
3	C	802	GOL	O2-C2-C3-O3
3	C	809	GOL	O1-C1-C2-C3
3	C	809	GOL	C1-C2-C3-O3
3	C	813	GOL	C1-C2-C3-O3
3	C	814	GOL	C1-C2-C3-O3
3	C	814	GOL	O2-C2-C3-O3
3	C	816	GOL	O1-C1-C2-C3
3	D	410	GOL	C1-C2-C3-O3
4	D	403	EDO	O1-C1-C2-O2
8	A	416	D8F	CAI-CAK-OAA-CAL
8	A	416	D8F	OAB-CAK-OAA-CAL
8	B	623	D8F	CAI-CAK-OAA-CAL
8	B	623	D8F	OAB-CAK-OAA-CAL
8	C	817	D8F	CAI-CAK-OAA-CAL
8	C	817	D8F	OAB-CAK-OAA-CAL
8	D	423	D8F	CAI-CAK-OAA-CAL
8	D	423	D8F	OAB-CAK-OAA-CAL
12	B	621	NPO	C2-C1-N1-O3
12	B	621	NPO	C6-C1-N1-O3
5	D	418	6NA	CA-CB-CG-CD
5	D	418	6NA	C-CA-CB-CG
5	A	403	6NA	CA-CB-CG-CD
5	C	810	6NA	CA-CB-CG-CD
3	A	401	GOL	O1-C1-C2-C3
3	D	402	GOL	C1-C2-C3-O3
3	D	410	GOL	O1-C1-C2-C3
3	B	619	GOL	O2-C2-C3-O3
3	C	809	GOL	O1-C1-C2-O2
3	C	813	GOL	O2-C2-C3-O3
3	D	402	GOL	O2-C2-C3-O3
3	D	410	GOL	O1-C1-C2-O2
3	D	410	GOL	O2-C2-C3-O3
4	B	601	EDO	O1-C1-C2-O2
4	B	605	EDO	O1-C1-C2-O2
4	B	606	EDO	O1-C1-C2-O2
4	C	805	EDO	O1-C1-C2-O2
4	D	422	EDO	O1-C1-C2-O2
8	B	623	D8F	CAF-CAG-CAI-CAK

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	809	GOL	O2-C2-C3-O3
5	C	810	6NA	C6-CD-CG-CB
4	B	624	EDO	O1-C1-C2-O2
4	C	818	EDO	O1-C1-C2-O2
4	D	407	EDO	O1-C1-C2-O2
8	B	623	D8F	CAM-CAL-OAA-CAK
5	A	417	6NA	CA-CB-CG-CD
8	D	423	D8F	CAH-CAF-CAG-CAI
8	B	623	D8F	CAN-CAL-OAA-CAK
3	C	802	GOL	O1-C1-C2-O2
5	D	412	6NA	C6-CD-CG-CB
8	A	416	D8F	CAM-CAL-OAA-CAK
8	A	416	D8F	CAN-CAL-OAA-CAK
4	A	404	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2
4	C	812	EDO	O1-C1-C2-O2
4	D	405	EDO	O1-C1-C2-O2
8	A	416	D8F	CAH-CAF-CAG-CAI
5	A	403	6NA	C-CA-CB-CG
8	C	817	D8F	CAM-CAL-OAA-CAK
8	B	623	D8F	CAG-CAF-CAH-CAJ
8	C	817	D8F	CAN-CAL-OAA-CAK
8	A	416	D8F	CAG-CAF-CAH-CAJ
8	B	623	D8F	CAH-CAF-CAG-CAI
4	D	414	EDO	O1-C1-C2-O2
5	C	810	6NA	O-C-CA-CB
5	A	403	6NA	OXT-C-CA-CB
11	B	615	BUA	C1-C2-C3-C4
5	A	403	6NA	O-C-CA-CB
5	C	810	6NA	OXT-C-CA-CB
8	D	423	D8F	CAF-CAG-CAI-CAK
5	D	418	6NA	OXT-C-CA-CB
4	A	402	EDO	O1-C1-C2-O2
4	C	806	EDO	O1-C1-C2-O2
4	C	815	EDO	O1-C1-C2-O2
5	D	418	6NA	O-C-CA-CB
5	D	412	6NA	O-C-CA-CB
8	C	817	D8F	CAH-CAF-CAG-CAI
8	D	423	D8F	CAG-CAF-CAH-CAJ
4	B	608	EDO	O1-C1-C2-O2
5	D	412	6NA	OXT-C-CA-CB

There are no ring outliers.

45 monomers are involved in 122 short contacts:

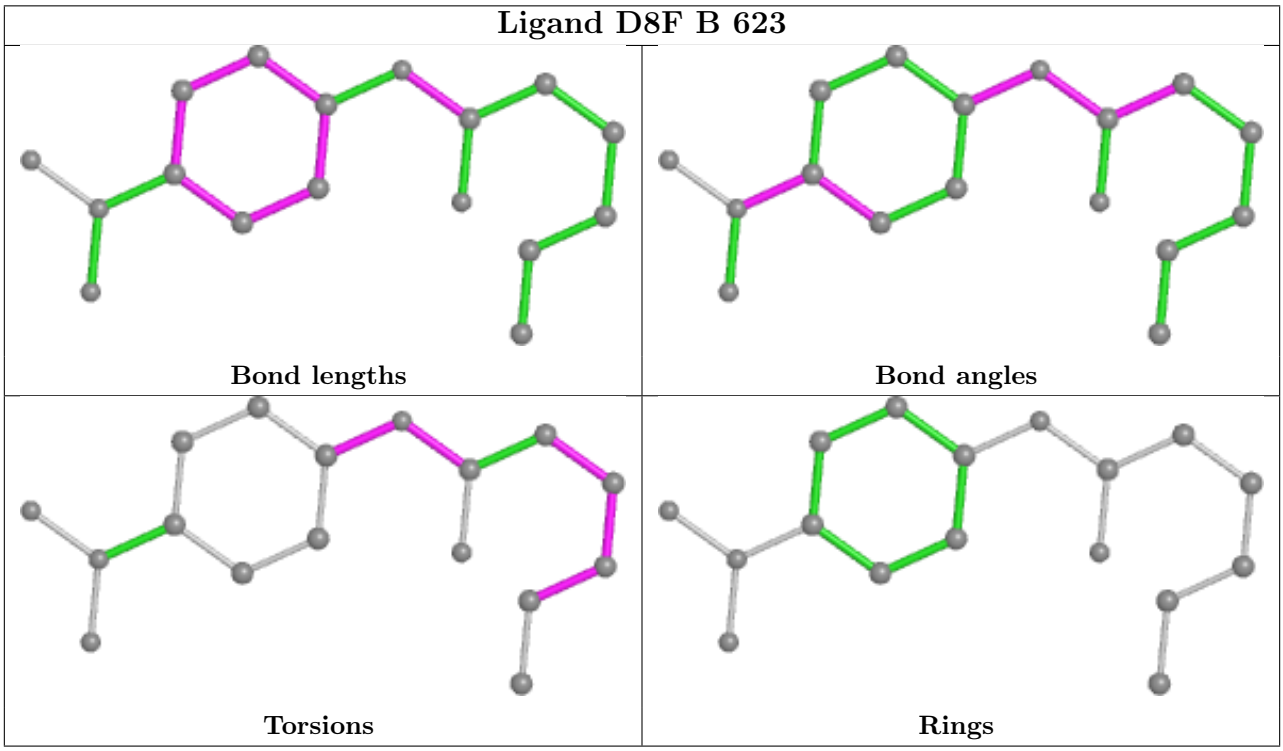
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	623	D8F	10	0
4	A	404	EDO	1	0
3	D	402	GOL	1	0
7	C	811	CCN	3	0
7	D	415	CCN	3	0
7	B	614	CCN	1	0
4	B	605	EDO	1	0
6	D	401	DMS	3	0
3	D	410	GOL	1	0
3	C	809	GOL	7	0
7	A	408	CCN	1	0
7	C	808	CCN	1	0
6	A	414	DMS	3	0
12	D	421	NPO	3	0
6	A	415	DMS	1	0
7	B	607	CCN	1	0
3	C	813	GOL	5	0
7	C	821	CCN	1	0
7	A	418	CCN	2	0
4	A	412	EDO	1	0
7	A	409	CCN	2	0
11	B	615	BUA	2	0
5	A	403	6NA	1	0
7	D	420	CCN	1	0
4	B	624	EDO	1	0
6	B	612	DMS	2	0
7	D	419	CCN	1	0
7	D	408	CCN	1	0
5	D	418	6NA	12	0
7	D	404	CCN	1	0
6	C	819	DMS	4	0
12	B	621	NPO	2	1
4	A	405	EDO	2	0
5	A	417	6NA	1	0
8	D	423	D8F	5	0
8	C	817	D8F	9	0
4	C	805	EDO	1	0
7	D	411	CCN	1	0
5	D	412	6NA	3	0
4	C	818	EDO	1	0
4	D	414	EDO	2	0
12	B	620	NPO	8	0

Continued on next page...

