Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 11:07 PM EDT

PDB ID	:	1LLR
Title	:	CHOLERA TOXIN B-PENTAMER WITH LIGAND BMSC-0012
Authors	:	Merritt, E.A.; Hol, W.G.J.
Deposited on	:	2002-04-30
Resolution	:	1.46 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:

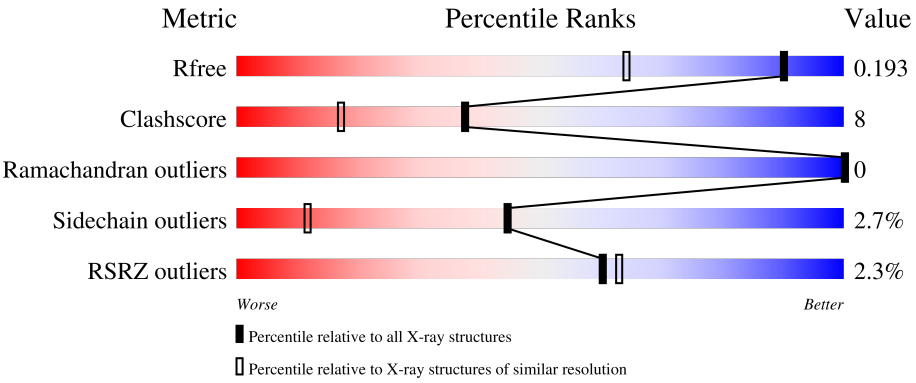
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.46 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	D	103	3% 82% 15%
1	E	103	2% 77% 21%
1	F	103	3% 77% 19%
1	G	103	3% 78% 21%
1	H	103	% 83% 13%

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
3	LNQ	F	105	-	-	-	X

2 Entry composition

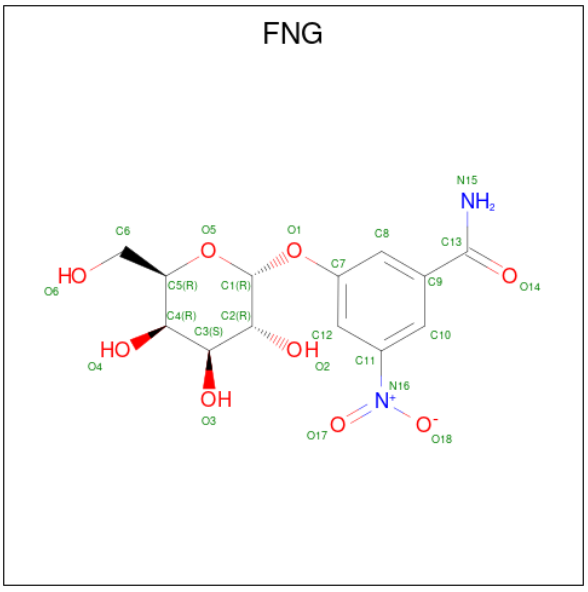
There are 4 unique types of molecules in this entry. The entry contains 4893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHOLERA TOXIN B SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	103	Total	C	N	O	S	0	3	0
			823	518	143	156	6			
1	E	103	Total	C	N	O	S	0	3	0
			823	518	143	156	6			
1	F	103	Total	C	N	O	S	0	1	0
			816	512	142	156	6			
1	G	103	Total	C	N	O	S	0	2	0
			818	514	142	156	6			
1	H	103	Total	C	N	O	S	0	2	0
			818	514	142	156	6			

- Molecule 2 is 5-aminocarbonyl-3-nitrophenyl alpha-D-galactopyranoside (three-letter code: FNG) (formula: $C_{13}H_{16}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			24	13	2	9		

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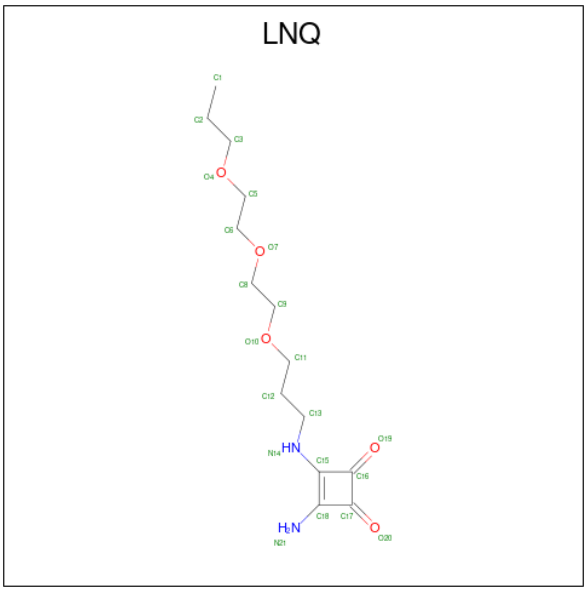
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			24	13	2	9		
2	F	1	Total	C	N	O	0	0
			24	13	2	9		
2	G	1	Total	C	N	O	0	0
			24	13	2	9		
2	H	1	Total	C	N	O	0	0
			24	13	2	9		

- Molecule 3 is 3-AMINO-4-{3-[2-(2-PROPOXY-ETHOXY)-ETHOXY]-PROPYLAMINO}-CYCLOBUT-3-ENE-1,2-DIONE (three-letter code: LNQ) (formula: $C_{14}H_{24}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	8	0
			21	14	2	5		
3	E	1	Total	C	N	O	8	0
			21	14	2	5		
3	F	1	Total	C	N	O	8	0
			21	14	2	5		
3	G	1	Total	C	N	O	8	0
			21	14	2	5		
3	H	1	Total	C	N	O	8	0
			21	14	2	5		

- Molecule 4 is water.

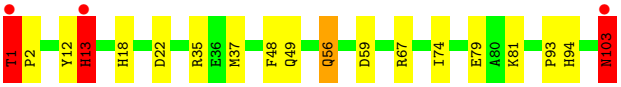
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	113	Total O 113 113	0	0
4	E	107	Total O 107 107	0	0
4	F	107	Total O 107 107	0	0
4	G	122	Total O 122 122	0	0
4	H	121	Total O 121 121	0	0

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.

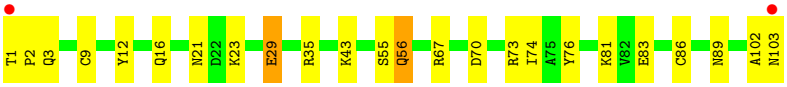
• Molecule 1: CHOLERA TOXIN B SUBUNIT

Chain D:



• Molecule 1: CHOLERA TOXIN B SUBUNIT

Chain E:

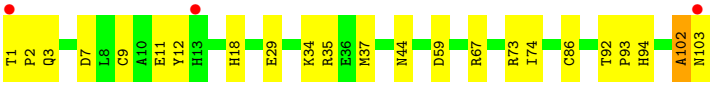


• Molecule 1: CHOLERA TOXIN B SUBUNIT

Chain F:

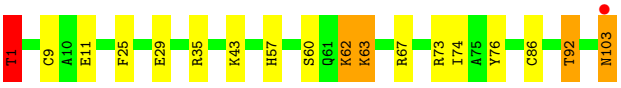
• Molecule 1: CHOLERA TOXIN B SUBUNIT

Chain G:



• Molecule 1: CHOLERA TOXIN B SUBUNIT

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	102.39Å 65.96Å 78.15Å 90.00° 105.97° 90.00°	Depositor
Resolution (Å)	27.00 – 1.46 26.53 – 1.46	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.00-1.46) 97.7 (26.53-1.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.46Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.149 , 0.191 0.153 , 0.193	Depositor DCC
R_{free} test set	4244 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 66.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4893	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LNQ, FNG

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	D	1.01	1/851 (0.1%)	1.72	16/1148 (1.4%)
1	E	0.98	1/851 (0.1%)	1.58	13/1148 (1.1%)
1	F	1.06	1/834 (0.1%)	1.68	13/1126 (1.2%)
1	G	1.05	1/842 (0.1%)	1.55	11/1137 (1.0%)
1	H	1.02	1/842 (0.1%)	1.69	16/1137 (1.4%)
All	All	1.03	5/4220 (0.1%)	1.65	69/5696 (1.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	29	GLU	CB-CG	-7.38	1.38	1.52
1	G	29	GLU	CB-CG	-5.89	1.41	1.52
1	H	29	GLU	CB-CG	-5.67	1.41	1.52
1	F	29	GLU	CB-CG	-5.49	1.41	1.52
1	D	79	GLU	CD-OE2	-5.04	1.20	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	35	ARG	NE-CZ-NH2	-17.72	111.44	120.30
1	H	103	ASN	CA-CB-CG	12.72	141.39	113.40
1	E	12	TYR	CB-CG-CD1	-12.12	113.72	121.00
1	D	35	ARG	NE-CZ-NH2	-11.83	114.39	120.30
1	G	67	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	E	29	GLU	OE1-CD-OE2	10.27	135.63	123.30
1	D	13	HIS	CA-CB-CG	9.75	130.17	113.60
1	H	62	LYS	CD-CE-NZ	9.70	134.00	111.70
1	F	12	TYR	CB-CG-CD1	-9.25	115.45	121.00
1	D	1	THR	CA-CB-CG2	-9.22	99.49	112.40
1	D	67	ARG	NE-CZ-NH2	-8.93	115.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	35	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	E	35	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	G	34	LYS	CB-CG-CD	8.67	134.15	111.60
1	H	67	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	G	35	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	D	1	THR	CA-CB-OG1	-7.95	92.31	109.00
1	G	7	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	103	ASN	CA-CB-CG	7.46	129.80	113.40
1	D	1	THR	OG1-CB-CG2	7.29	126.77	110.00
1	E	29	GLU	CA-CB-CG	7.21	129.26	113.40
1	F	73	ARG	CD-NE-CZ	7.13	133.58	123.60
1	H	35	ARG	NH1-CZ-NH2	7.12	127.23	119.40
1	E	35	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	E	83	GLU	OE1-CD-OE2	-7.05	114.83	123.30
1	F	7	ASP	CB-CG-OD1	7.02	124.62	118.30
1	G	11	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	D	12	TYR	CZ-CE2-CD2	-6.84	113.65	119.80
1	D	22	ASP	CB-CG-OD1	6.76	124.39	118.30
1	H	76	TYR	CZ-CE2-CD2	-6.68	113.78	119.80
1	F	67	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	G	12	TYR	CB-CG-CD1	-6.63	117.02	121.00
1	F	34	LYS	CB-CG-CD	6.60	128.76	111.60
1	E	67	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	81[A]	LYS	CG-CD-CE	6.46	131.28	111.90
1	D	81[B]	LYS	CG-CD-CE	6.46	131.28	111.90
1	F	48	PHE	CB-CG-CD1	-6.45	116.29	120.80
1	F	62	LYS	CB-CG-CD	6.45	128.36	111.60
1	H	60	SER	O-C-N	-6.44	112.40	122.70
1	F	1	THR	N-CA-CB	-6.36	98.22	110.30
1	F	102	ALA	O-C-N	6.34	132.85	122.70
1	G	73	ARG	CD-NE-CZ	6.22	132.30	123.60
1	E	29	GLU	CG-CD-OE2	-6.08	106.14	118.30
1	H	76	TYR	CG-CD2-CE2	6.05	126.14	121.30
1	F	11	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	E	12	TYR	CB-CG-CD2	6.00	124.60	121.00
1	E	76	TYR	CB-CG-CD1	5.97	124.58	121.00
1	G	44	ASN	N-CA-CB	-5.94	99.90	110.60
1	E	70	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	G	44	ASN	O-C-N	-5.90	113.17	123.20
1	G	102	ALA	O-C-N	5.79	131.96	122.70
1	H	29	GLU	OE1-CD-OE2	5.75	130.19	123.30
1	D	12	TYR	CG-CD2-CE2	5.62	125.79	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	59	ASP	CB-CG-OD1	5.61	123.35	118.30
1	F	6	THR	CA-CB-CG2	-5.61	104.54	112.40
1	H	92	THR	CA-CB-CG2	-5.58	104.58	112.40
1	H	25	PHE	CB-CG-CD1	-5.57	116.90	120.80
1	E	3	GLN	CA-CB-CG	-5.57	101.14	113.40
1	H	1	THR	CA-CB-OG1	-5.56	97.33	109.00
1	G	34	LYS	CD-CE-NZ	5.54	124.45	111.70
1	F	79	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	E	73	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	H	63	LYS	N-CA-CB	5.33	120.20	110.60
1	H	60	SER	CA-C-O	5.33	131.29	120.10
1	H	67	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	F	103	ASN	CA-CB-CG	5.16	124.76	113.40
1	D	48	PHE	CB-CG-CD2	5.08	124.35	120.80
1	H	73	ARG	CD-NE-CZ	5.05	130.67	123.60
1	D	59	ASP	CA-C-O	5.00	130.61	120.10

