Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2025 – 12:19 pm GMT

PDB ID	:	8S34
Title	:	Ferric-mycobactin receptor (FemA) in complex with aeruginic acid
Authors	:	Moynie, L.
Deposited on	:	2024-02-19
Resolution	:	1.86 Å(reported)

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

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

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

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

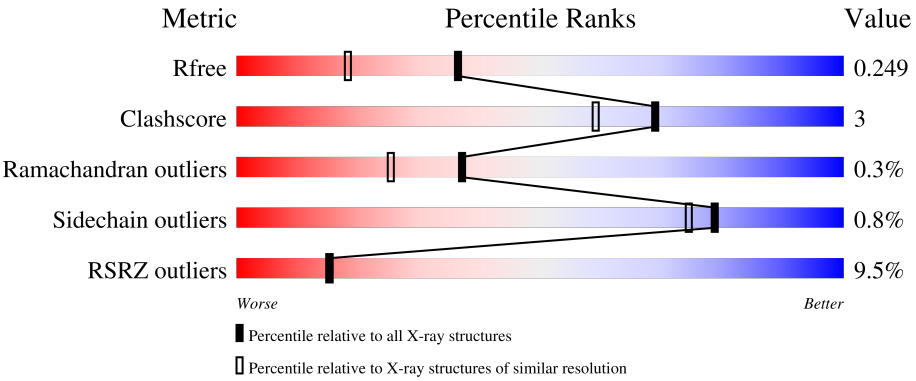
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	780	9% 79% 7% 14%
1	B	780	8% 79% 8% 14%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11194 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.

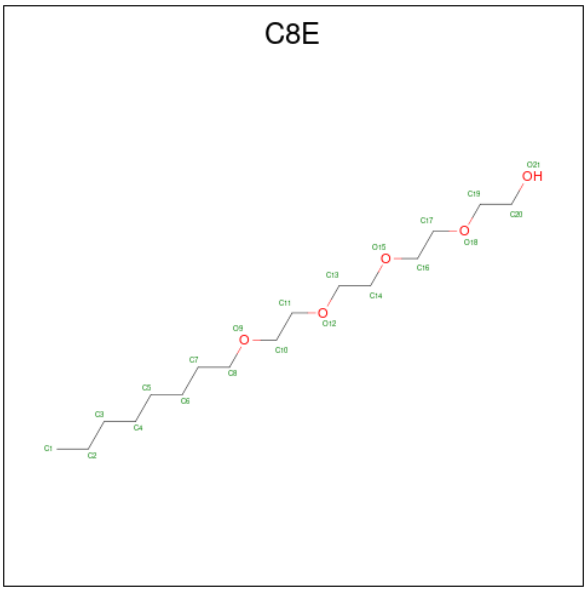
- Molecule 1 is a protein called Ferric-mycobactin receptor, FemA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	674	Total	C	N	O	S	0	5	0
			5209	3247	943	1010	9			
1	A	674	Total	C	N	O	S	0	2	0
			5179	3229	936	1005	9			

There are 8 discrepancies between the modelled and reference sequences:

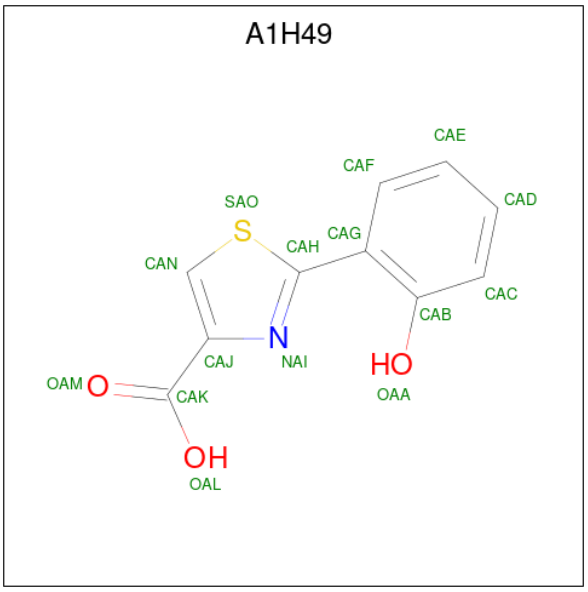
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9I2J4
B	-1	ALA	-	expression tag	UNP Q9I2J4
B	0	MET	-	expression tag	UNP Q9I2J4
B	1	THR	-	expression tag	UNP Q9I2J4
A	-2	GLY	-	expression tag	UNP Q9I2J4
A	-1	ALA	-	expression tag	UNP Q9I2J4
A	0	MET	-	expression tag	UNP Q9I2J4
A	1	THR	-	expression tag	UNP Q9I2J4