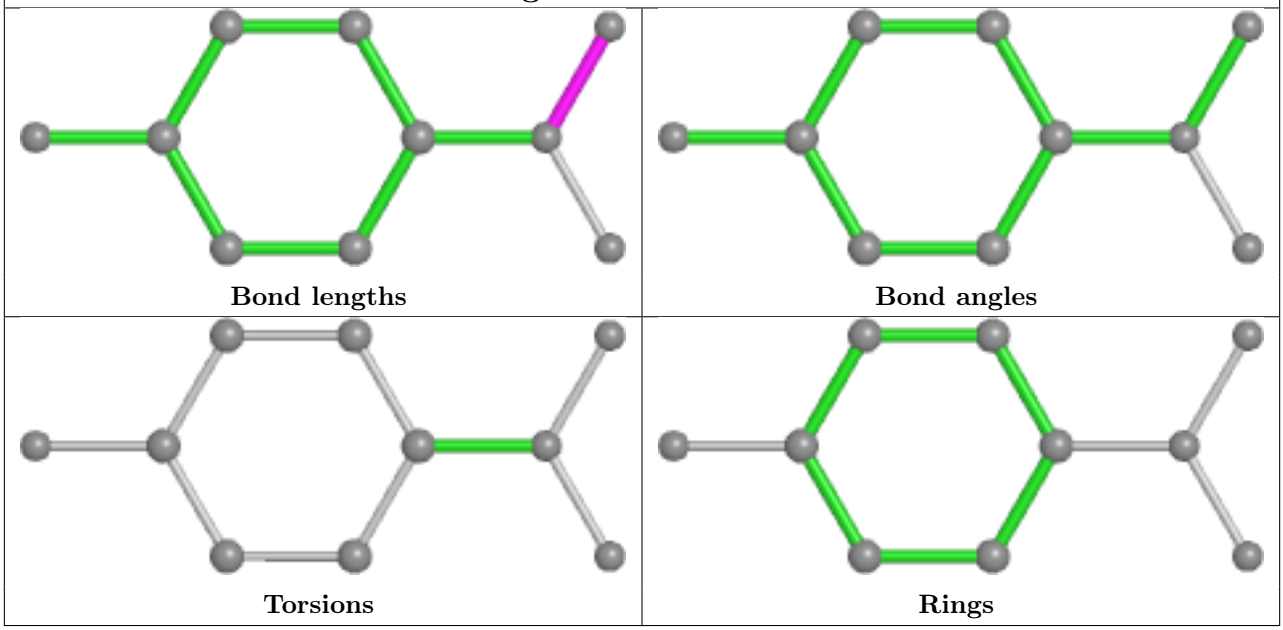
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	618	CCN	4	0
8	A	416	D8F	6	0
6	A	406	DMS	2	0

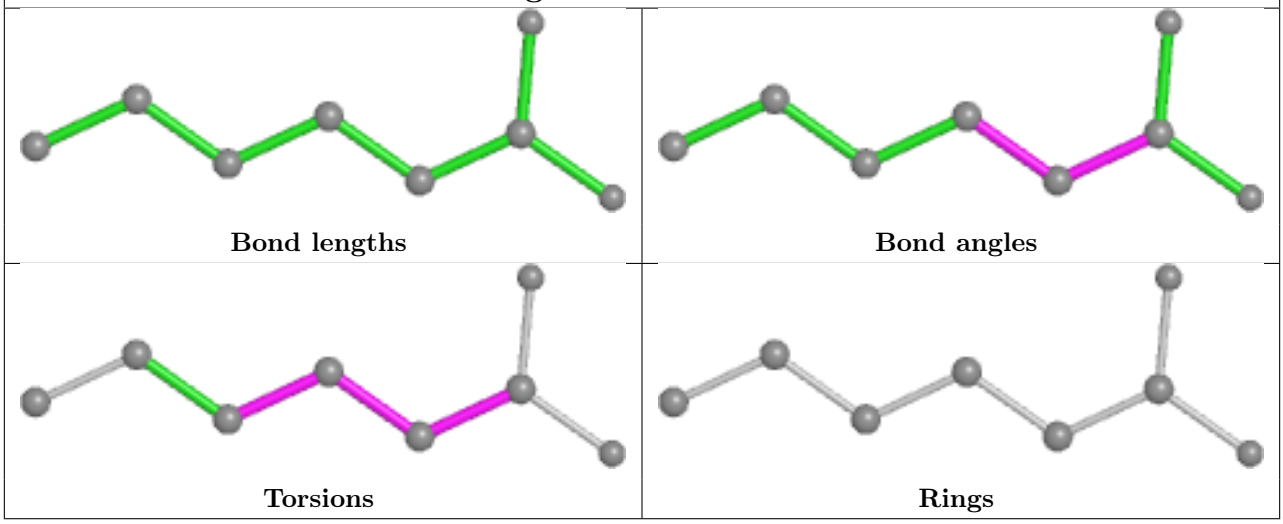
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