There are no chirality outliers.

There are no planarity outliers.

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	D	823	0	827	14	0
1	E	823	0	828	20	1
1	F	816	0	817	17	0
1	G	818	0	819	15	1
1	H	818	0	819	9	1
2	D	24	0	15	0	0
2	E	24	0	14	0	0
2	F	24	0	15	1	0
2	G	24	0	15	0	0
2	H	24	0	15	0	0
3	D	21	0	23	1	0
3	E	21	0	22	0	0
3	F	21	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	21	0	23	1	0
3	H	21	0	23	1	0
4	D	113	0	0	3	1
4	E	107	0	0	2	1
4	F	107	0	0	1	1
4	G	122	0	0	3	0
4	H	121	0	0	5	0
All	All	4893	0	4297	64	3

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 8.

All (64) 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:E:81[A]:LYS:HE2	1:E:103:ASN:HB2	1.37	1.07
1:E:81[A]:LYS:HE3	1:E:102:ALA:O	1.59	1.00
1:E:74[B]:ILE:HD12	1:F:77:LEU:HD13	1.42	0.99
1:E:56:GLN:HE21	1:E:56:GLN:H	1.14	0.96
1:E:81[A]:LYS:CE	1:E:102:ALA:O	2.15	0.95
1:D:56:GLN:HE21	1:D:56:GLN:H	1.10	0.94
1:D:18:HIS:HE1	1:D:94:HIS:HD2	1.24	0.84
1:F:3:GLN:HE22	1:G:92:THR:HG22	1.46	0.79
1:E:1:THR:HG22	1:F:93:PRO:HD2	1.64	0.79
1:G:1:THR:HG23	4:H:1005:HOH:O	1.80	0.79
1:E:16:GLN:OE1	1:E:89:ASN:ND2	2.12	0.79
1:E:74[B]:ILE:HD12	1:F:77:LEU:CD1	2.13	0.79
1:F:1:THR:HG23	1:F:2:PRO:HD2	1.66	0.76
1:D:103:ASN:HD22	1:D:103:ASN:H	1.32	0.74
1:E:1:THR:OG1	1:E:2:PRO:HD2	1.87	0.73
1:F:9[B]:CYS:SG	1:F:15:THR:HB	2.30	0.71
1:D:18:HIS:CE1	1:D:94:HIS:HD2	2.08	0.70
1:D:93:PRO:HD2	1:H:1:THR:HG22	1.73	0.69
4:D:191:HOH:O	1:H:74[A]:ILE:HD13	1.96	0.65
1:E:74[B]:ILE:CD1	1:F:77:LEU:HD13	2.23	0.64
1:H:11:GLU:HG2	4:H:1472:HOH:O	2.00	0.61
1:G:18:HIS:HE1	1:G:94:HIS:HD2	1.48	0.61
1:D:13:HIS:HD2	4:D:218:HOH:O	1.84	0.61
1:E:1:THR:CG2	1:F:93:PRO:HD2	2.31	0.61
1:E:81[A]:LYS:HE2	1:E:102:ALA:O	2.00	0.59
1:D:74[B]:ILE:HD13	4:E:165:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:105:LNQ:H31	4:G:1731:HOH:O	2.02	0.59
1:E:81[B]:LYS:HD2	1:E:103:ASN:OXT	2.03	0.58
1:D:18:HIS:HE1	1:D:94:HIS:CD2	2.14	0.57
1:G:18:HIS:CE1	1:G:94:HIS:HD2	2.23	0.57
1:G:1:THR:HB	1:G:2:PRO:HD2	1.88	0.56
1:D:103:ASN:H	1:D:103:ASN:ND2	1.96	0.54
1:G:74[B]:ILE:HD13	4:H:1387:HOH:O	2.07	0.54
1:F:102:ALA:O	1:F:103:ASN:HB2	2.08	0.53
1:F:18:HIS:HE1	1:F:94:HIS:ND1	2.07	0.53
3:D:105:LNQ:H132	4:D:180:HOH:O	2.11	0.51
1:G:102:ALA:HB1	4:G:1463:HOH:O	2.11	0.51
3:H:105:LNQ:H31	4:H:1732:HOH:O	2.10	0.51
1:F:3:GLN:NE2	1:G:92:THR:HG22	2.21	0.50
1:F:92:THR:HG23	4:F:1388:HOH:O	2.12	0.50
1:H:9[B]:CYS:SG	1:H:86:CYS:CB	3.02	0.48
1:E:21:ASN:OD1	1:E:81[A]:LYS:NZ	2.40	0.47
1:D:18:HIS:CE1	1:D:94:HIS:CD2	2.97	0.47
1:G:9[B]:CYS:HB2	1:G:86:CYS:SG	2.55	0.47
1:F:9[B]:CYS:SG	1:F:15:THR:CB	3.03	0.46
1:E:9[B]:CYS:SG	1:E:86:CYS:CB	3.04	0.46
1:E:23:LYS:HE3	4:E:181:HOH:O	2.15	0.46
1:H:63:LYS:HG3	4:H:1605:HOH:O	2.15	0.46
1:D:37:MET:HE3	1:H:1:THR:HG21	1.98	0.46
1:E:56:GLN:HE21	1:E:56:GLN:N	1.97	0.46
1:G:92:THR:HA	1:G:93:PRO:C	2.37	0.45
1:D:56:GLN:HE21	1:D:56:GLN:N	1.94	0.43
2:F:104:FNG:H121	2:F:104:FNG:H51	1.99	0.43
1:G:3:GLN:NE2	4:G:1502:HOH:O	2.45	0.43
1:E:1:THR:HG22	1:F:93:PRO:CD	2.43	0.42
1:D:1:THR:HA	1:D:2:PRO:HD3	1.67	0.42
1:G:3:GLN:OE1	1:H:92:THR:HG22	2.20	0.42
1:F:1:THR:HG21	1:G:37:MET:CE	2.49	0.42
1:H:57:HIS:HB2	1:H:62:LYS:HE2	2.01	0.41
1:F:1:THR:CG2	1:G:37:MET:HE1	2.50	0.41
1:D:49:GLN:OE1	1:H:1:THR:HG21	2.20	0.41
1:F:1:THR:CG2	1:G:37:MET:CE	2.99	0.40

All (3) 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)
4:D:170:HOH:O	4:E:177:HOH:O[4_445]	1.87	0.33
1:H:43:LYS:NZ	4:F:1376:HOH:O[4_546]	1.88	0.32
1:E:55:SER:OG	1:G:59:ASP:OD1[2_555]	2.19	0.01

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	D	104/103 (101%)	102 (98%)	2 (2%)	0	100	100
1	E	104/103 (101%)	103 (99%)	1 (1%)	0	100	100
1	F	102/103 (99%)	101 (99%)	1 (1%)	0	100	100
1	G	103/103 (100%)	101 (98%)	2 (2%)	0	100	100
1	H	103/103 (100%)	102 (99%)	1 (1%)	0	100	100
All	All	516/515 (100%)	509 (99%)	7 (1%)	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	D	92/89 (103%)	88 (96%)	4 (4%)	29	3
1	E	92/89 (103%)	89 (97%)	3 (3%)	38	7
1	F	90/89 (101%)	88 (98%)	2 (2%)	52	18
1	G	91/89 (102%)	90 (99%)	1 (1%)	73	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	91/89 (102%)	89 (98%)	2 (2%)	52 18
All	All	456/445 (102%)	444 (97%)	12 (3%)	44 13

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1	THR
1	D	13	HIS
1	D	56	GLN
1	D	103	ASN
1	E	29	GLU
1	E	43	LYS
1	E	56	GLN
1	F	62	LYS
1	F	81	LYS
1	G	103	ASN
1	H	1	THR
1	H	103	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	13	HIS
1	D	18	HIS
1	D	56	GLN
1	D	94	HIS
1	D	103	ASN
1	E	56	GLN
1	E	103	ASN
1	F	3	GLN
1	F	13	HIS
1	F	18	HIS
1	G	3	GLN
1	G	18	HIS
1	G	94	HIS

5.3.3 RNA

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)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FNG	D	104	3	24,25,25	1.42	3 (12%)	34,36,36	1.82	8 (23%)
2	FNG	F	104	3	24,25,25	1.53	5 (20%)	34,36,36	2.32	14 (41%)
3	LNQ	H	105	2	17,21,21	1.24	1 (5%)	13,25,25	2.58	5 (38%)
3	LNQ	F	105	2	17,21,21	1.26	2 (11%)	13,25,25	2.21	6 (46%)
2	FNG	E	104	3	24,25,25	1.90	5 (20%)	34,36,36	1.94	9 (26%)
3	LNQ	G	105	2	17,21,21	0.98	2 (11%)	13,25,25	2.34	6 (46%)
3	LNQ	E	105	2	17,21,21	1.03	2 (11%)	13,25,25	2.16	2 (15%)
3	LNQ	D	105	2	17,21,21	1.18	1 (5%)	13,25,25	1.82	2 (15%)
2	FNG	G	104	3	24,25,25	1.82	8 (33%)	34,36,36	2.40	11 (32%)
2	FNG	H	104	3	24,25,25	1.72	5 (20%)	34,36,36	2.63	17 (50%)