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



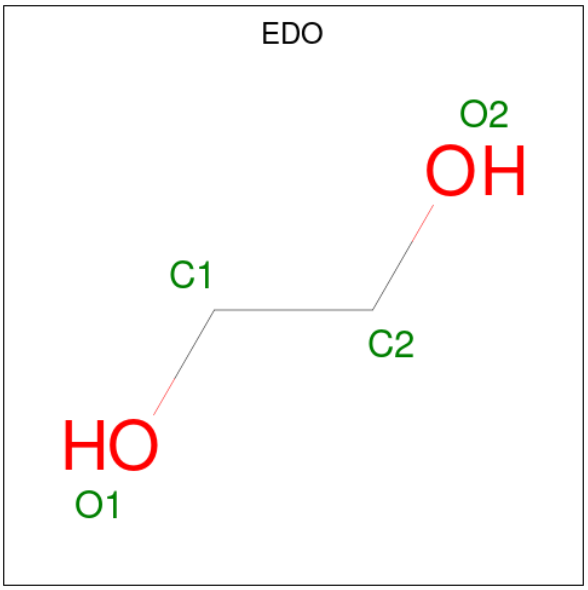
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 12 10 2	0	0
2	B	1	Total C O 15 12 3	0	0
2	B	1	Total C O 13 8 5	0	0
2	B	1	Total C O 12 10 2	0	0
2	A	1	Total C O 12 10 2	0	0
2	A	1	Total C O 21 16 5	0	0
2	A	1	Total C O 15 12 3	0	0

- Molecule 3 is 2-(2-hydroxyphenyl)-1,3-thiazole-4-carboxylic acid (three-letter code: A1H49) (formula: $C_{10}H_7NO_3S$) (labeled as "Ligand of Interest" by depositor).



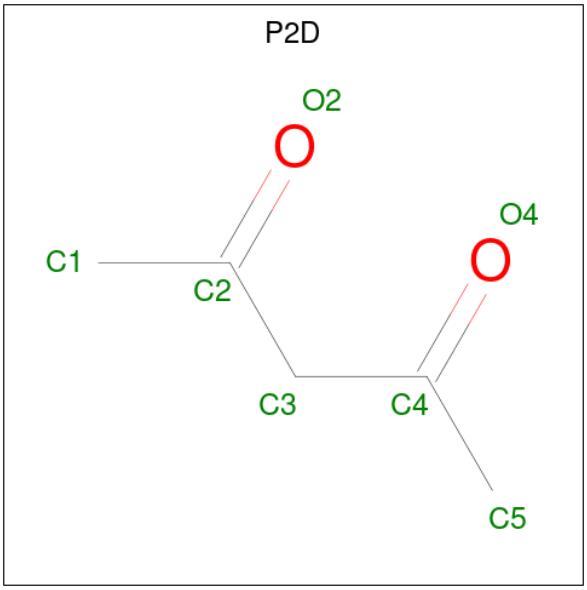
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			15	10	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			15	10	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			15	10	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			15	10	1	3	1		

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



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

- Molecule 5 is pentane-2,4-dione (three-letter code: P2D) (formula: $C_5H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 5 2	0	0
5	A	1	Total C O 7 5 2	0	0

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Fe 1 1	0	0
6	A	1	Total Fe 1 1	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	6	Total K 6 6	0	0
7	A	8	Total K 8 8	0	0

- Molecule 8 is water.

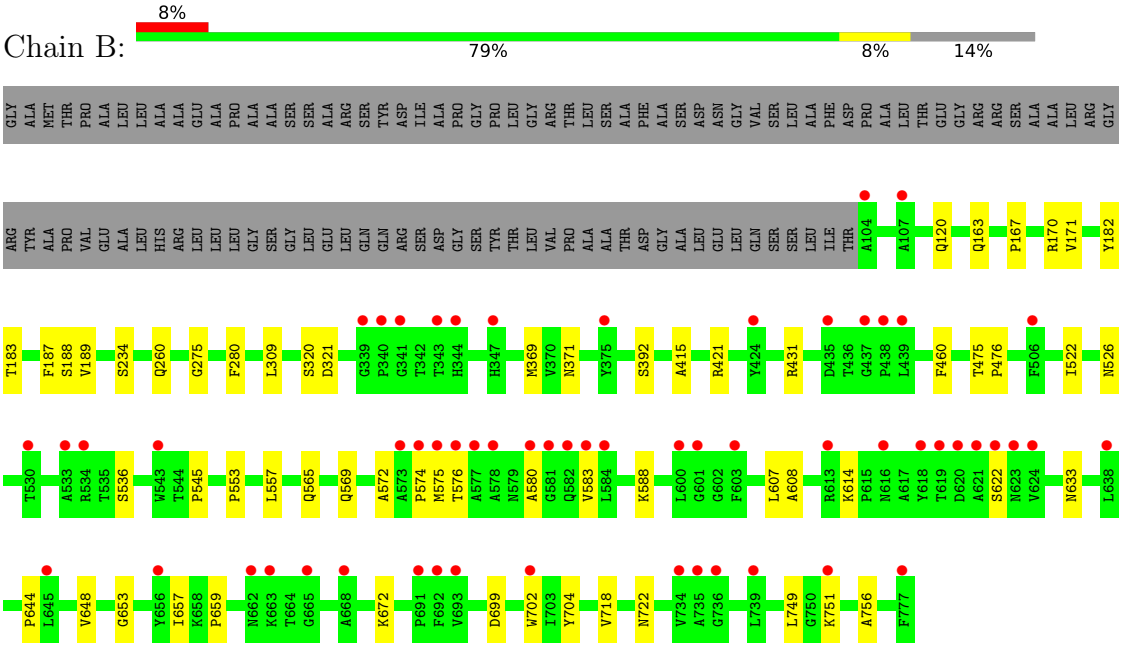
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	306	Total O 306 306	0	0
8	A	298	Total O 298 298	0	0