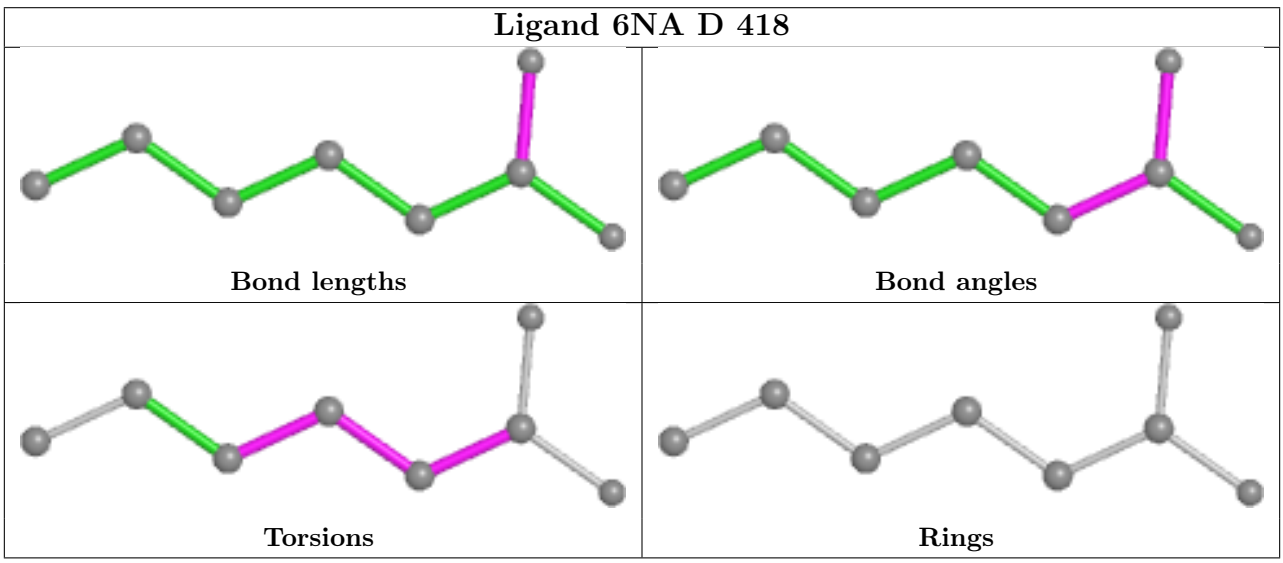
Ligand NPO D 421



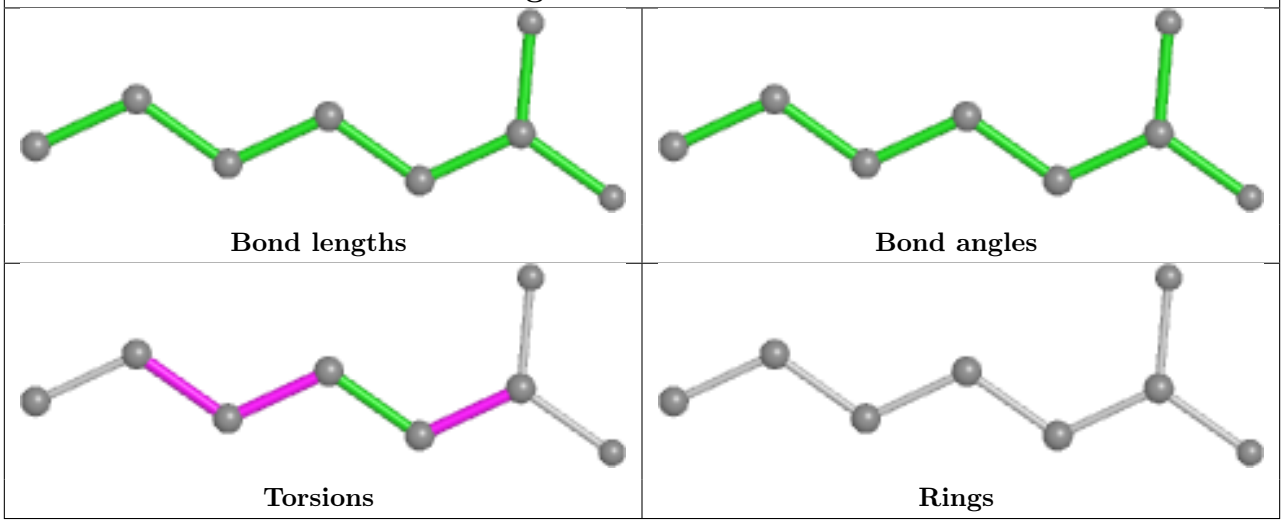
Ligand 6NA A 403



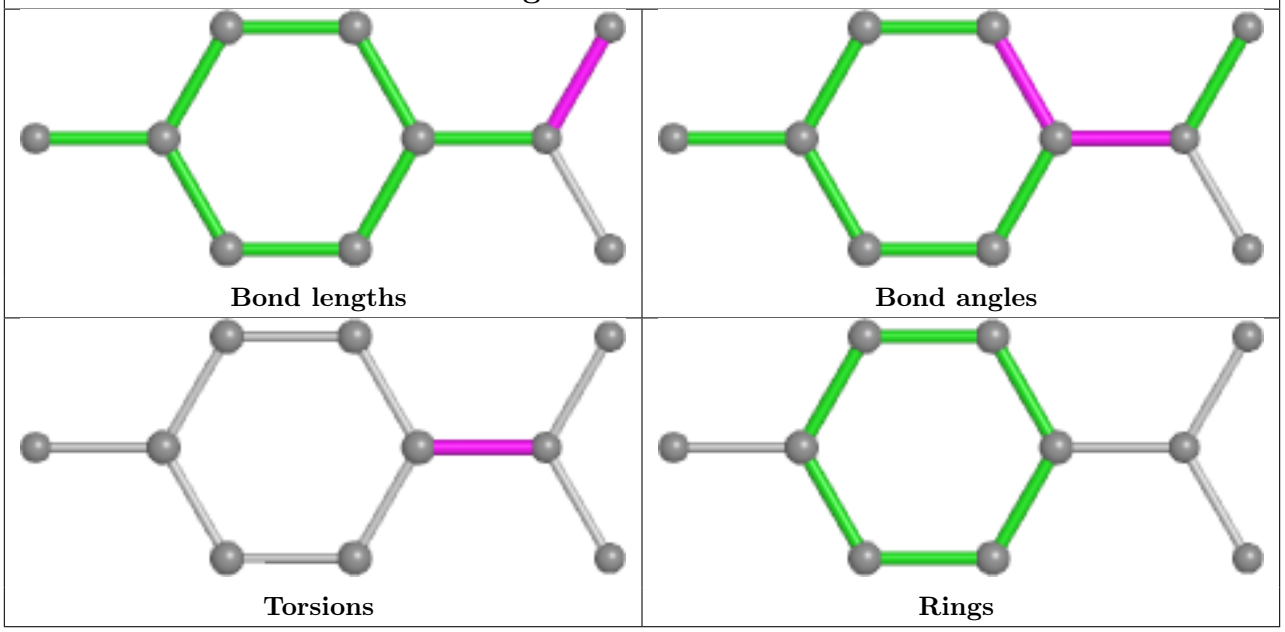
Ligand 6NA D 418



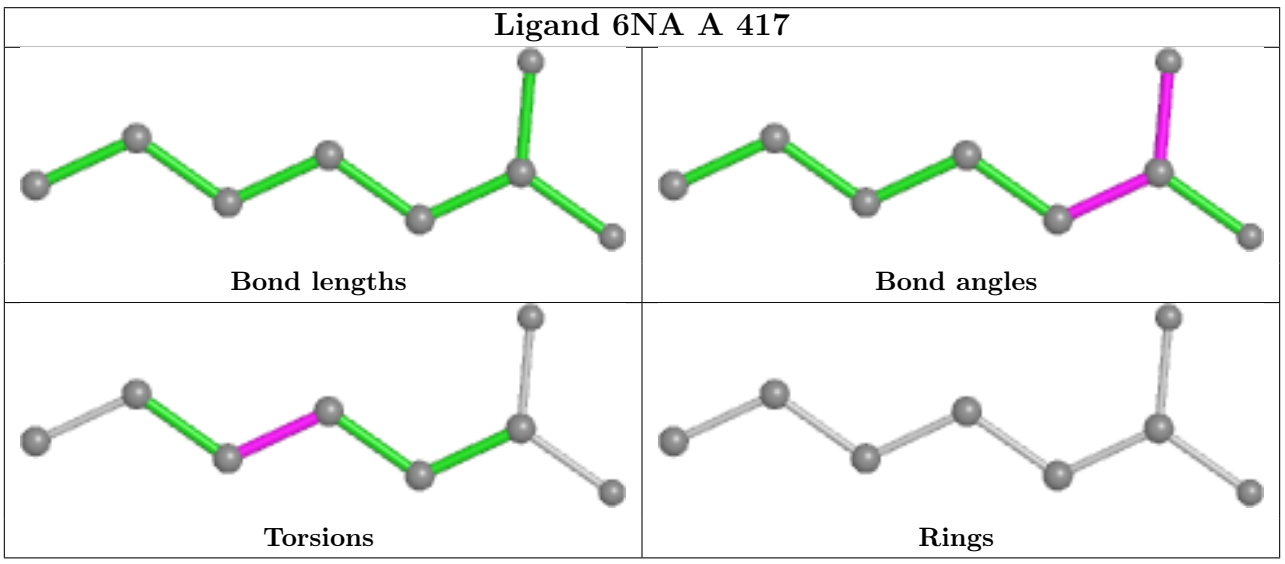
Ligand 6NA C 810



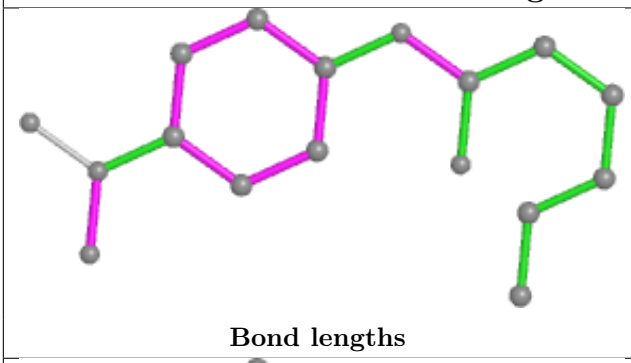
Ligand NPO B 621



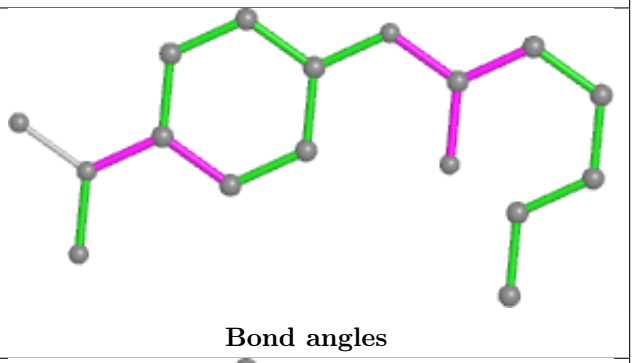
Ligand 6NA A 417



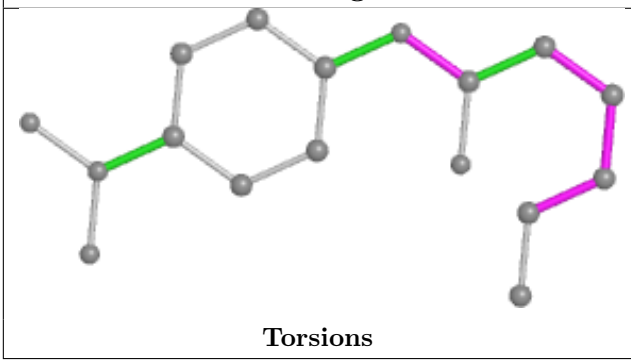
Ligand D8F D 423



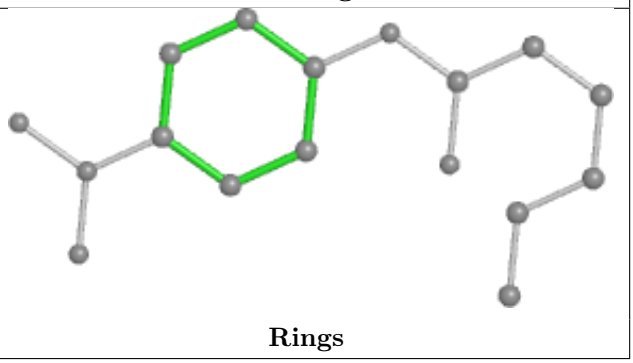
Bond lengths



Bond angles

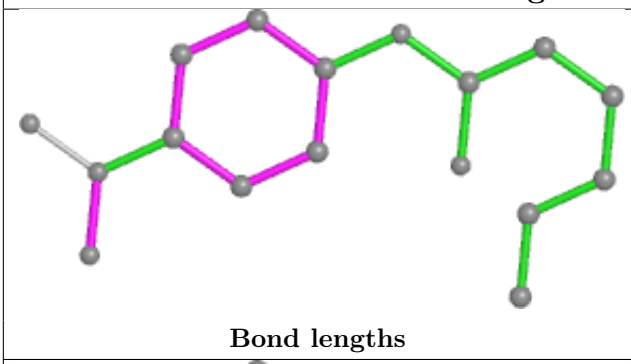


Torsions

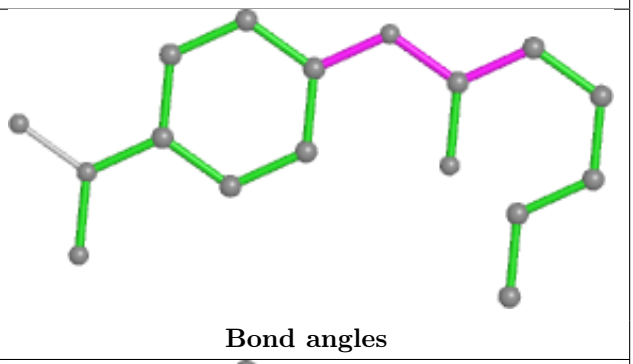


Rings

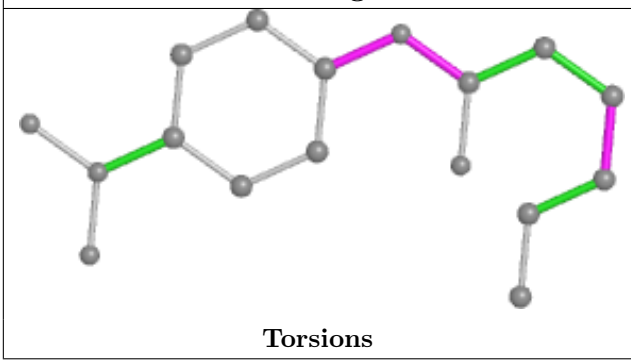
Ligand D8F C 817



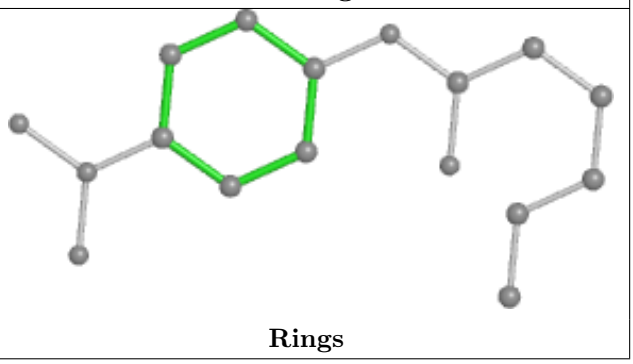
Bond lengths



Bond angles

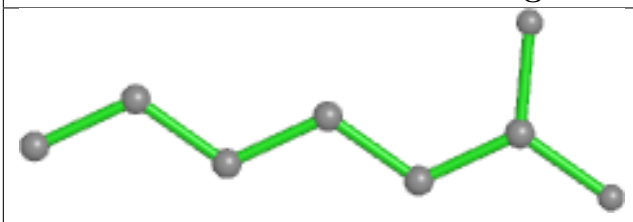


Torsions

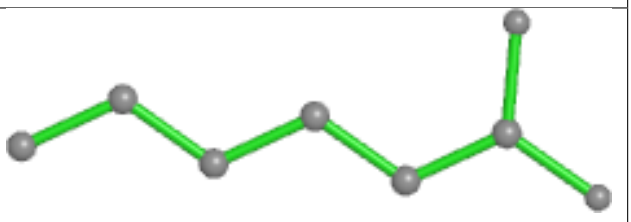


Rings

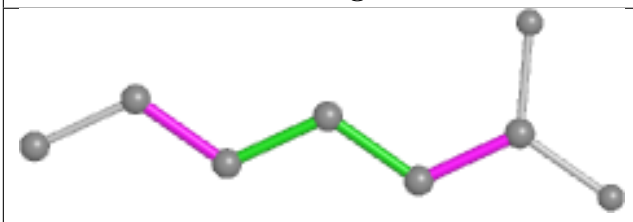
Ligand 6NA D 412



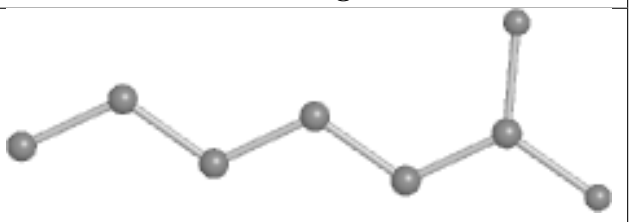
Bond lengths



Bond angles

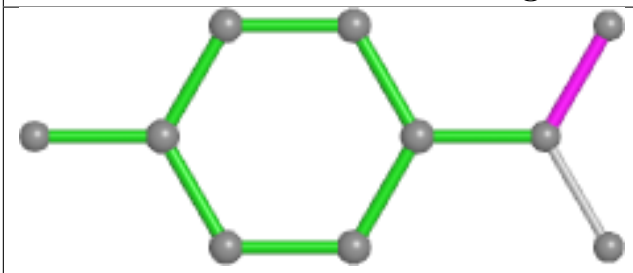


Torsions

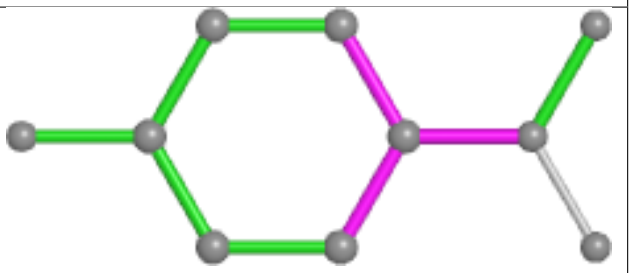


Rings

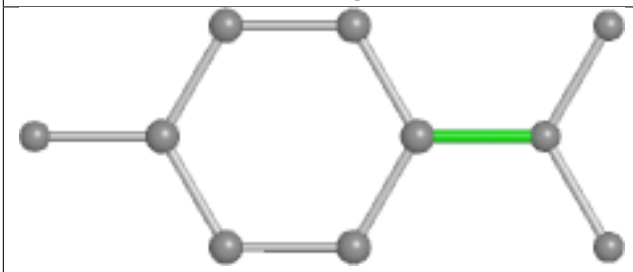
Ligand NPO B 620



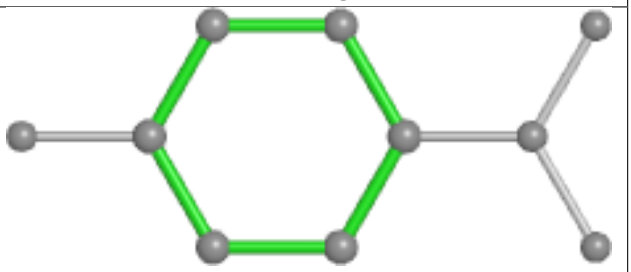
Bond lengths



Bond angles

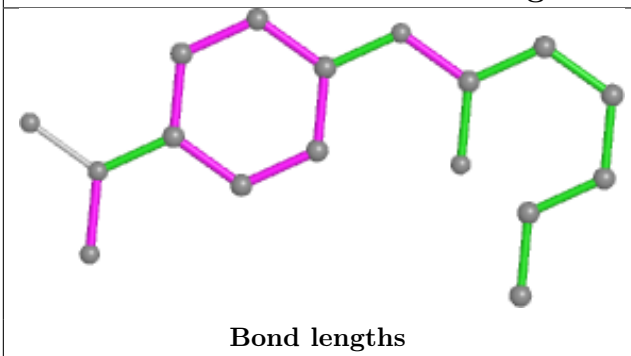


Torsions

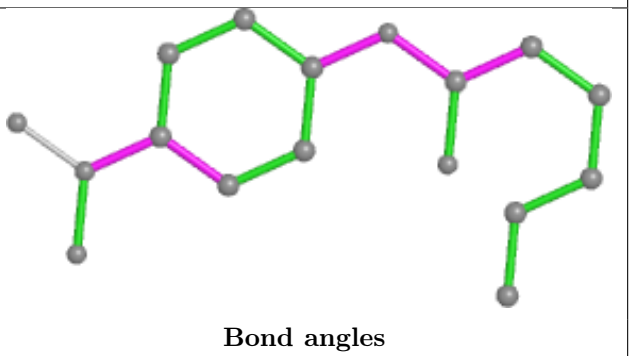


Rings

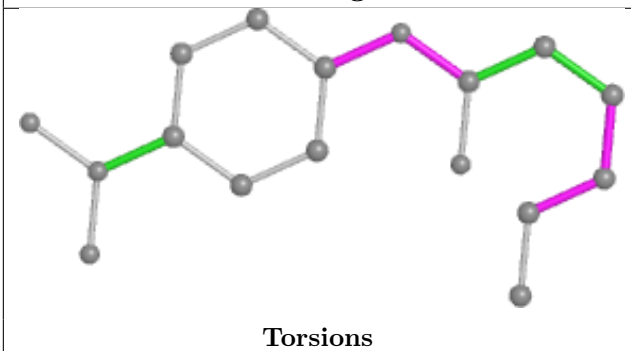
Ligand D8F A 416



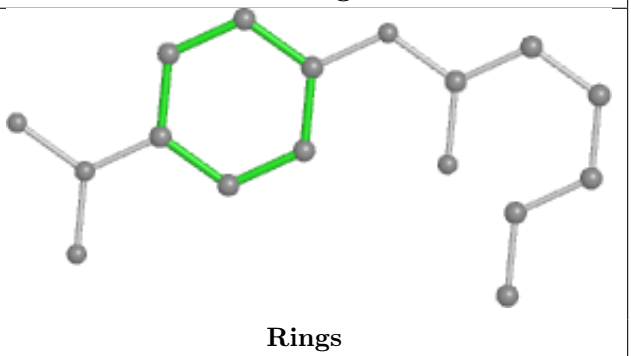
Bond lengths



Bond angles



Torsions



Rings

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	309/314 (98%)	-0.12	4 (1%) 77 83	20, 25, 41, 58	0
1	B	309/314 (98%)	-0.09	1 (0%) 94 95	22, 29, 48, 62	0
1	D	309/314 (98%)	0.12	11 (3%) 42 49	22, 30, 52, 65	0
2	C	309/314 (98%)	-0.04	5 (1%) 72 79	19, 25, 41, 58	0
All	All	1236/1256 (98%)	-0.03	21 (1%) 70 77	19, 27, 46, 65	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	LEU	4.3
1	D	27	ALA	3.5
1	D	26	LEU	3.2
1	D	30	THR	3.2
2	C	77	SER	2.8
1	D	28	GLU	2.7
1	A	77	SER	2.7
2	C	149	LEU	2.7
1	D	24	PRO	2.7
1	D	22	ALA	2.6
1	D	247	ILE	2.4
1	D	275	VAL	2.4
1	A	147	SER	2.3
1	A	23	GLY	2.3
1	D	219	PHE	2.3
2	C	274	VAL	2.2
2	C	4	THR	2.2
1	A	149	LEU	2.2
1	D	25	THR	2.1
2	C	275	VAL	2.0
1	B	32	GLU	2.0

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

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

6.3 Carbohydrates (i)

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
12	NPO	B	621	10/10	-0.06	1.01	135,164,197,201	15
6	DMS	A	414	4/4	0.36	0.32	42,50,56,71	10
6	DMS	A	415	4/4	0.56	0.26	23,30,53,68	10
5	6NA	D	412	8/8	0.60	0.50	54,65,78,78	0
13	NA	C	820	1/1	0.61	0.15	64,64,64,64	0
3	GOL	C	813	6/6	0.63	0.28	48,54,67,67	0