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	FNG	D	104	3	-	2/12/34/34	0/2/2/2
2	FNG	F	104	3	-	2/12/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LNQ	H	105	2	-	9/12/30/30	0/1/1/1
3	LNQ	F	105	2	-	7/12/30/30	0/1/1/1
2	FNG	E	104	3	-	2/12/34/34	0/2/2/2
3	LNQ	G	105	2	-	8/12/30/30	0/1/1/1
3	LNQ	E	105	2	-	9/12/30/30	0/1/1/1
3	LNQ	D	105	2	-	9/12/30/30	0/1/1/1
2	FNG	G	104	3	-	2/12/34/34	0/2/2/2
2	FNG	H	104	3	-	2/12/34/34	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	104	FNG	C13-N15	-6.18	1.21	1.33
2	H	104	FNG	O2-C2	4.51	1.53	1.43
2	F	104	FNG	O1-C7	4.00	1.46	1.38
2	G	104	FNG	O1-C7	4.00	1.46	1.38
2	E	104	FNG	O1-C7	3.97	1.46	1.38
2	D	104	FNG	C13-N15	-3.89	1.25	1.33
2	G	104	FNG	C13-N15	-3.72	1.25	1.33
2	H	104	FNG	C9-C13	-3.71	1.45	1.50
3	D	105	LNQ	C13-N14	3.68	1.53	1.45
2	F	104	FNG	C13-N15	-3.64	1.26	1.33
3	F	105	LNQ	C13-N14	3.33	1.52	1.45
3	H	105	LNQ	C13-N14	3.23	1.52	1.45
2	H	104	FNG	O1-C7	2.93	1.44	1.38
2	G	104	FNG	C9-C13	-2.85	1.46	1.50
2	H	104	FNG	C13-N15	-2.56	1.28	1.33
3	G	105	LNQ	C13-N14	2.42	1.50	1.45
3	E	105	LNQ	C13-N14	2.42	1.50	1.45
3	F	105	LNQ	C15-N14	-2.35	1.31	1.41
2	E	104	FNG	C3-C2	2.32	1.58	1.52
2	F	104	FNG	C9-C13	-2.32	1.47	1.50
2	G	104	FNG	C8-C7	-2.32	1.34	1.38
2	D	104	FNG	O1-C7	2.30	1.42	1.38
2	F	104	FNG	C3-C2	2.26	1.58	1.52
2	D	104	FNG	C3-C2	2.25	1.58	1.52
2	G	104	FNG	C8-C9	2.18	1.42	1.39
2	G	104	FNG	C3-C2	2.18	1.57	1.52
2	G	104	FNG	C11-N16	2.18	1.50	1.45
3	G	105	LNQ	C15-N14	-2.09	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	104	FNG	O2-C2	2.07	1.47	1.43
2	H	104	FNG	O14-C13	2.07	1.28	1.24
2	G	104	FNG	C12-C11	-2.06	1.35	1.39
2	E	104	FNG	O2-C2	2.01	1.47	1.43
3	E	105	LNQ	C15-N14	-2.01	1.32	1.41
2	E	104	FNG	C6-C5	2.01	1.58	1.51

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	104	FNG	O17-N16-C11	-8.22	107.16	118.80
3	E	105	LNQ	C8-O7-C6	6.64	142.08	113.29
3	H	105	LNQ	C13-C12-C11	6.64	137.30	113.61
2	H	104	FNG	C11-C12-C7	-5.75	112.61	119.19
2	E	104	FNG	C12-C11-N16	-5.64	113.78	118.75
2	F	104	FNG	C9-C13-N15	5.37	124.19	117.75
2	E	104	FNG	C9-C10-C11	-5.29	113.89	119.87
3	G	105	LNQ	C8-O7-C6	5.27	136.14	113.29
2	H	104	FNG	O17-N16-C11	-5.06	111.64	118.80
2	F	104	FNG	C9-C8-C7	-4.98	114.26	119.57
2	H	104	FNG	O14-C13-N15	-4.72	115.88	122.58
2	G	104	FNG	C11-C12-C7	-4.70	113.81	119.19
2	F	104	FNG	O17-N16-C11	-4.56	112.34	118.80
2	G	104	FNG	O14-C13-N15	-4.51	116.17	122.58
3	D	105	LNQ	C8-O7-C6	4.45	132.57	113.29
2	H	104	FNG	C12-C11-N16	-4.43	114.84	118.75
2	D	104	FNG	C11-C12-C7	-4.35	114.21	119.19
2	F	104	FNG	C10-C11-N16	4.26	122.50	118.75
2	H	104	FNG	C3-C4-C5	-4.15	102.84	110.24
2	G	104	FNG	C8-C7-C12	4.04	127.42	120.98
3	F	105	LNQ	C8-O7-C6	3.93	130.30	113.29
2	D	104	FNG	C9-C8-C7	-3.74	115.58	119.57
2	G	104	FNG	C9-C8-C7	-3.69	115.64	119.57
2	F	104	FNG	C8-C7-C12	3.69	126.87	120.98
2	H	104	FNG	O5-C1-C2	-3.66	102.61	110.35
2	H	104	FNG	O1-C1-C2	3.59	112.35	107.14
2	D	104	FNG	C8-C7-C12	3.44	126.47	120.98
2	D	104	FNG	O17-N16-C11	-3.44	113.94	118.80
3	H	105	LNQ	C12-C13-N14	3.40	120.64	111.49
2	H	104	FNG	C10-C11-C12	3.40	126.27	120.78
3	D	105	LNQ	C12-C13-N14	3.37	120.56	111.49
2	E	104	FNG	C7-O1-C1	-3.30	112.96	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	105	LNQ	C5-O4-C3	3.19	127.09	113.29
2	H	104	FNG	O2-C2-C3	-3.07	103.25	110.35
2	H	104	FNG	C9-C13-N15	3.06	121.43	117.75
2	F	104	FNG	O14-C13-C9	-3.04	115.99	119.63
2	H	104	FNG	C6-C5-C4	-3.03	105.92	113.00
2	F	104	FNG	O1-C1-C2	-3.01	102.77	107.14
3	G	105	LNQ	C12-C13-N14	2.99	119.52	111.49
3	H	105	LNQ	C8-O7-C6	2.97	126.14	113.29
3	F	105	LNQ	C11-O10-C9	2.89	125.80	113.29
2	E	104	FNG	C6-C5-C4	-2.83	106.39	113.00
2	E	104	FNG	C10-C11-C12	2.82	125.33	120.78
3	G	105	LNQ	O4-C5-C6	-2.78	97.86	110.39
3	H	105	LNQ	C11-O10-C9	2.76	125.25	113.29
3	G	105	LNQ	C11-O10-C9	2.76	125.25	113.29
2	G	104	FNG	C9-C13-N15	2.74	121.03	117.75
2	H	104	FNG	O5-C5-C4	2.74	114.66	109.69
2	H	104	FNG	C8-C7-C12	2.67	125.23	120.98
2	G	104	FNG	C10-C11-C12	2.66	125.06	120.78
2	D	104	FNG	O14-C13-N15	2.64	126.33	122.58
2	H	104	FNG	C9-C10-C11	-2.63	116.90	119.87
2	G	104	FNG	C12-C11-N16	-2.53	116.52	118.75
2	H	104	FNG	O14-C13-C9	2.51	122.64	119.63
3	G	105	LNQ	C1-C2-C3	2.51	127.53	112.32
2	H	104	FNG	O4-C4-C3	-2.46	104.67	110.35
3	G	105	LNQ	C5-O4-C3	2.44	123.86	113.29
2	F	104	FNG	C3-C4-C5	-2.44	105.89	110.24
2	E	104	FNG	C10-C11-N16	2.43	120.89	118.75
2	D	104	FNG	C9-C13-N15	-2.41	114.86	117.75
3	F	105	LNQ	O4-C5-C6	-2.40	99.56	110.39
2	D	104	FNG	C8-C9-C10	2.39	122.52	119.63
2	E	104	FNG	C8-C9-C10	2.36	122.47	119.63
3	F	105	LNQ	O10-C9-C8	-2.35	99.81	110.39
2	D	104	FNG	C12-C11-N16	-2.35	116.68	118.75
2	E	104	FNG	C3-C4-C5	-2.29	106.16	110.24
2	H	104	FNG	O2-C2-C1	-2.29	104.49	110.05
2	F	104	FNG	C4-C3-C2	-2.27	106.85	110.82
2	E	104	FNG	C11-C12-C7	-2.22	116.65	119.19
2	G	104	FNG	C9-C10-C11	-2.21	117.37	119.87
2	F	104	FNG	O6-C6-C5	-2.16	103.86	111.29
3	H	105	LNQ	C13-N14-C15	-2.16	110.29	121.78
3	F	105	LNQ	O7-C8-C9	-2.15	100.70	110.39
2	F	104	FNG	O2-C2-C3	-2.11	105.46	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	104	FNG	O3-C3-C4	-2.11	105.48	110.35
2	F	104	FNG	O5-C5-C4	2.10	113.51	109.69
3	E	105	LNQ	O7-C8-C9	-2.05	101.13	110.39
2	G	104	FNG	C4-C3-C2	-2.05	107.25	110.82
2	F	104	FNG	C6-C5-C4	-2.04	108.23	113.00
2	G	104	FNG	O2-C2-C3	-2.02	105.67	110.35

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	105	LNQ	C11-C12-C13-N14
3	H	105	LNQ	C11-C12-C13-N14
3	E	105	LNQ	O7-C8-C9-O10
3	F	105	LNQ	O7-C8-C9-O10
3	E	105	LNQ	O10-C11-C12-C13
3	D	105	LNQ	O4-C5-C6-O7
3	D	105	LNQ	C1-C2-C3-O4
3	D	105	LNQ	C5-C6-O7-C8
3	H	105	LNQ	C1-C2-C3-O4
3	F	105	LNQ	C1-C2-C3-O4
3	D	105	LNQ	O10-C11-C12-C13
3	G	105	LNQ	C1-C2-C3-O4
3	H	105	LNQ	O7-C8-C9-O10
3	E	105	LNQ	C1-C2-C3-O4
3	G	105	LNQ	O7-C8-C9-O10
3	G	105	LNQ	O4-C5-C6-O7
3	H	105	LNQ	O10-C11-C12-C13
3	E	105	LNQ	O4-C5-C6-O7
3	G	105	LNQ	C12-C13-N14-C15
3	D	105	LNQ	C11-C12-C13-N14
3	E	105	LNQ	C12-C13-N14-C15
3	H	105	LNQ	C6-C5-O4-C3
3	H	105	LNQ	C9-C8-O7-C6
2	E	104	FNG	C8-C7-O1-C1
3	G	105	LNQ	O10-C11-C12-C13
3	F	105	LNQ	C11-C12-C13-N14
3	D	105	LNQ	C2-C3-O4-C5
3	F	105	LNQ	C5-C6-O7-C8
3	H	105	LNQ	C8-C9-O10-C11
3	E	105	LNQ	C2-C3-O4-C5
3	F	105	LNQ	C9-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
3	H	105	LNQ	O4-C5-C6-O7
2	E	104	FNG	C12-C7-O1-C1
2	H	104	FNG	C8-C7-O1-C1
3	D	105	LNQ	O7-C8-C9-O10
3	D	105	LNQ	C12-C13-N14-C15
2	H	104	FNG	C12-C7-O1-C1
3	G	105	LNQ	C9-C8-O7-C6
3	D	105	LNQ	C6-C5-O4-C3
2	D	104	FNG	C12-C7-O1-C1
2	D	104	FNG	C8-C7-O1-C1
2	F	104	FNG	C12-C7-O1-C1
2	F	104	FNG	C8-C7-O1-C1
3	G	105	LNQ	C2-C3-O4-C5
2	G	104	FNG	C12-C7-O1-C1
2	G	104	FNG	C8-C7-O1-C1
3	F	105	LNQ	C6-C5-O4-C3
3	H	105	LNQ	C12-C13-N14-C15
3	G	105	LNQ	C6-C5-O4-C3
3	E	105	LNQ	C6-C5-O4-C3
3	F	105	LNQ	O4-C5-C6-O7
3	E	105	LNQ	C9-C8-O7-C6

There are no ring outliers.