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.

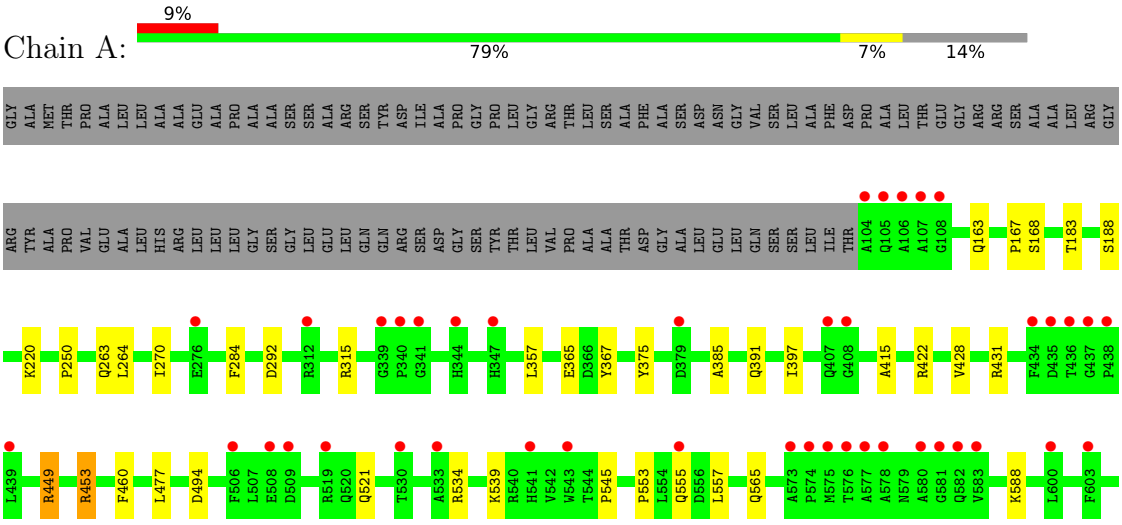
• Molecule 1: Ferric-mycobactin receptor, FemA

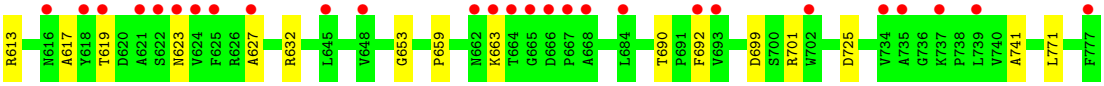
Chain B:



• Molecule 1: Ferric-mycobactin receptor, FemA

Chain A:




R613
N616
A617
Y618
T619
D620
A621
S622
N623
V624
F625
R626
A627
R632
L645
V648
G653
P659
N662
K663
T664
G665
D666
P667
A668
L684
T690
P691
F692
V693
D699
S700
R701
W702
D725
V734
A735
G736
K737
P738
L739
V740
A741
L771
F777

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	83.86Å 84.88Å 86.86Å 90.01° 118.53° 113.70°	Depositor
Resolution (Å)	75.47 – 1.86 75.47 – 1.86	Depositor EDS
% Data completeness (in resolution range)	94.3 (75.47-1.86) 94.5 (75.47-1.86)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.213 , 0.249 0.213 , 0.249	Depositor DCC
R_{free} test set	15375 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11194	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.43% 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: K, EDO, C8E, P2D, A1H49, FE

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	0.39	0/5288	0.58	0/7185
1	B	0.40	0/5319	0.59	0/7227
All	All	0.39	0/10607	0.59	0/14412