11	BUA	B	615	6/6	0.64	0.14	36,50,60,60	0
12	NPO	B	620	10/10	0.64	0.87	143,155,193,196	15
5	6NA	C	810	8/8	0.64	0.24	49,61,71,71	0
7	CCN	D	411	3/3	0.64	0.46	43,52,52,54	0
6	DMS	D	413	4/4	0.67	0.28	67,90,102,104	0
4	EDO	A	412	4/4	0.67	0.29	47,56,64,64	0
12	NPO	D	421	10/10	0.69	0.21	55,66,86,86	15
7	CCN	A	413	3/3	0.72	0.18	45,54,54,54	0
7	CCN	B	607	3/3	0.72	0.24	55,56,67,67	0
3	GOL	B	619	6/6	0.72	0.29	46,53,64,64	0
7	CCN	A	411	3/3	0.72	0.19	47,53,57,57	0
4	EDO	C	806	4/4	0.73	0.31	52,63,71,71	0
5	6NA	A	417	8/8	0.74	0.30	50,60,78,78	0
7	CCN	B	613	3/3	0.74	0.29	45,54,55,56	0
7	CCN	C	807	3/3	0.75	0.45	47,50,57,57	0
8	D8F	A	416	17/17	0.76	0.19	28,46,55,57	0
6	DMS	A	406	4/4	0.76	0.38	51,61,72,85	0
4	EDO	B	608	4/4	0.76	0.14	53,66,74,83	0
7	CCN	D	408	3/3	0.77	0.21	42,51,51,53	0
4	EDO	B	605	4/4	0.78	0.38	43,52,57,69	0
6	DMS	A	407	4/4	0.79	0.45	61,73,80,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	816	6/6	0.79	0.27	47,53,67,72	0
4	EDO	C	812	4/4	0.79	0.29	50,61,67,74	0
8	D8F	B	623	17/17	0.79	0.19	38,54,66,70	0
8	D8F	D	423	17/17	0.79	0.16	38,52,61,62	0
7	CCN	A	409	3/3	0.80	0.15	45,48,54,54	0
4	EDO	D	403	4/4	0.81	0.20	43,51,58,63	0
7	CCN	D	404	3/3	0.81	0.16	39,47,48,48	0
7	CCN	A	410	3/3	0.82	0.35	42,45,54,54	0
3	GOL	D	410	6/6	0.82	0.23	51,56,68,68	0
4	EDO	C	818	4/4	0.82	0.28	42,51,65,78	0
8	D8F	C	817	17/17	0.82	0.18	27,43,53,54	0
5	6NA	D	418	8/8	0.82	0.34	24,34,41,41	19
6	DMS	B	616	4/4	0.83	0.33	59,84,88,88	0
7	CCN	C	821	3/3	0.83	0.18	27,32,40,41	0
6	DMS	B	622	4/4	0.83	0.38	47,57,58,77	0
4	EDO	B	606	4/4	0.83	0.42	56,68,80,80	0
7	CCN	A	408	3/3	0.83	0.27	40,47,48,48	0
7	CCN	D	415	3/3	0.83	0.14	39,47,47,50	0
7	CCN	D	416	3/3	0.83	0.20	36,41,44,44	0
4	EDO	C	815	4/4	0.83	0.18	48,57,63,64	0
7	CCN	D	417	3/3	0.84	0.26	38,46,55,55	0
4	EDO	A	405	4/4	0.84	0.27	38,46,56,64	0
7	CCN	C	808	3/3	0.84	0.46	46,54,65,65	0
7	CCN	B	610	3/3	0.84	0.16	45,48,58,58	0
6	DMS	D	409	4/4	0.84	0.40	70,86,96,96	0
3	GOL	C	814	6/6	0.85	0.12	41,45,54,54	0
7	CCN	B	614	3/3	0.85	0.47	40,48,48,53	0
7	CCN	B	609	3/3	0.86	0.15	46,49,56,56	0
4	EDO	D	422	4/4	0.86	0.17	41,50,59,60	0
7	CCN	D	420	3/3	0.87	0.12	45,52,63,63	0
7	CCN	C	811	3/3	0.87	0.28	34,41,44,47	0
4	EDO	B	624	4/4	0.87	0.12	38,46,49,52	0
7	CCN	A	418	3/3	0.87	0.15	36,44,44,50	0
5	6NA	A	403	8/8	0.87	0.16	37,47,63,63	0
3	GOL	C	809	6/6	0.88	0.17	28,36,41,42	8
4	EDO	D	414	4/4	0.88	0.11	33,40,48,52	0
6	DMS	D	401	4/4	0.88	0.22	56,67,83,83	0
4	EDO	B	601	4/4	0.89	0.13	41,49,59,67	0
6	DMS	C	819	4/4	0.89	0.17	58,70,80,87	0
7	CCN	B	618	3/3	0.90	0.43	35,38,46,46	0
7	CCN	D	419	3/3	0.90	0.21	38,44,49,49	0
4	EDO	C	805	4/4	0.90	0.24	40,49,56,68	0