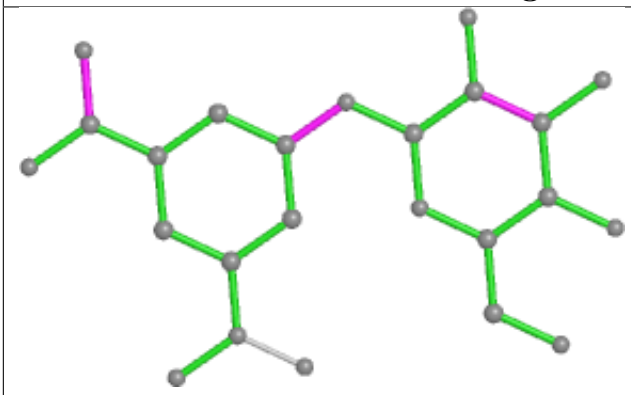
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	104	FNG	1	0
3	H	105	LNQ	1	0
3	G	105	LNQ	1	0
3	D	105	LNQ	1	0

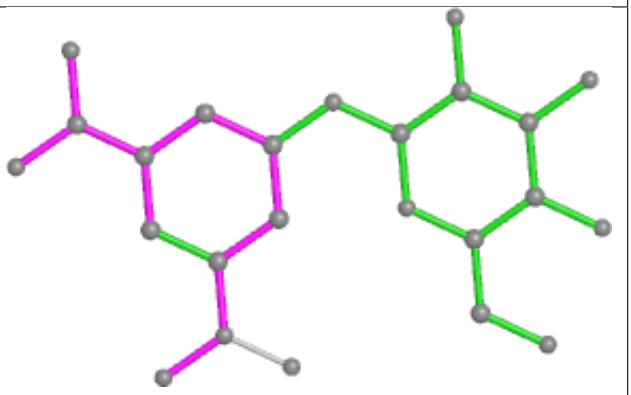
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