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5179	0	5035	33	0
1	B	5209	0	5058	37	0
2	A	48	0	80	5	0
2	B	52	0	84	8	0
3	A	30	0	0	0	0
3	B	30	0	0	1	0
4	A	8	0	12	1	0
4	B	4	0	6	0	0
5	A	7	0	8	0	0
5	B	7	0	8	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	8	0	0	0	0
7	B	6	0	0	0	0
8	A	298	0	0	6	0
8	B	306	0	0	7	0
All	All	11194	0	10291	70	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (70) 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:188:SER:HB2	2:B:805:C8E:H142	1.72	0.71
1:A:431:ARG:NH1	8:A:903:HOH:O	2.24	0.70
1:B:187:PHE:HD1	2:B:805:C8E:H171	1.54	0.69
1:A:565:GLN:OE1	1:A:588:LYS:HD2	2.00	0.62
1:A:453:ARG:NH1	8:A:901:HOH:O	2.21	0.61
1:B:565:GLN:OE1	1:B:588:LYS:HD2	2.01	0.60
1:B:614:LYS:HE3	2:B:805:C8E:H191	1.83	0.60
1:B:633:ASN:HB3	1:B:657:ILE:HD11	1.83	0.60
1:A:167:PRO:HG3	1:A:653:GLY:HA3	1.83	0.58
1:B:120:GLN:NE2	8:B:903:HOH:O	2.31	0.57
1:B:522:ILE:HG21	1:B:569:GLN:HG3	1.87	0.55
1:A:449:ARG:NH1	1:A:494:ASP:OD2	2.33	0.54
1:A:250:PRO:HG3	8:A:1190:HOH:O	2.07	0.54
1:B:309:LEU:HB3	2:B:804:C8E:H22	1.90	0.54
1:B:260:GLN:NE2	8:B:909:HOH:O	2.41	0.53
1:A:188:SER:H	4:A:806:EDO:H22	1.73	0.53
1:B:572:ALA:HA	1:B:583:VAL:HA	1.89	0.53
1:B:722:ASN:O	1:B:751:LYS:HE3	2.08	0.52
1:A:168:SER:HB2	1:A:220:LYS:HE2	1.91	0.52
1:A:741:ALA:HB1	2:A:802:C8E:H162	1.91	0.52
1:B:167:PRO:HG3	1:B:653:GLY:HA3	1.91	0.51
1:B:320:SER:HB2	2:B:804:C8E:H81	1.93	0.51
1:A:357:LEU:HD21	1:A:477:LEU:HD21	1.92	0.51
1:A:553:PRO:HG2	1:A:557:LEU:HD23	1.93	0.51
1:B:583:VAL:HG13	8:B:1109:HOH:O	2.10	0.51
1:A:367:TYR:HD2	2:A:801:C8E:H61	1.74	0.51
1:B:553:PRO:HG2	1:B:557:LEU:HD23	1.91	0.51
1:B:163[B]:GLN:OE1	1:B:170:ARG:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PHE:HD2	2:B:804:C8E:H32	1.75	0.50
1:A:391:GLN:OE1	1:A:422:ARG:HG2	2.11	0.50
1:A:555:GLN:CD	1:A:555:GLN:H	2.15	0.49
1:B:575:MET:HA	1:B:580:ALA:HB1	1.94	0.49
1:B:183:THR:HG21	8:B:1004:HOH:O	2.12	0.48
1:A:264:LEU:HB3	2:A:802:C8E:H31	1.95	0.48
1:B:431:ARG:NH1	8:B:905:HOH:O	2.46	0.47
1:A:690:THR:HB	1:A:692:PHE:CE1	2.49	0.47
1:A:619:THR:HG22	1:A:623:ASN:HA	1.97	0.47
1:B:275:GLY:HA2	1:A:365:GLU:OE1	2.15	0.47
1:A:453:ARG:HD2	8:A:1120:HOH:O	2.15	0.47
1:A:701:ARG:HB2	1:A:725:ASP:HB2	1.98	0.46
1:A:397:ILE:HG21	1:A:477:LEU:HD22	1.98	0.46
1:B:574:PRO:C	1:B:576:THR:H	2.19	0.45
1:B:371:ASN:HB3	2:B:804:C8E:H111	1.98	0.45
1:A:264:LEU:HD22	2:A:802:C8E:H51	1.98	0.45
1:A:613:ARG:HG2	1:A:632:ARG:HG3	1.99	0.45
1:A:263:GLN:HG3	1:A:292:ASP:O	2.17	0.44
1:A:521:GLN:OE1	1:A:539:LYS:NZ	2.48	0.44
1:A:315:ARG:NH2	1:A:375:TYR:OH	2.35	0.44
1:A:771:LEU:HB3	2:A:802:C8E:H131	2.00	0.43
1:B:749:LEU:HB2	1:B:751:LYS:HE2	1.99	0.43
1:B:475:THR:HB	1:B:476:PRO:HD2	2.00	0.43
1:A:270:ILE:HD12	1:A:284:PHE:HD2	1.82	0.43
1:A:220:LYS:HE3	8:A:1005:HOH:O	2.17	0.43
1:B:182:TYR:O	1:B:189:VAL:N	2.43	0.43
1:A:385:ALA:HB2	1:A:428:VAL:HG23	2.00	0.43
1:A:183:THR:HG21	8:A:1046:HOH:O	2.18	0.42
1:B:415:ALA:HB2	1:B:460:PHE:CD2	2.54	0.42
1:A:415:ALA:HB2	1:A:460:PHE:CD2	2.55	0.42
3:B:803:A1H49:OAM	8:B:901:HOH:O	2.22	0.42
1:B:163[B]:GLN:NE2	8:B:922:HOH:O	2.51	0.41
1:B:718:VAL:HG21	1:B:756:ALA:HB2	2.02	0.41
1:B:607:LEU:HG	1:B:608:ALA:N	2.35	0.41
1:B:644:PRO:HD2	1:B:648:VAL:O	2.20	0.41
1:A:617:ALA:HA	1:A:627:ALA:HA	2.02	0.41
1:B:163[B]:GLN:OE1	1:B:171:VAL:N	2.54	0.41
1:B:321:ASP:O	1:B:369:MET:HA	2.21	0.41
1:B:526:ASN:HD22	1:B:536:SER:HG	1.68	0.41
1:B:702:TRP:CZ2	1:B:704:TYR:HB2	2.56	0.41
1:B:234:SER:HA	2:B:805:C8E:H202	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:SER:HB3	1:B:421:ARG:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	674/780 (86%)	659 (98%)	13 (2%)	2 (0%)	37	25
1	B	677/780 (87%)	657 (97%)	18 (3%)	2 (0%)	37	25
All	All	1351/1560 (87%)	1316 (97%)	31 (2%)	4 (0%)	37	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	545	PRO
1	A	545	PRO
1	B	659	PRO
1	A	659	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	538/612 (88%)	531 (99%)	7 (1%)	65	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	541/612 (88%)	538 (99%)	3 (1%)	84 81
All	All	1079/1224 (88%)	1069 (99%)	10 (1%)	79 70