Continued on next page...

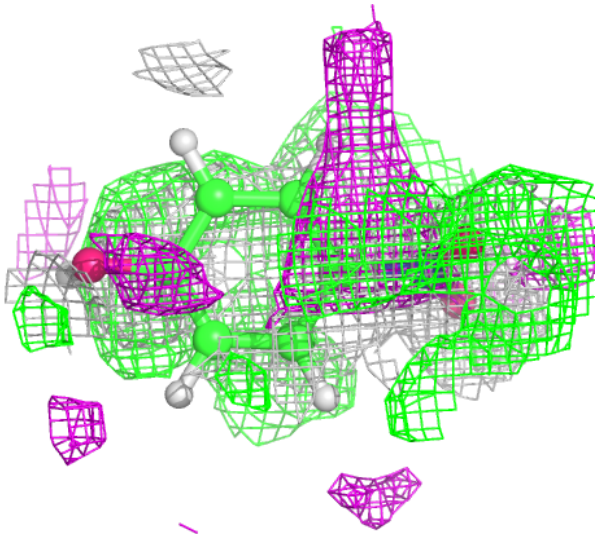
Continued from previous page...

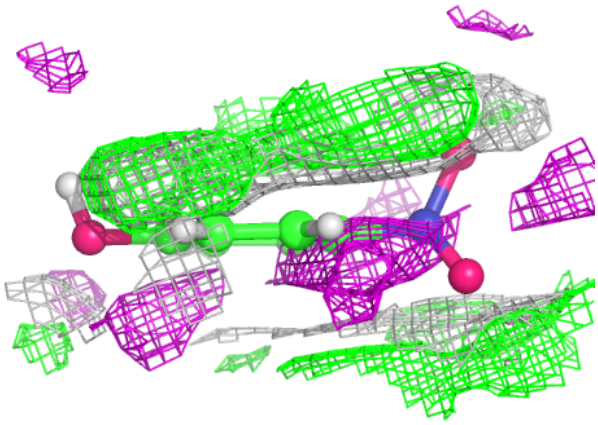
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	404	4/4	0.90	0.10	39,47,54,64	0
4	EDO	C	803	4/4	0.90	0.16	56,68,77,92	0
4	EDO	D	406	4/4	0.90	0.17	37,45,53,54	0
4	EDO	D	407	4/4	0.91	0.14	37,47,63,71	0
3	GOL	C	802	6/6	0.92	0.12	30,35,41,43	0
4	EDO	C	804	4/4	0.92	0.16	34,46,56,56	0
4	EDO	A	402	4/4	0.92	0.14	36,43,51,51	0
6	DMS	B	617	4/4	0.93	0.21	51,62,66,69	0
3	GOL	D	402	6/6	0.93	0.16	35,42,49,55	0
4	EDO	D	405	4/4	0.93	0.13	34,52,53,64	0
4	EDO	C	801	4/4	0.94	0.09	40,48,55,56	0
6	DMS	B	611	4/4	0.94	0.27	68,81,92,92	0
3	GOL	A	401	6/6	0.94	0.11	30,36,40,48	0
4	EDO	B	603	4/4	0.95	0.29	36,50,60,60	0
6	DMS	B	612	4/4	0.95	0.15	48,59,72,72	0
9	SO4	A	419	5/5	0.96	0.12	52,52,63,63	0
9	SO4	A	420	5/5	0.96	0.30	60,65,78,93	0
10	DIO	B	604	6/6	0.96	0.10	36,43,46,46	0
4	EDO	B	602	4/4	0.96	0.18	31,43,51,51	0

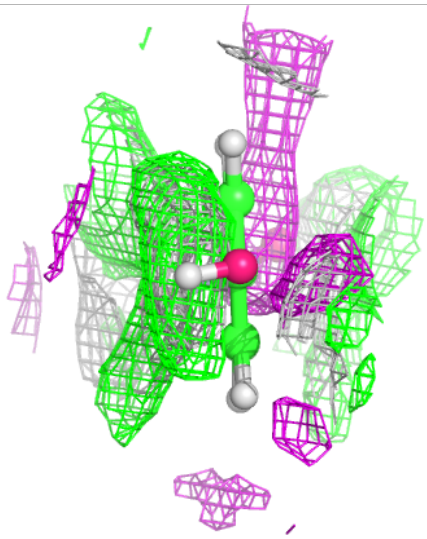
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NPO B 621:

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

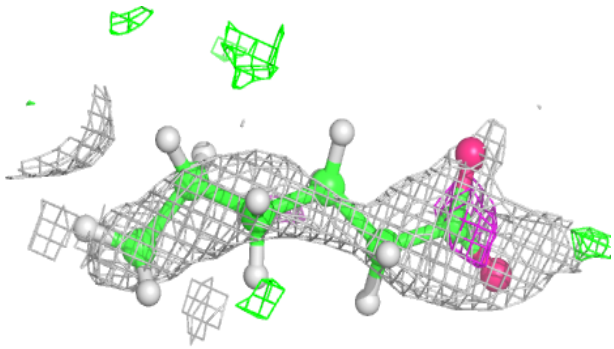


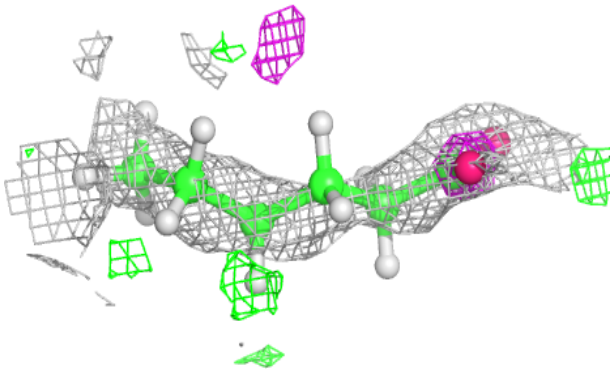


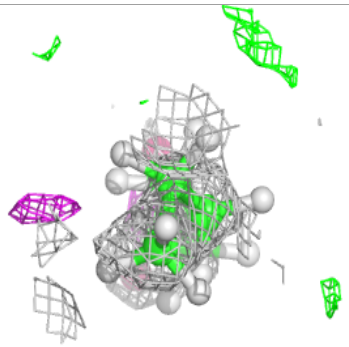


Electron density around 6NA D 412:

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

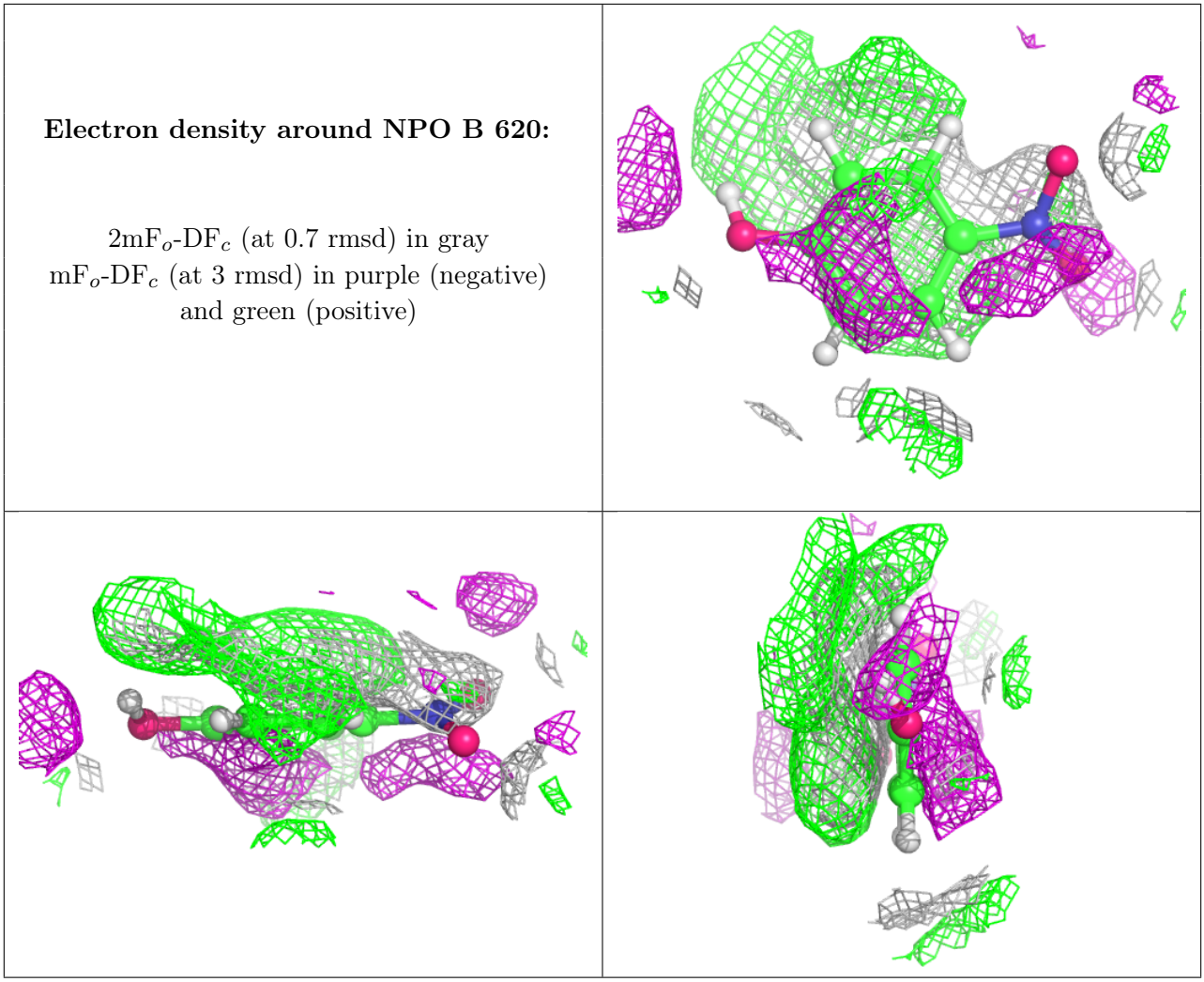






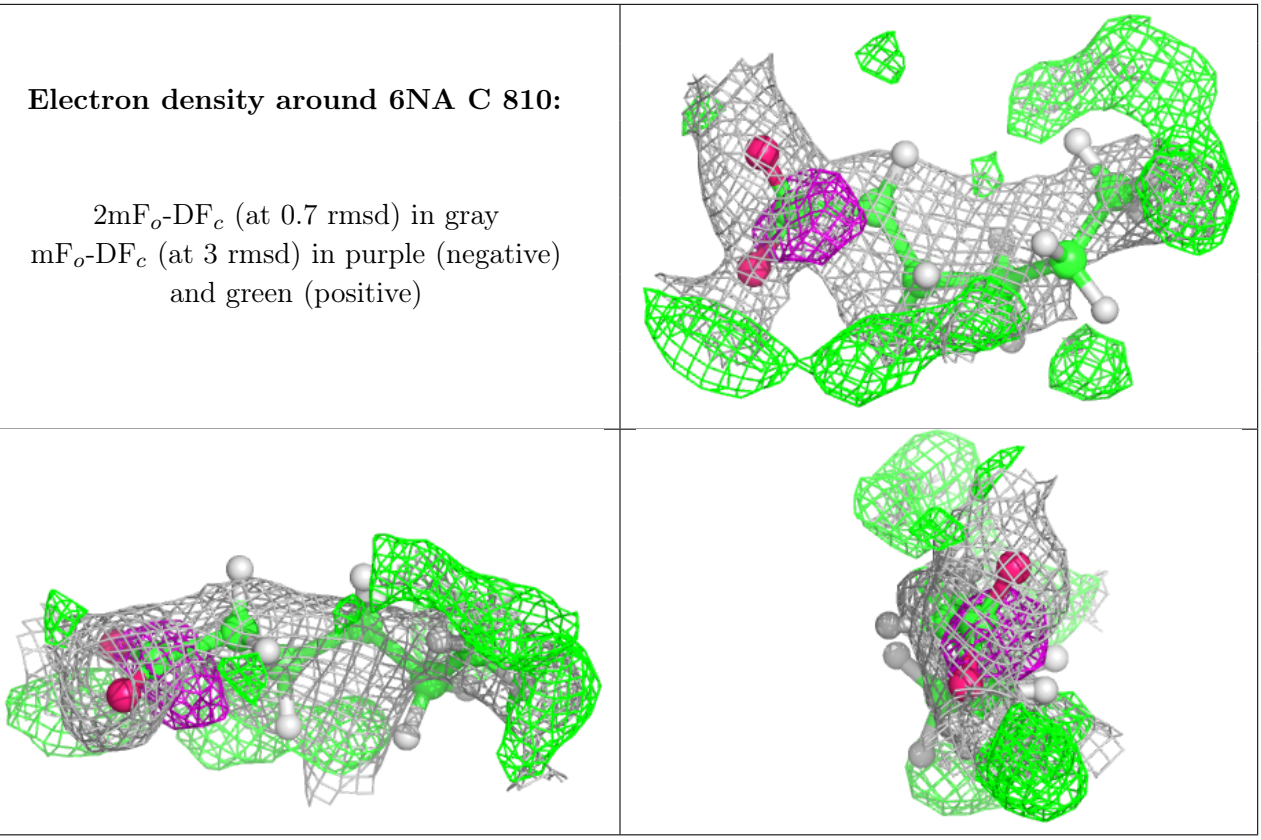
Electron density around NPO B 620:

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



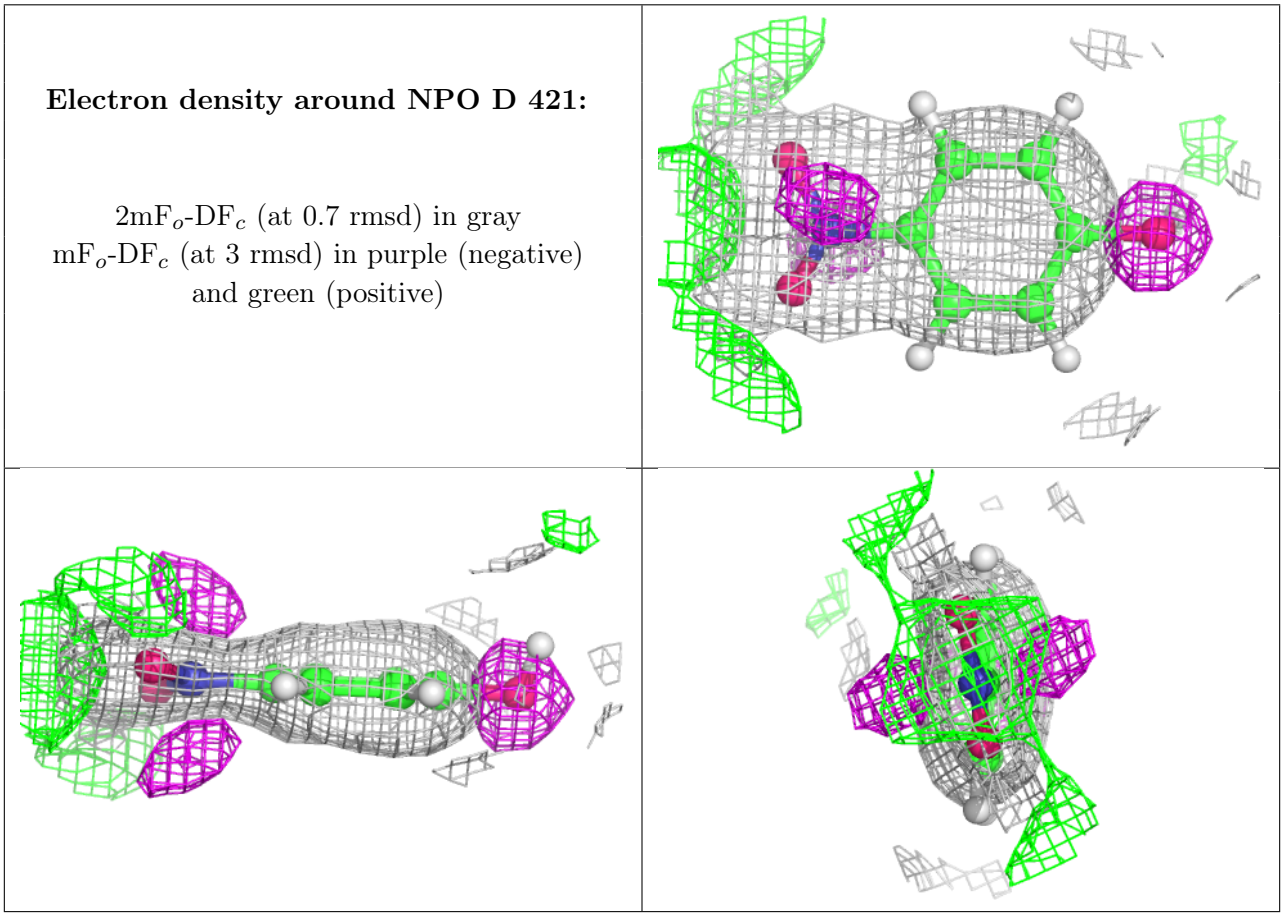
Electron density around 6NA C 810:

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



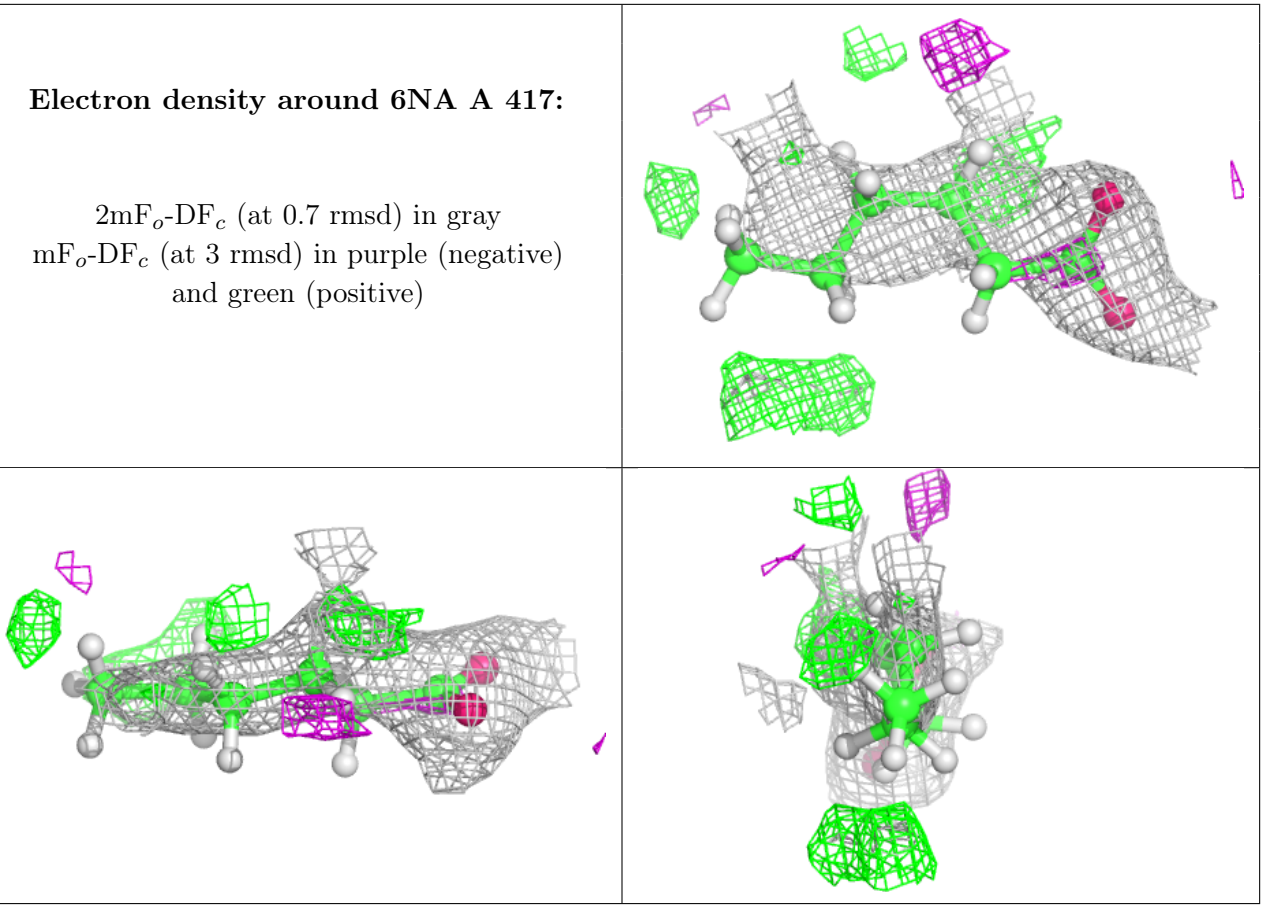
Electron density around NPO D 421:

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



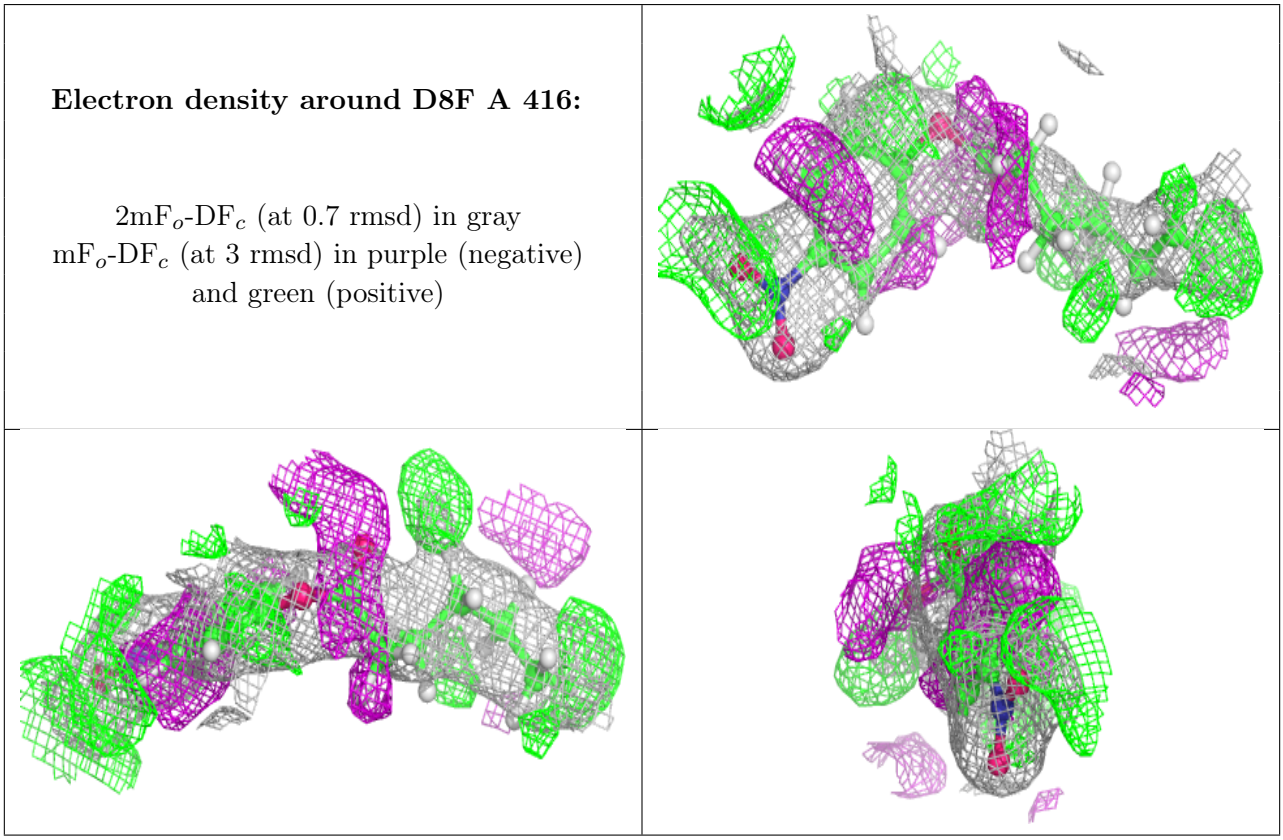
Electron density around 6NA A 417:

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



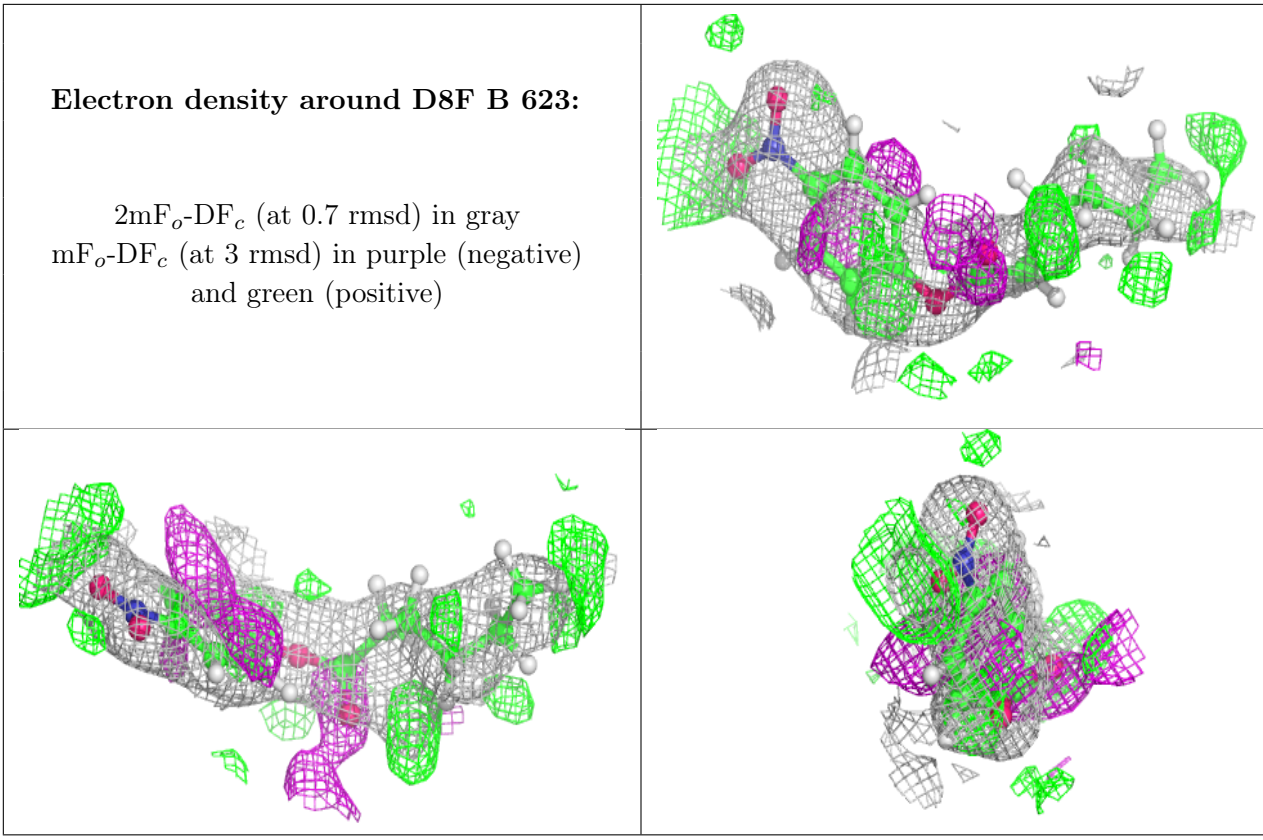
Electron density around D8F A 416:

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



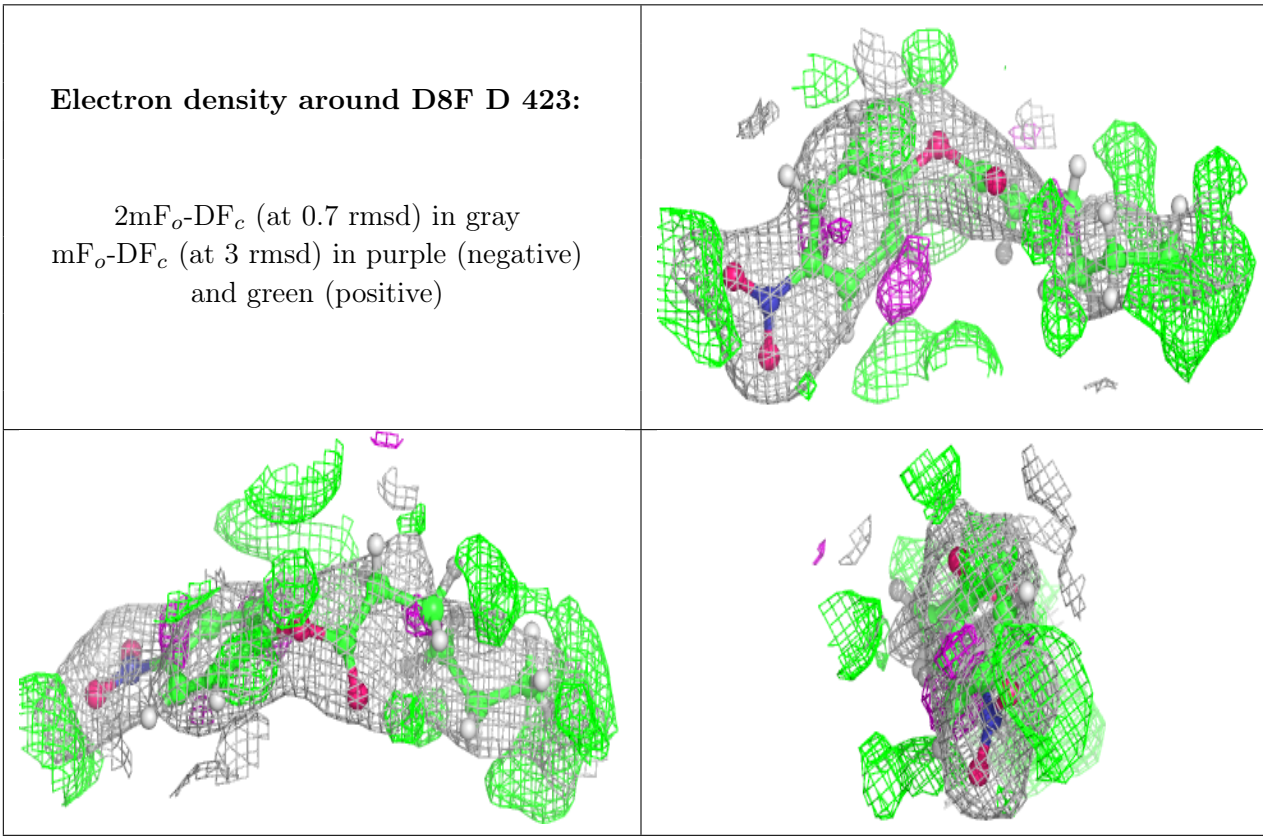
Electron density around D8F B 623:

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



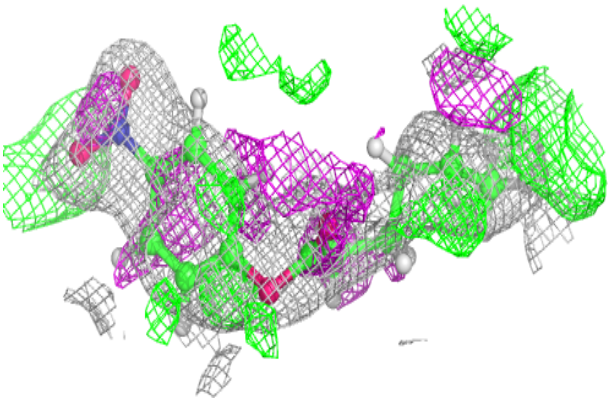
Electron density around D8F D 423:

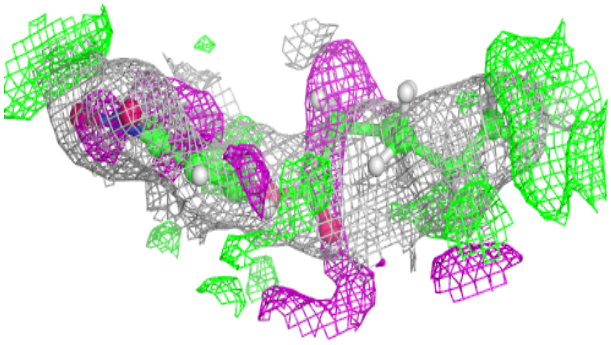
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

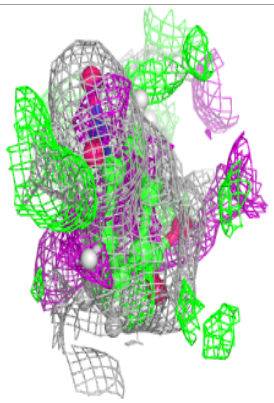


Electron density around D8F C 817:

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

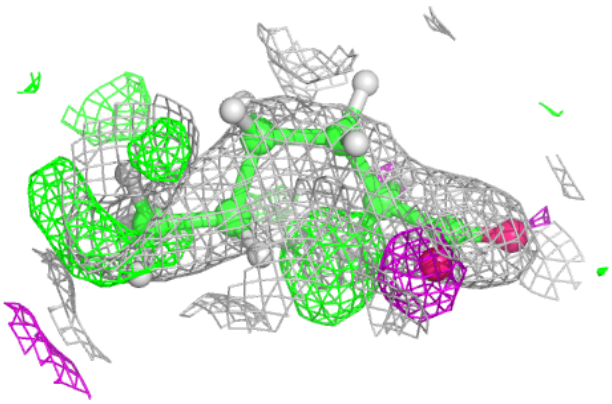


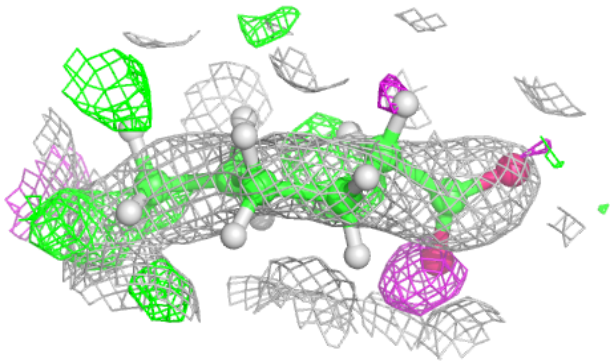


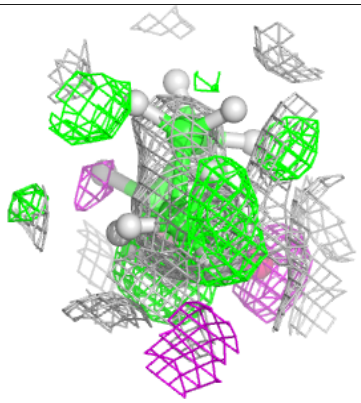


Electron density around 6NA D 418:

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

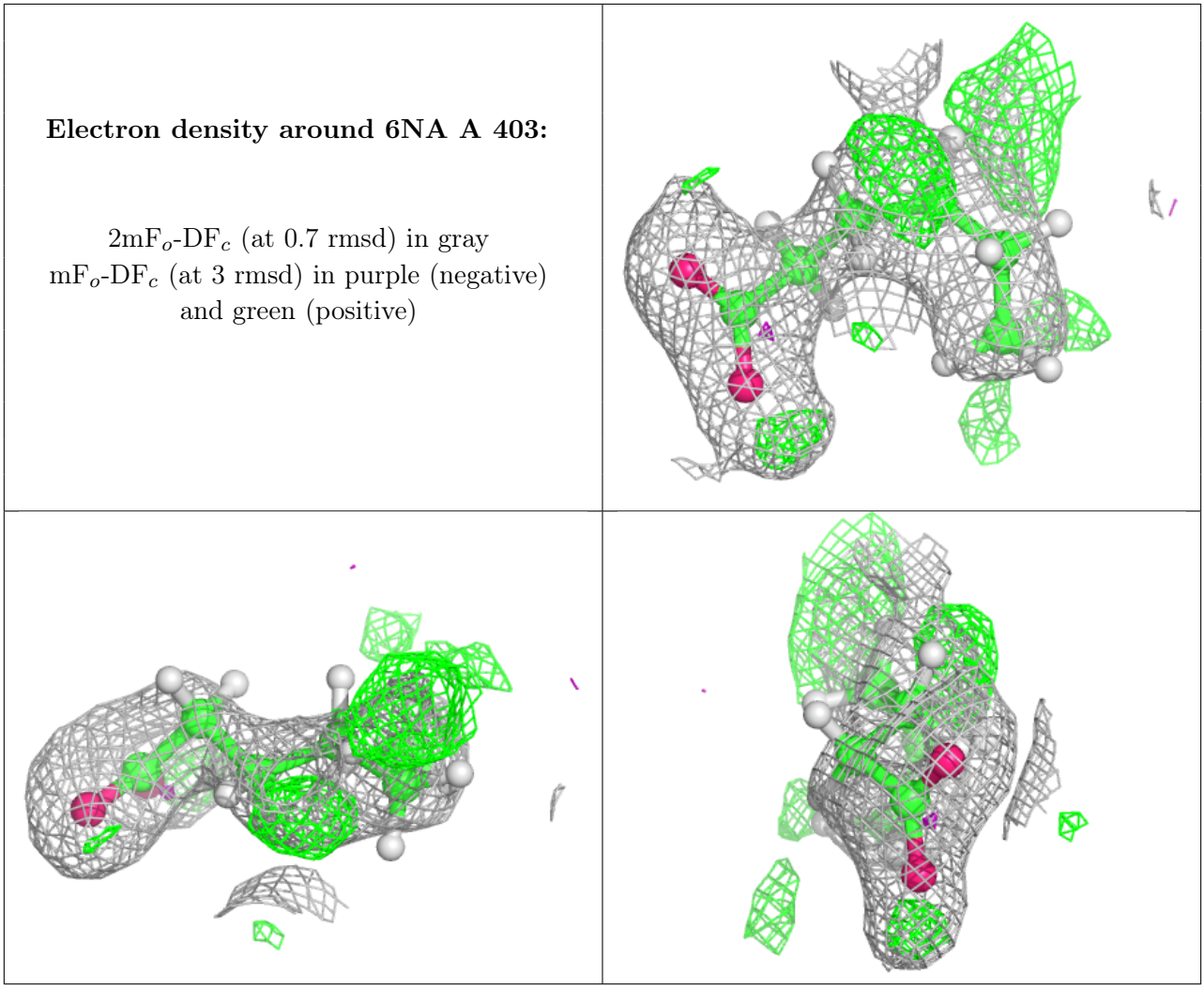






Electron density around 6NA A 403:

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



6.5 Other polymers

There are no such residues in this entry.