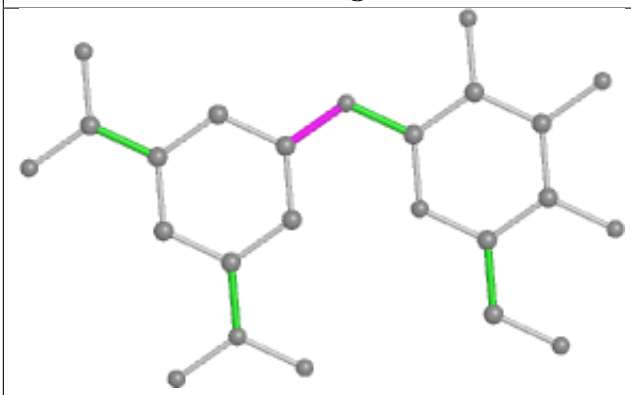
Ligand FNG D 104



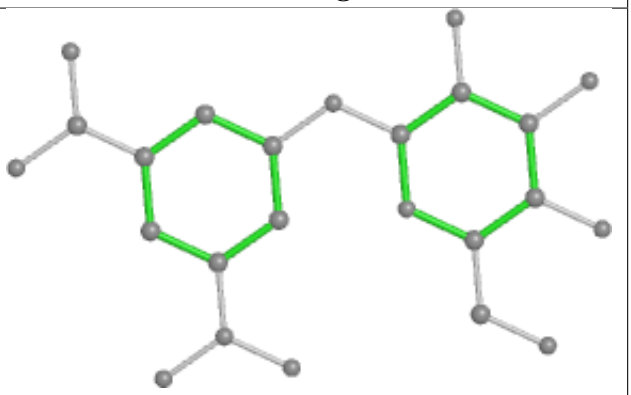
Bond lengths



Bond angles

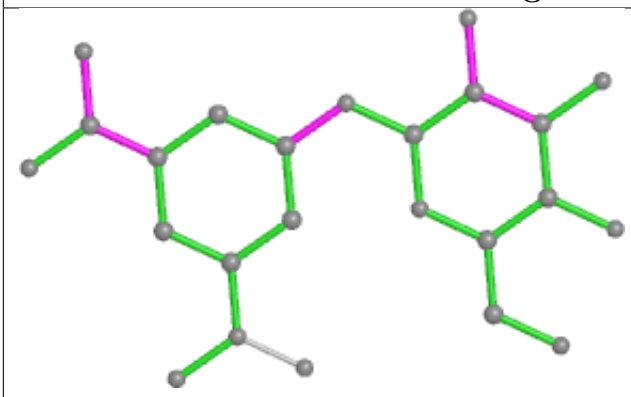


Torsions

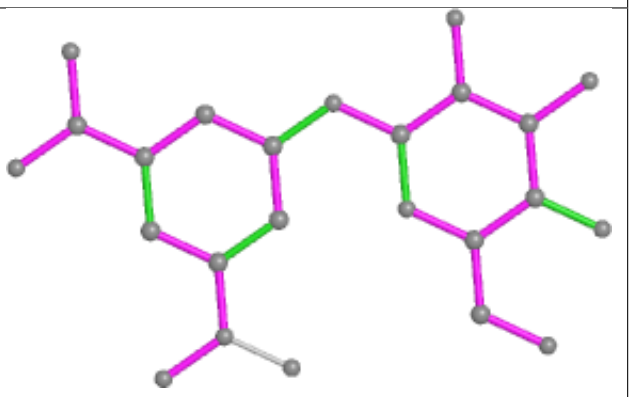


Rings

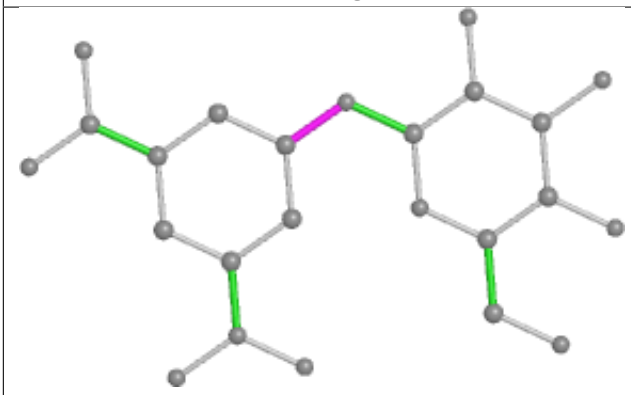
Ligand FNG F 104



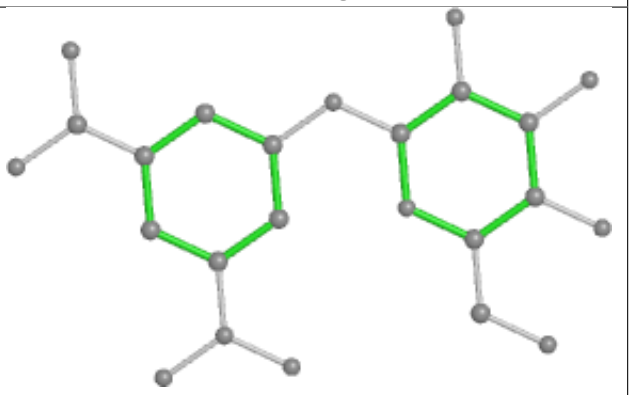
Bond lengths



Bond angles

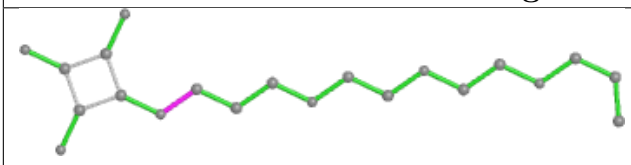


Torsions

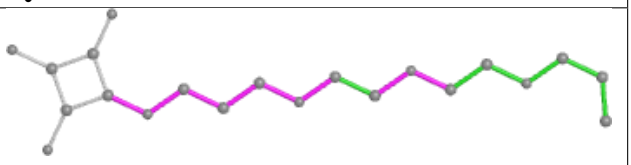


Rings

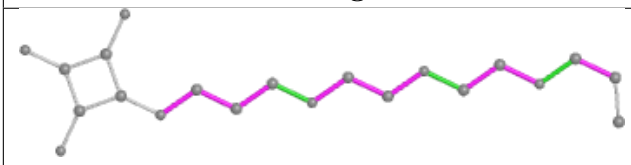
Ligand LNQ H 105



Bond lengths



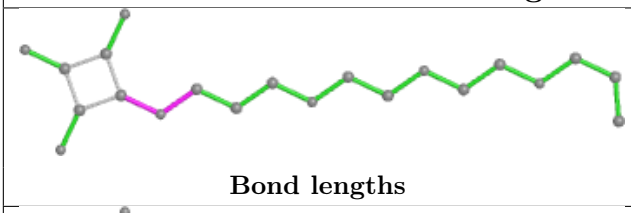
Bond angles



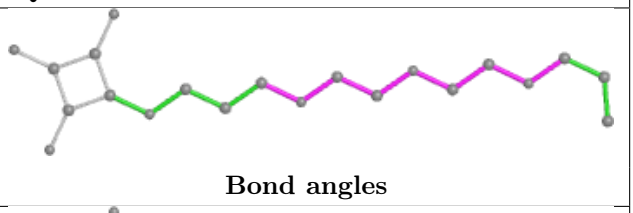
Torsions

Rings

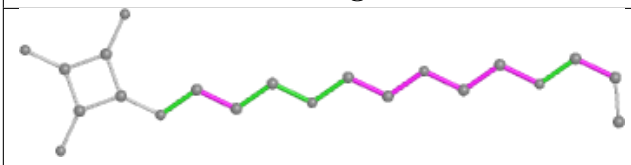
Ligand LNQ F 105



Bond lengths



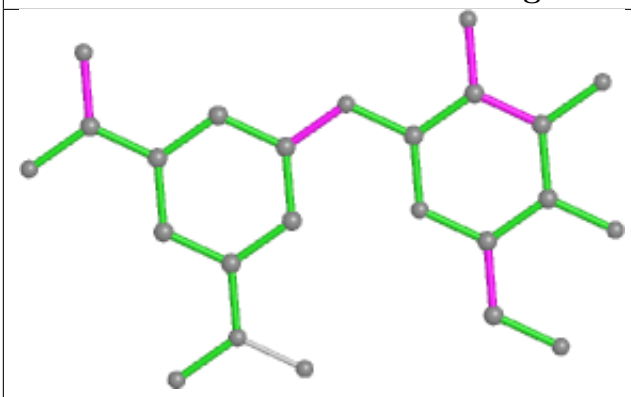
Bond angles



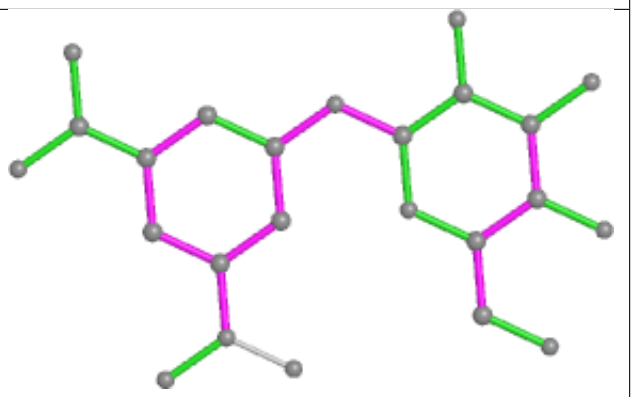
Torsions

Rings

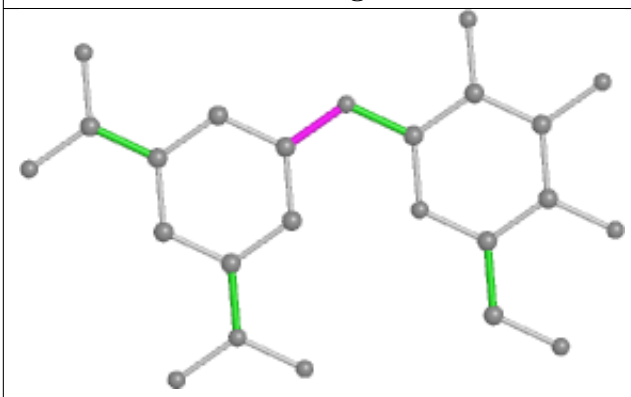
Ligand FNG E 104



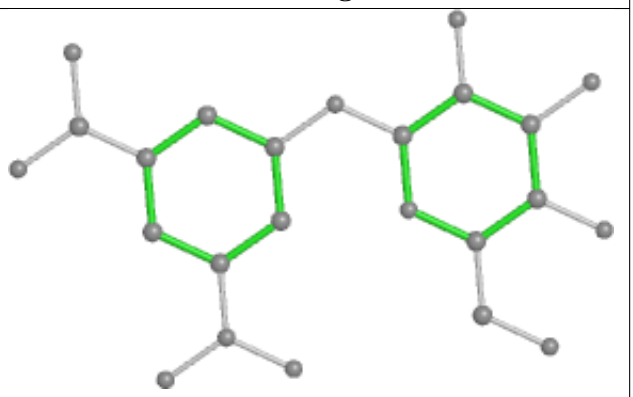
Bond lengths



Bond angles

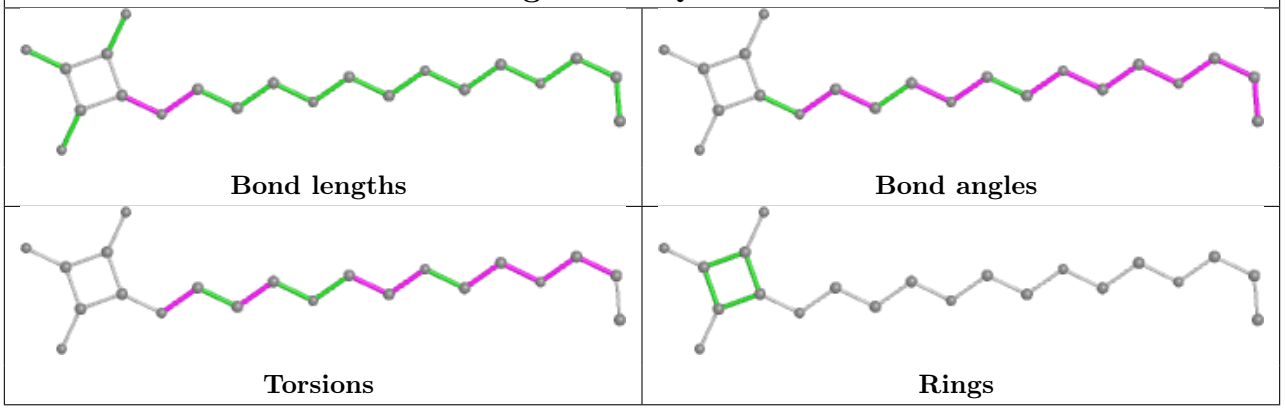


Torsions

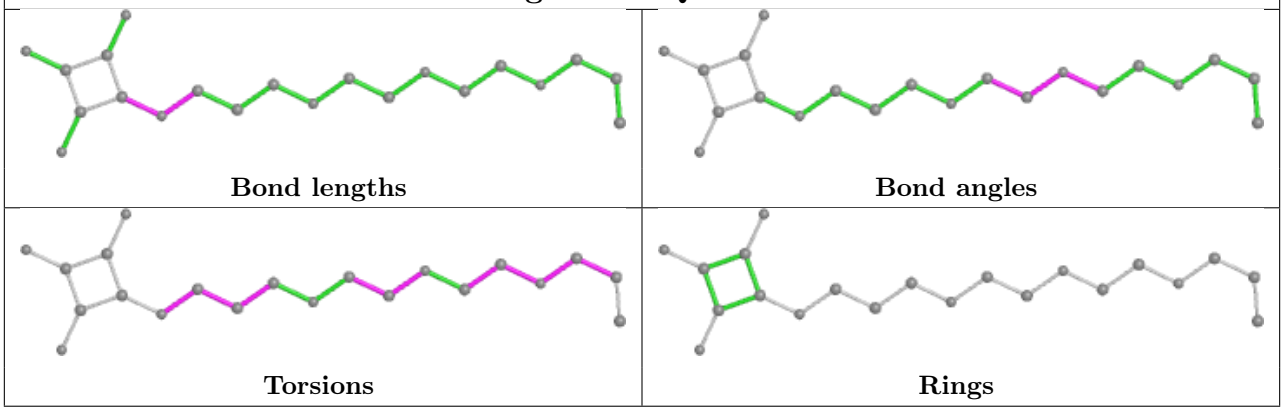


Rings

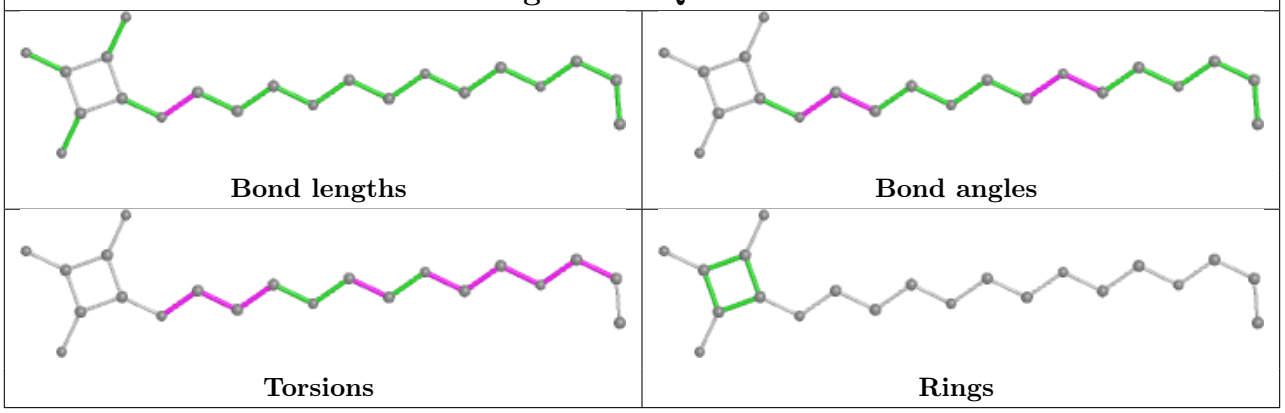
Ligand LNQ G 105



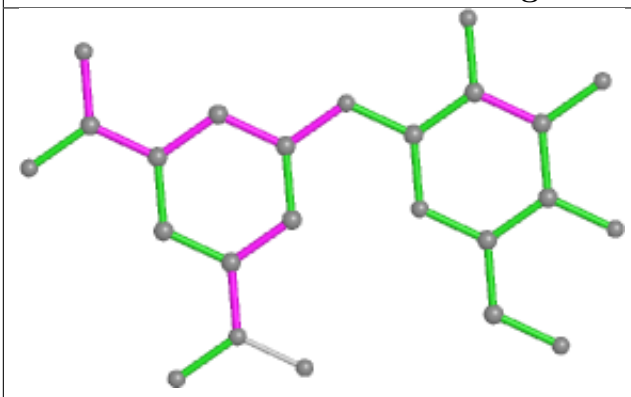
Ligand LNQ E 105



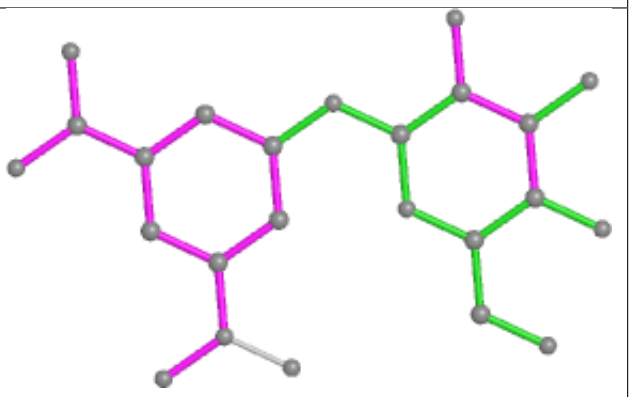
Ligand LNQ D 105



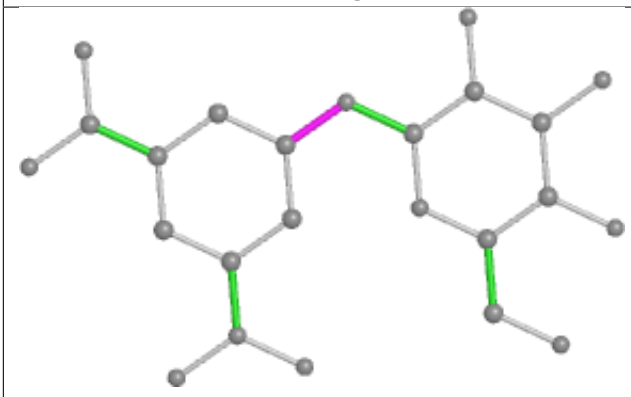
Ligand FNG G 104



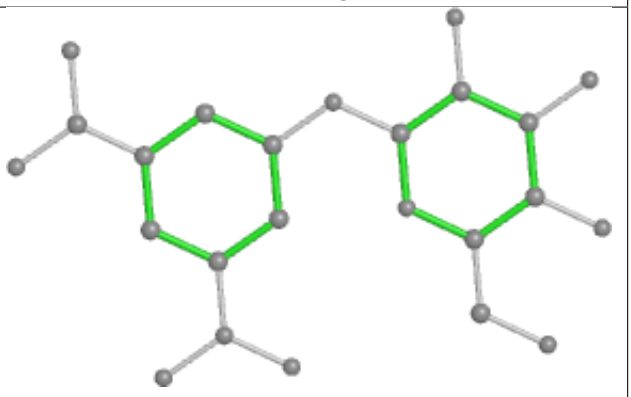
Bond lengths



Bond angles

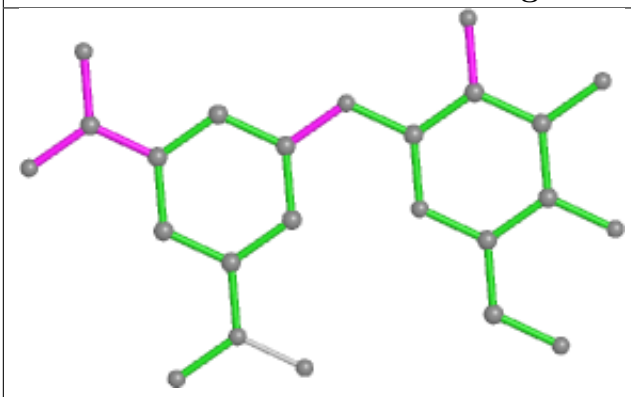