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

Mol	Chain	Res	Type
1	B	622	SER
1	B	672	LYS
1	B	699	ASP
1	A	163[A]	GLN
1	A	163[B]	GLN
1	A	449	ARG
1	A	453	ARG
1	A	534	ARG
1	A	663	LYS
1	A	699	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	HIS
1	A	733	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
4	EDO	A	806	-	3,3,3	0.46	0	2,2,2	0.39	0
5	P2D	B	807	-	6,6,6	2.17	1 (16%)	6,7,7	0.61	0
3	A1H49	A	803	6	14,16,16	3.28	2 (14%)	13,22,22	1.51	3 (23%)
4	EDO	B	806	-	3,3,3	0.53	0	2,2,2	0.15	0
2	C8E	B	804	-	14,14,20	0.30	0	13,13,19	0.55	0
3	A1H49	A	804	6	14,16,16	3.33	2 (14%)	13,22,22	1.61	3 (23%)
3	A1H49	B	803	6	14,16,16	3.56	2 (14%)	13,22,22	1.68	2 (15%)
4	EDO	A	805	-	3,3,3	0.47	0	2,2,2	0.18	0
2	C8E	B	808	-	11,11,20	0.29	0	10,10,19	0.48	0
2	C8E	A	801	-	11,11,20	0.26	0	10,10,19	0.59	0
5	P2D	A	807	-	6,6,6	2.21	1 (16%)	6,7,7	0.77	0
2	C8E	B	801	-	11,11,20	0.28	0	10,10,19	0.61	0
3	A1H49	B	802	6	14,16,16	3.31	2 (14%)	13,22,22	1.53	3 (23%)
2	C8E	B	805	-	12,12,20	0.45	0	11,11,19	0.31	0
2	C8E	A	808	-	14,14,20	0.32	0	13,13,19	0.71	0
2	C8E	A	802	-	20,20,20	0.37	0	19,19,19	0.53	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
4	EDO	A	806	-	-	1/1/1/1	-
5	P2D	B	807	-	-	4/4/4/4	-
3	A1H49	A	803	6	-	0/4/8/8	0/2/2/2
4	EDO	B	806	-	-	0/1/1/1	-
2	C8E	B	804	-	-	5/12/12/18	-
3	A1H49	A	804	6	-	0/4/8/8	0/2/2/2
3	A1H49	B	803	6	-	0/4/8/8	0/2/2/2
4	EDO	A	805	-	-	1/1/1/1	-
2	C8E	B	808	-	-	5/9/9/18	-
2	C8E	A	801	-	-	3/9/9/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	P2D	A	807	-	-	4/4/4/4	-
2	C8E	B	801	-	-	8/9/9/18	-
3	A1H49	B	802	6	-	0/4/8/8	0/2/2/2
2	C8E	B	805	-	-	6/10/10/18	-
2	C8E	A	808	-	-	8/12/12/18	-
2	C8E	A	802	-	-	9/18/18/18	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	A1H49	CAJ-CAK	-11.86	1.34	1.50
3	B	803	A1H49	CAJ-CAK	-11.82	1.34	1.50
3	B	802	A1H49	CAJ-CAK	-11.33	1.34	1.50
3	A	803	A1H49	CAJ-CAK	-11.27	1.35	1.50
3	B	803	A1H49	CAH-SAO	-5.45	1.66	1.73
5	A	807	P2D	O4-C4	4.91	1.40	1.21
5	B	807	P2D	O4-C4	4.84	1.40	1.21
3	B	802	A1H49	CAH-SAO	-4.00	1.68	1.73
3	A	803	A1H49	CAH-SAO	-3.98	1.68	1.73
3	A	804	A1H49	CAH-NAI	2.62	1.35	1.31