Torsions

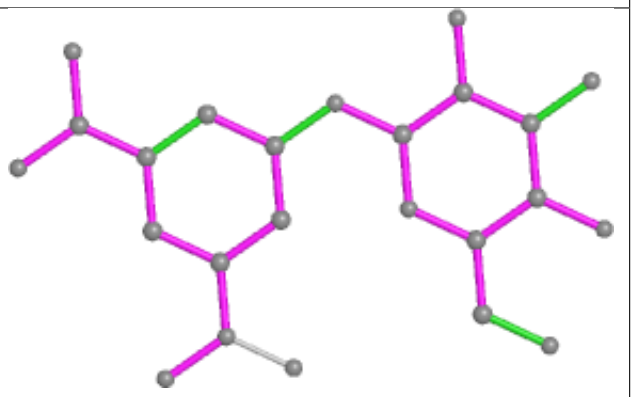


Rings

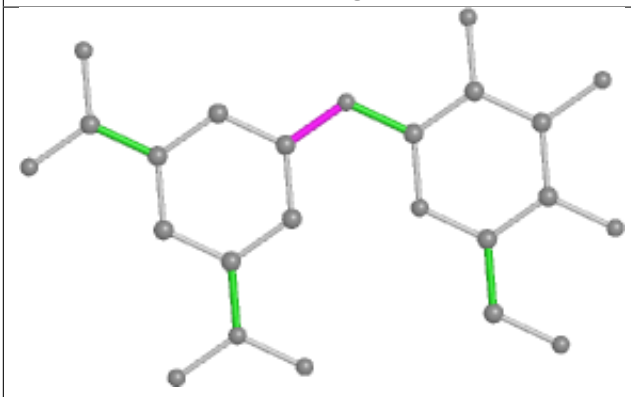
Ligand FNG H 104



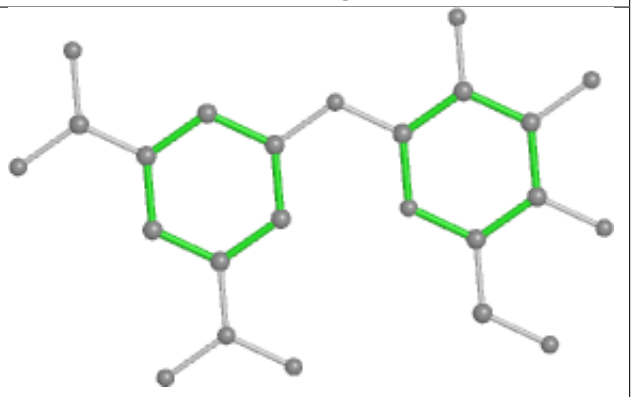
Bond lengths



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	D	103/103 (100%)	0.04	3 (2%)	51	53	8, 13, 22, 32	0
1	E	103/103 (100%)	-0.00	2 (1%)	66	68	9, 14, 22, 28	0
1	F	103/103 (100%)	0.14	3 (2%)	51	53	10, 16, 22, 31	0
1	G	103/103 (100%)	-0.08	3 (2%)	51	53	9, 13, 20, 30	0
1	H	103/103 (100%)	-0.14	1 (0%)	82	84	8, 12, 19, 31	0
All	All	515/515 (100%)	-0.01	12 (2%)	60	63	8, 13, 22, 32	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	THR	7.8
1	F	13	HIS	4.9
1	H	103	ASN	4.9
1	D	103	ASN	4.7
1	G	103	ASN	4.6
1	F	103	ASN	4.6
1	E	103	ASN	4.5
1	D	13	HIS	3.9
1	E	1	THR	3.6
1	G	1	THR	3.3
1	F	1	THR	2.6
1	G	13	HIS	2.0

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

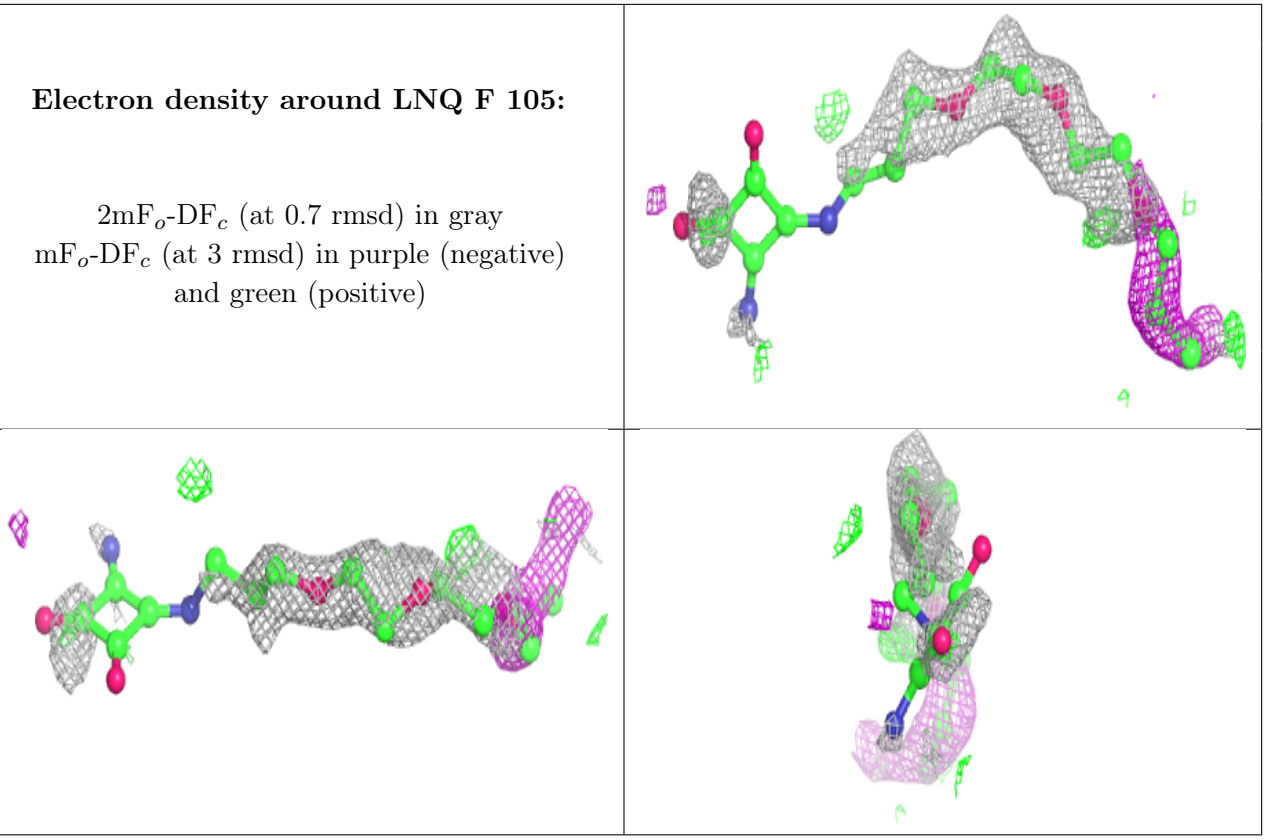
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	LNQ	F	105	21/21	0.46	0.46	31,36,36,36	8
3	LNQ	H	105	21/21	0.57	0.39	27,35,37,37	8
3	LNQ	G	105	21/21	0.59	0.36	28,35,35,36	8
3	LNQ	D	105	21/21	0.60	0.37	29,35,36,37	8
3	LNQ	E	105	21/21	0.65	0.36	29,35,36,36	8
2	FNG	F	104	24/24	0.81	0.17	19,23,30,32	0
2	FNG	H	104	24/24	0.87	0.13	16,20,26,28	0
2	FNG	G	104	24/24	0.87	0.14	14,18,27,29	0
2	FNG	E	104	24/24	0.88	0.14	19,22,29,30	0
2	FNG	D	104	24/24	0.90	0.13	17,21,28,29	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.