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	803	A1H49	CAJ-CAN-SAO	-4.63	106.11	111.79
3	A	803	A1H49	CAJ-CAN-SAO	-3.87	107.04	111.79
3	A	804	A1H49	CAJ-CAN-SAO	-3.73	107.21	111.79
3	B	802	A1H49	CAJ-CAN-SAO	-3.64	107.32	111.79
3	A	804	A1H49	OAL-CAK-CAJ	2.55	120.50	114.69
3	B	802	A1H49	OAL-CAK-CAJ	2.49	120.36	114.69
3	A	804	A1H49	CAN-CAJ-CAK	-2.37	121.45	128.42
3	B	802	A1H49	OAL-CAK-OAM	-2.35	118.14	123.35
3	B	803	A1H49	OAL-CAK-CAJ	2.32	119.96	114.69
3	A	803	A1H49	OAL-CAK-CAJ	2.30	119.92	114.69
3	A	803	A1H49	OAL-CAK-OAM	-2.28	118.29	123.35

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	807	P2D	C1-C2-C3-C4
5	B	807	P2D	O2-C2-C3-C4
5	A	807	P2D	C2-C3-C4-C5
5	A	807	P2D	C2-C3-C4-O4
2	A	802	C8E	O15-C16-C17-O18
2	B	805	C8E	O12-C13-C14-O15
2	A	808	C8E	O12-C13-C14-O15
2	A	802	C8E	O12-C13-C14-O15
2	A	802	C8E	C6-C7-C8-O9
2	B	801	C8E	C6-C7-C8-O9
2	A	808	C8E	C6-C7-C8-O9
2	B	804	C8E	O12-C13-C14-O15
2	B	805	C8E	O18-C19-C20-O21
2	A	802	C8E	C2-C3-C4-C5
2	B	801	C8E	C2-C3-C4-C5
2	A	808	C8E	C3-C4-C5-C6
2	A	801	C8E	C3-C4-C5-C6
2	B	801	C8E	C3-C4-C5-C6
2	B	804	C8E	C3-C4-C5-C6
2	B	801	C8E	O9-C10-C11-O12
2	A	802	C8E	O18-C19-C20-O21
2	B	805	C8E	O9-C10-C11-O12
4	A	806	EDO	O1-C1-C2-O2
2	A	808	C8E	O9-C10-C11-O12
2	A	801	C8E	C2-C3-C4-C5
2	B	808	C8E	O9-C10-C11-O12
2	A	801	C8E	O9-C10-C11-O12
2	B	801	C8E	C1-C2-C3-C4
2	B	801	C8E	C4-C5-C6-C7
2	B	808	C8E	C2-C3-C4-C5
2	B	808	C8E	C3-C4-C5-C6
2	A	808	C8E	C1-C2-C3-C4
2	A	802	C8E	C3-C4-C5-C6
2	A	808	C8E	C5-C6-C7-C8
4	A	805	EDO	O1-C1-C2-O2
2	B	805	C8E	C20-C19-O18-C17
2	A	802	C8E	C11-C10-O9-C8
2	A	802	C8E	C7-C8-O9-C10
5	B	807	P2D	C2-C3-C4-C5
2	A	802	C8E	C16-C17-O18-C19
2	A	808	C8E	C11-C10-O9-C8
2	B	805	C8E	C13-C14-O15-C16
2	B	801	C8E	C11-C10-O9-C8

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Mol	Chain	Res	Type	Atoms
2	B	801	C8E	C7-C8-O9-C10
2	B	804	C8E	C7-C8-O9-C10
2	A	808	C8E	C7-C8-O9-C10
2	B	804	C8E	C6-C7-C8-O9
2	B	805	C8E	C10-C11-O12-C13
2	B	808	C8E	C7-C8-O9-C10
2	B	804	C8E	O9-C10-C11-O12
5	B	807	P2D	C2-C3-C4-O4
5	A	807	P2D	C1-C2-C3-C4
5	A	807	P2D	O2-C2-C3-C4
2	B	808	C8E	C11-C10-O9-C8

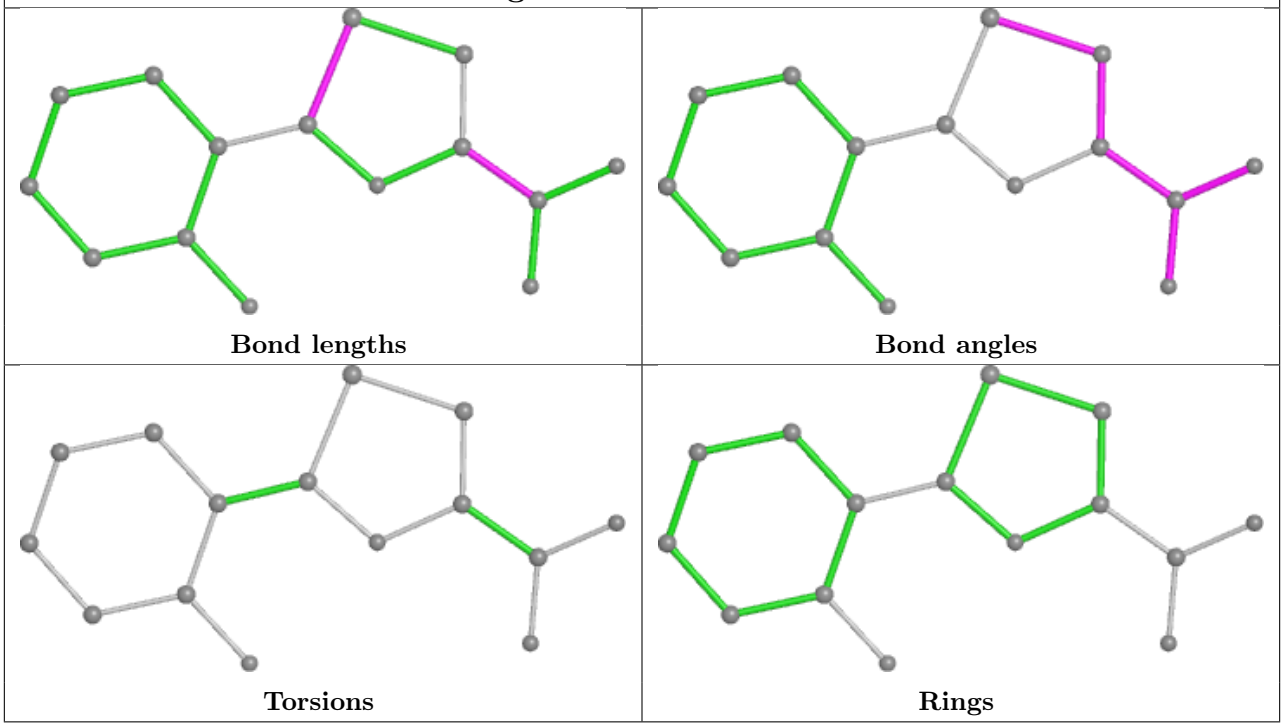
There are no ring outliers.

6 monomers are involved in 15 short contacts:

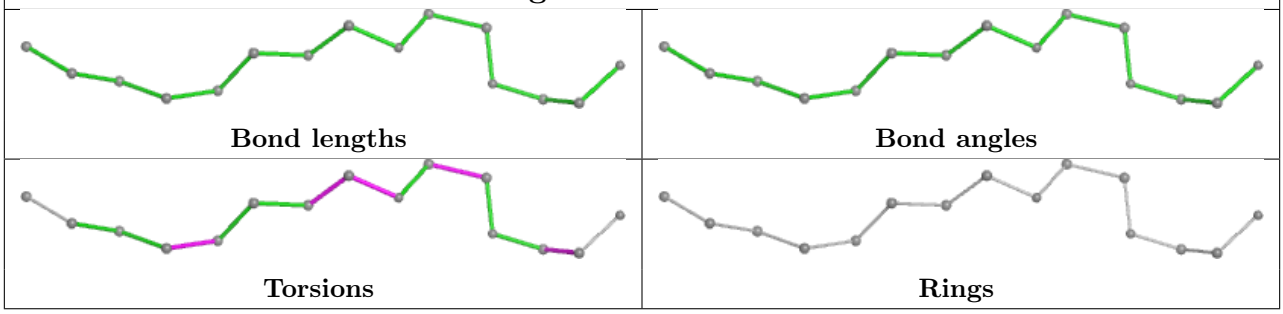
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	806	EDO	1	0
2	B	804	C8E	4	0
3	B	803	A1H49	1	0
2	A	801	C8E	1	0
2	B	805	C8E	4	0
2	A	802	C8E	4	0

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.