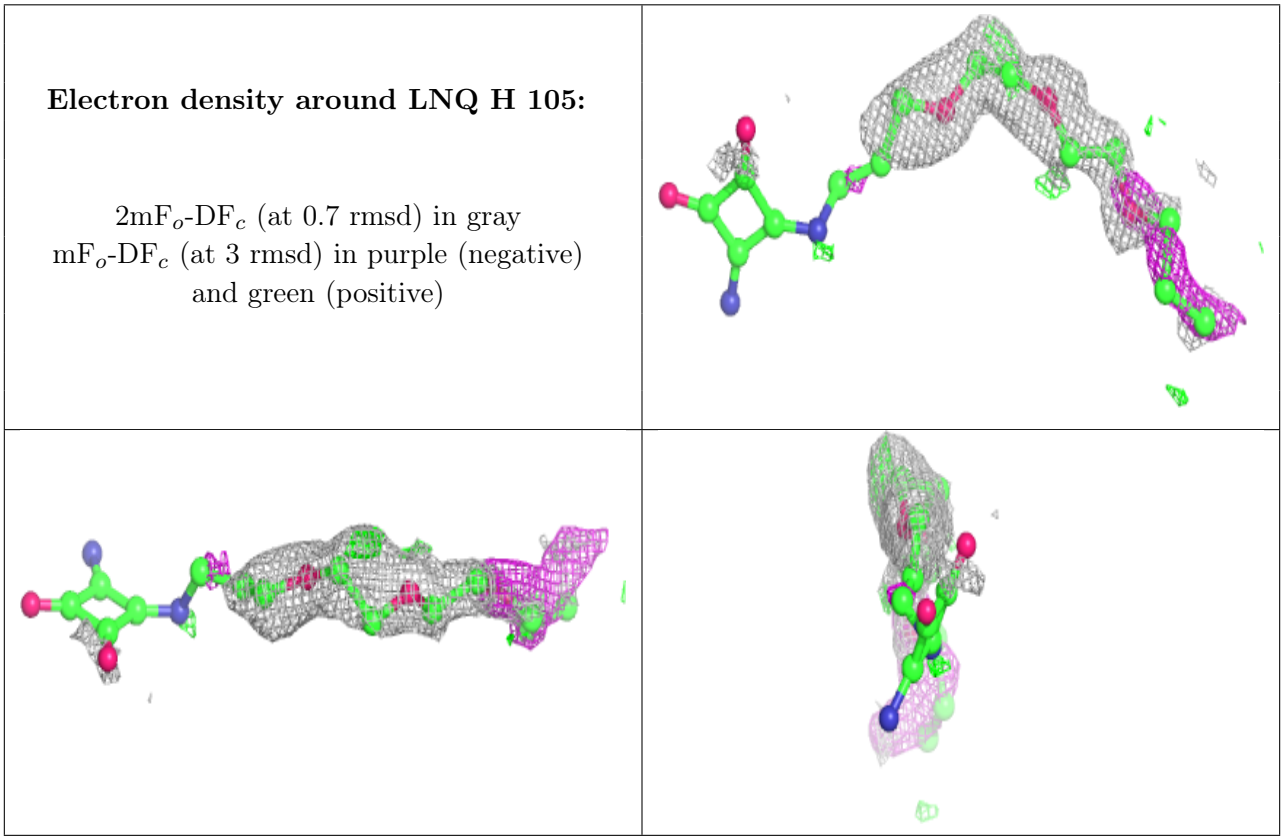
Electron density around LNQ F 105:

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



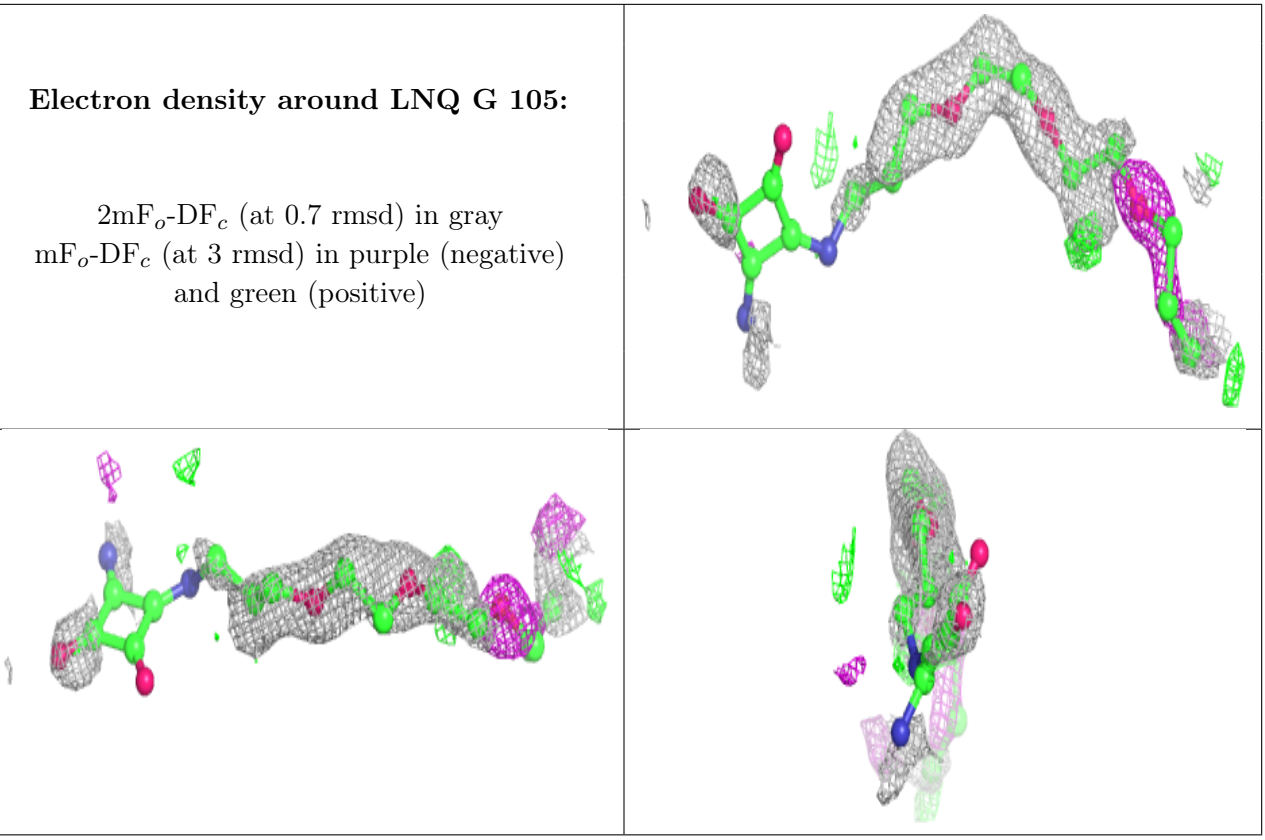
Electron density around LNQ H 105:

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



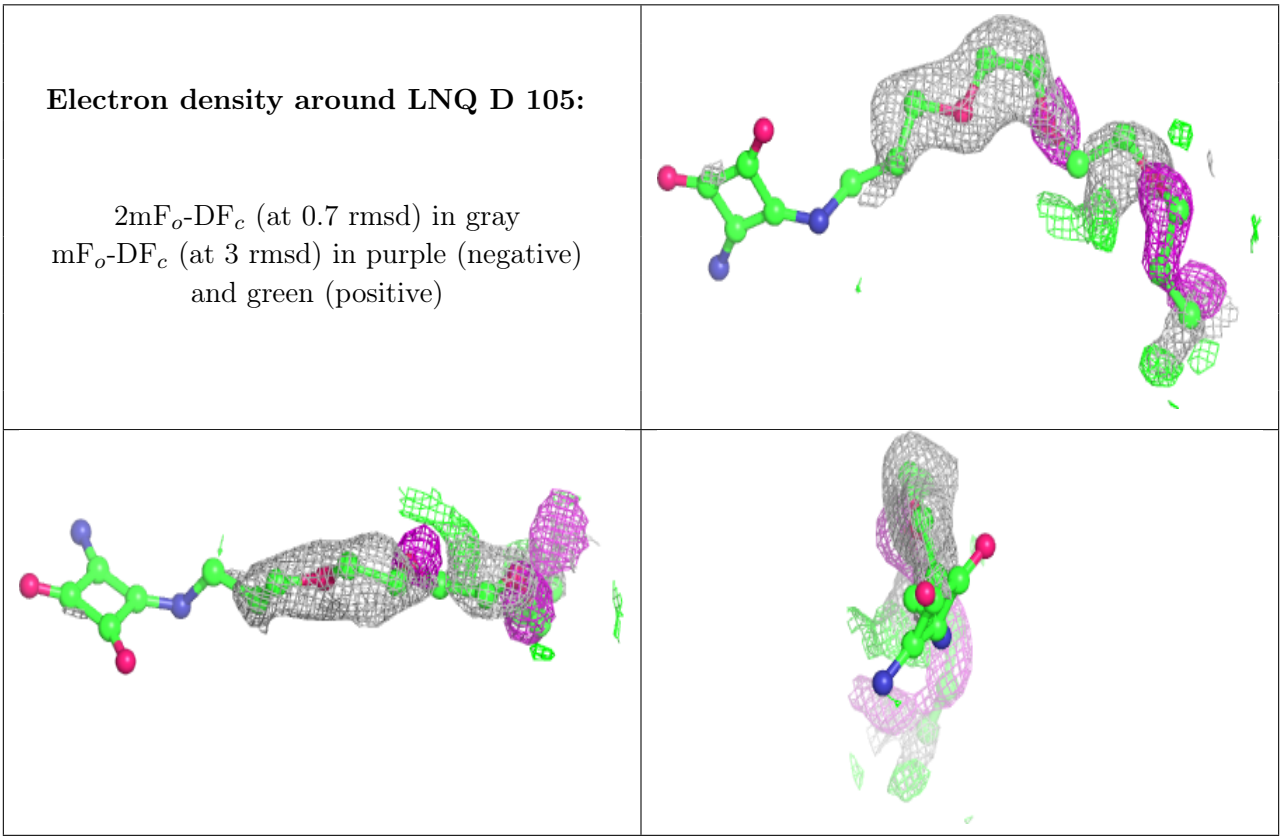
Electron density around LNQ G 105:

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



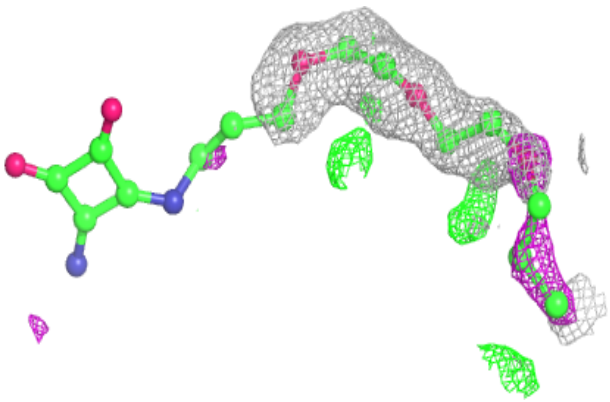
Electron density around LNQ D 105:

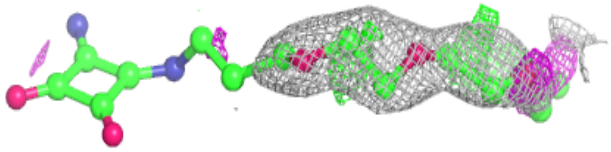
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

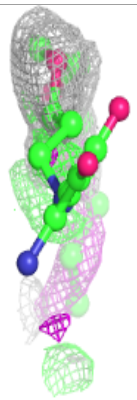


Electron density around LNQ E 105:

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

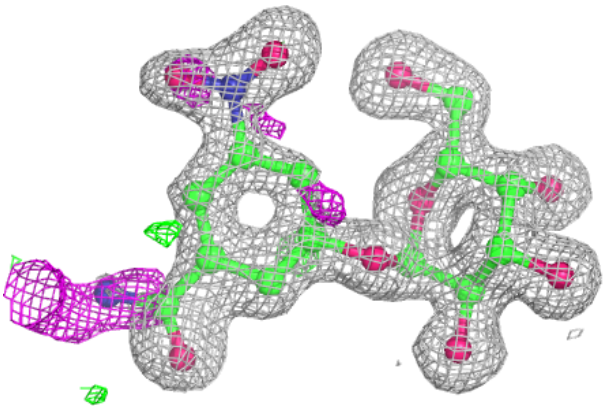


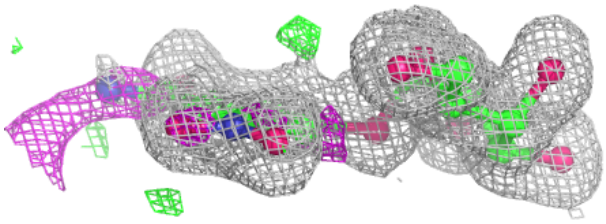


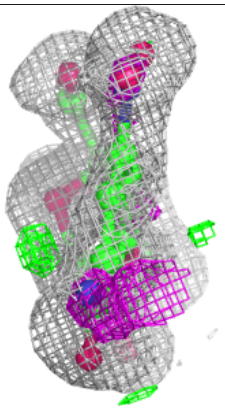


Electron density around FNG F 104:

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

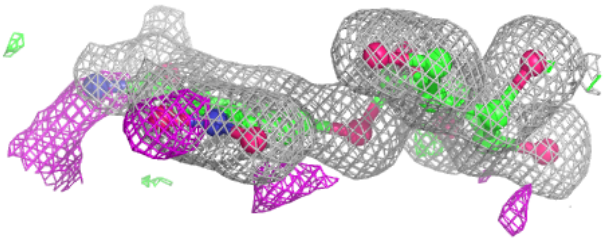


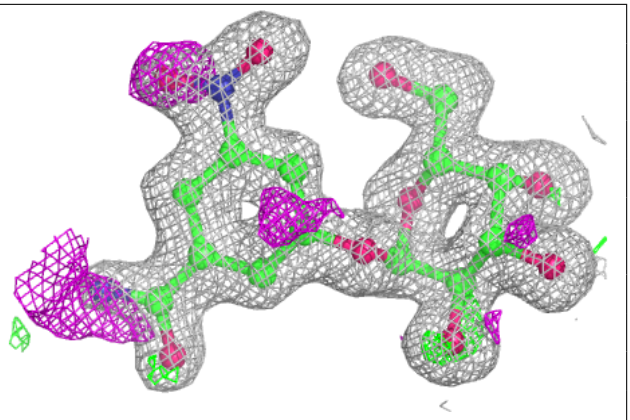


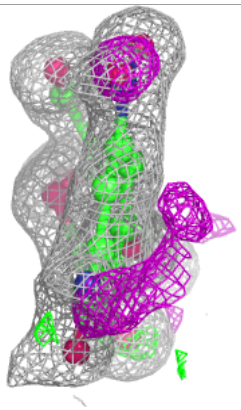


Electron density around FNG H 104:

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

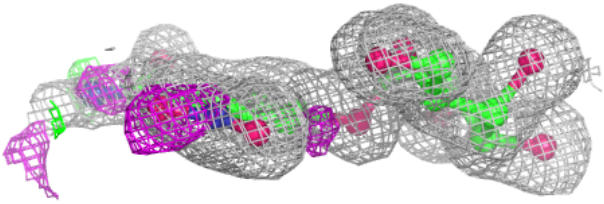


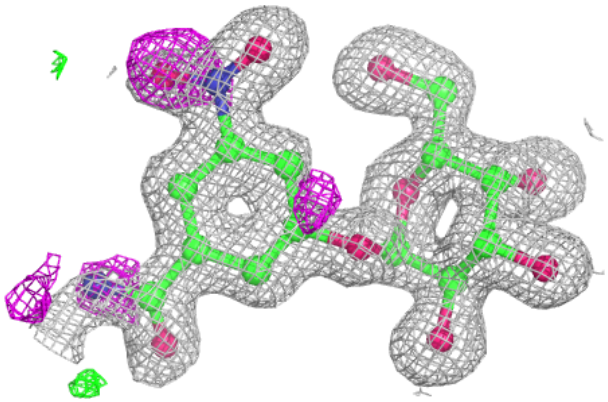


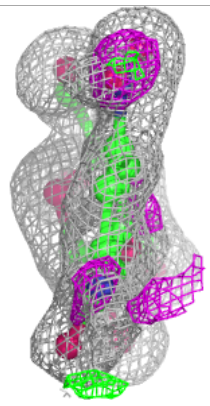


Electron density around FNG G 104:

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

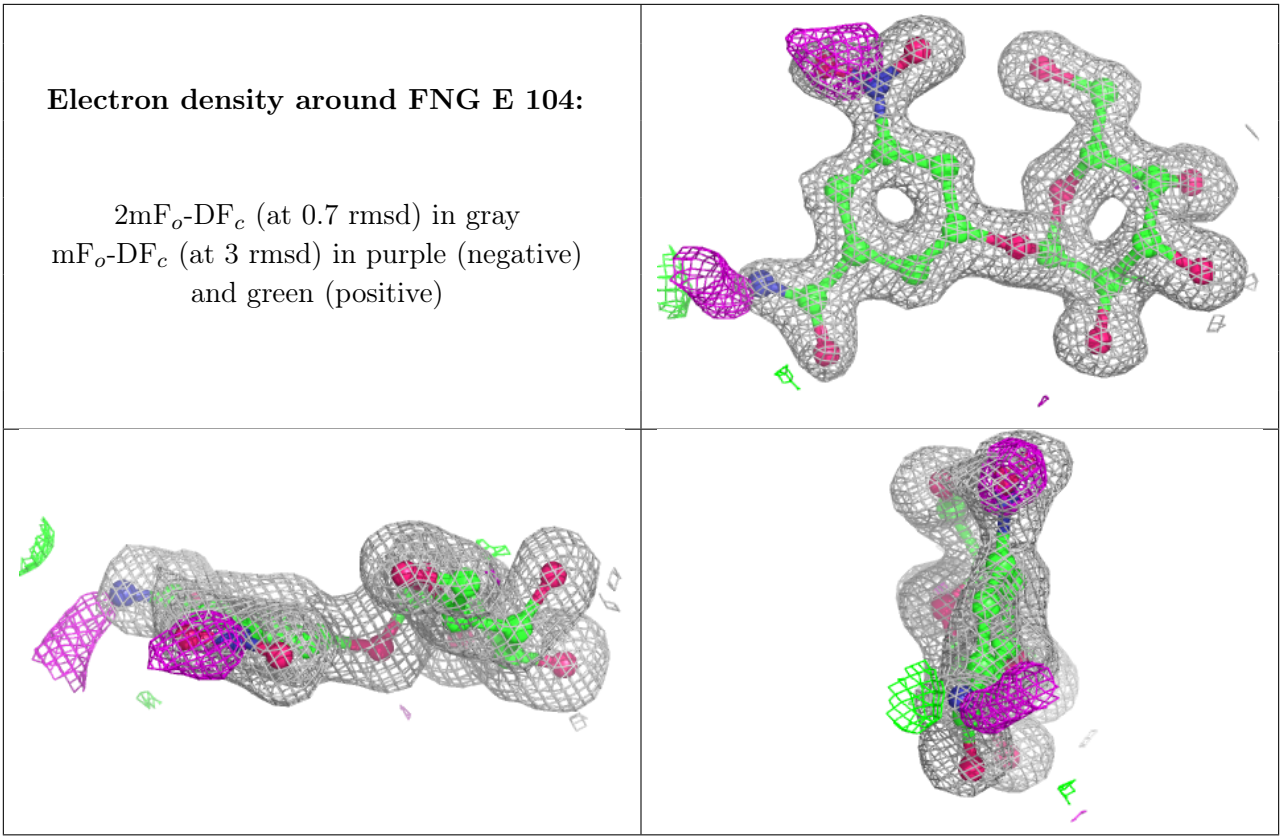






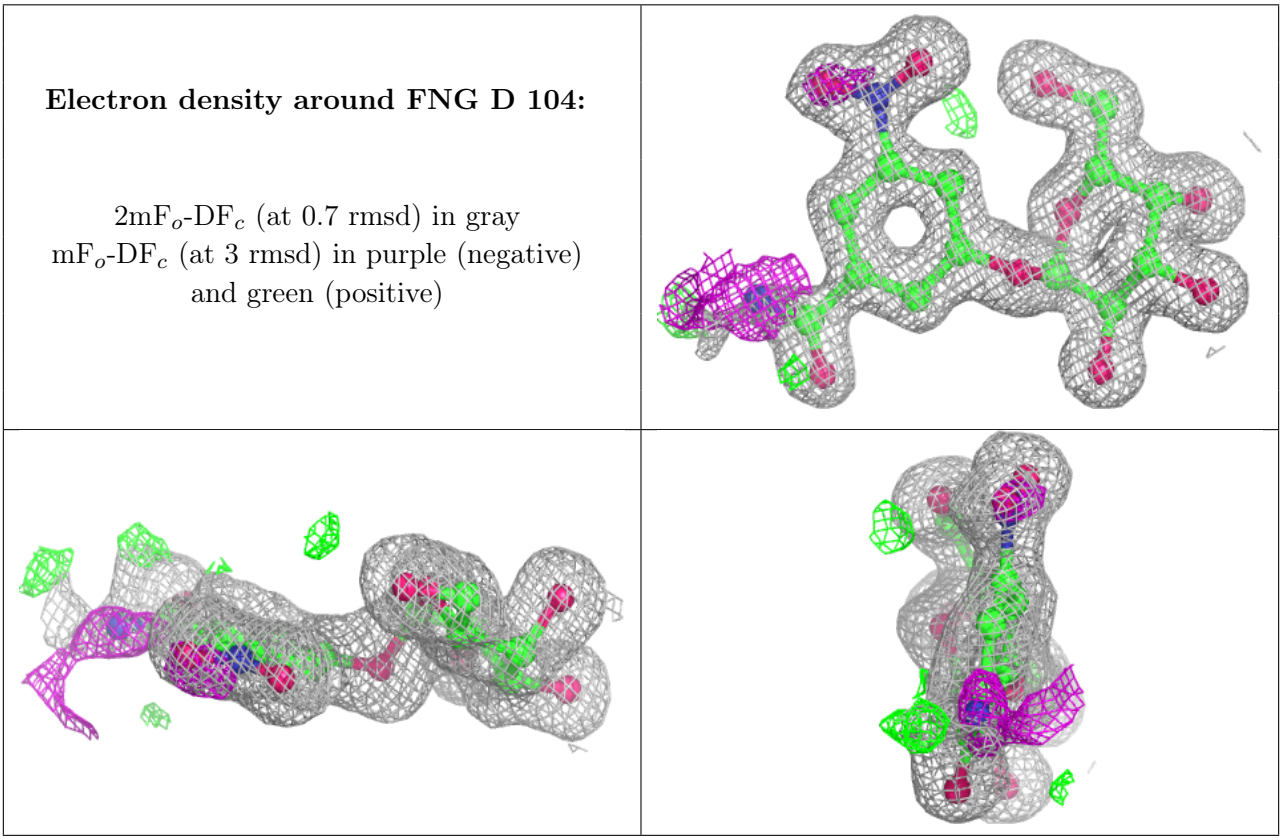
Electron density around FNG E 104:

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



Electron density around FNG D 104:

$2mF_o$-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.