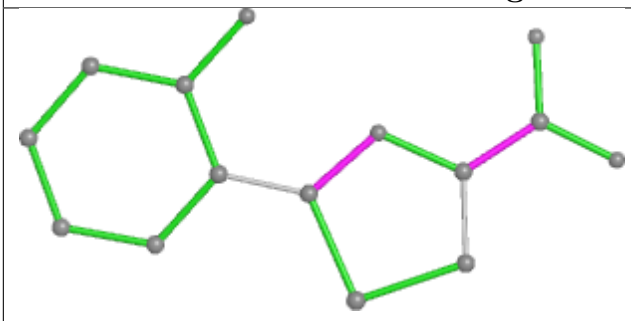
Ligand A1H49 A 803



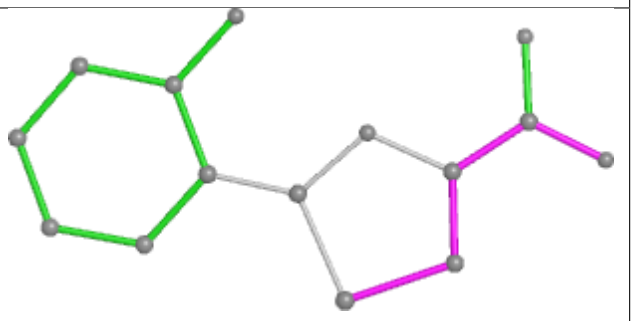
Ligand C8E B 804



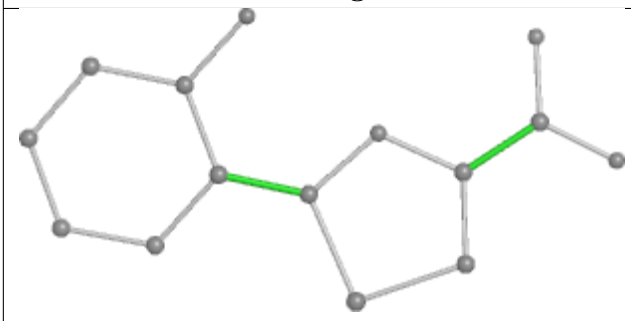
Ligand A1H49 A 804



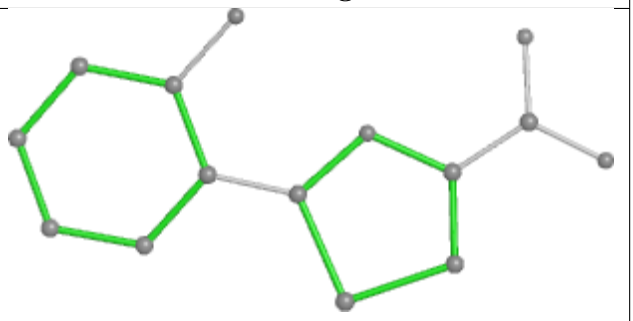
Bond lengths



Bond angles

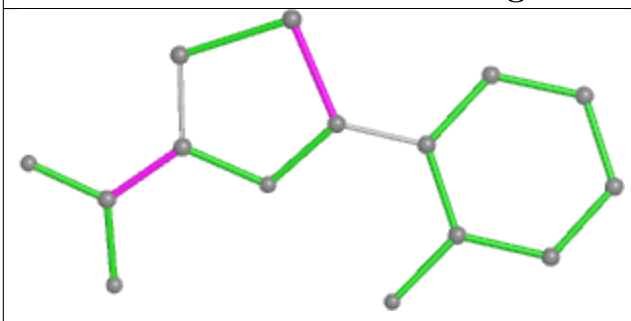


Torsions

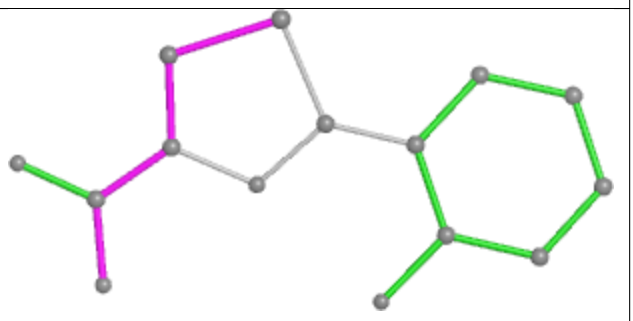


Rings

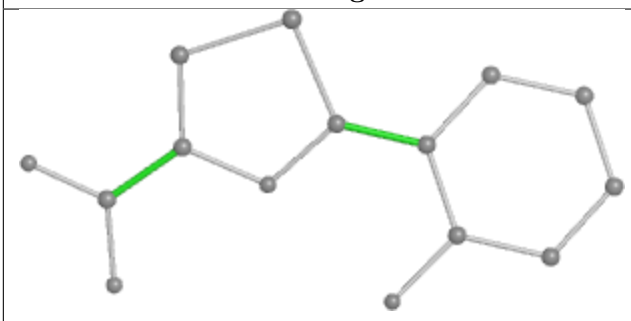
Ligand A1H49 B 803



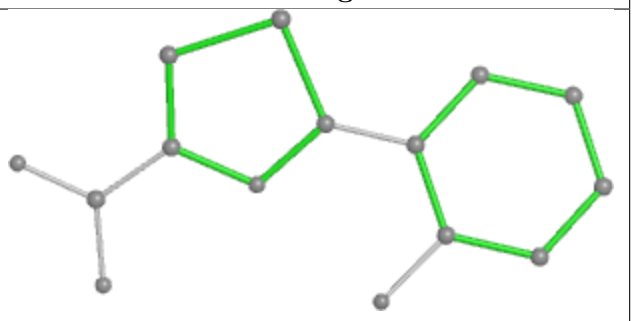
Bond lengths



Bond angles

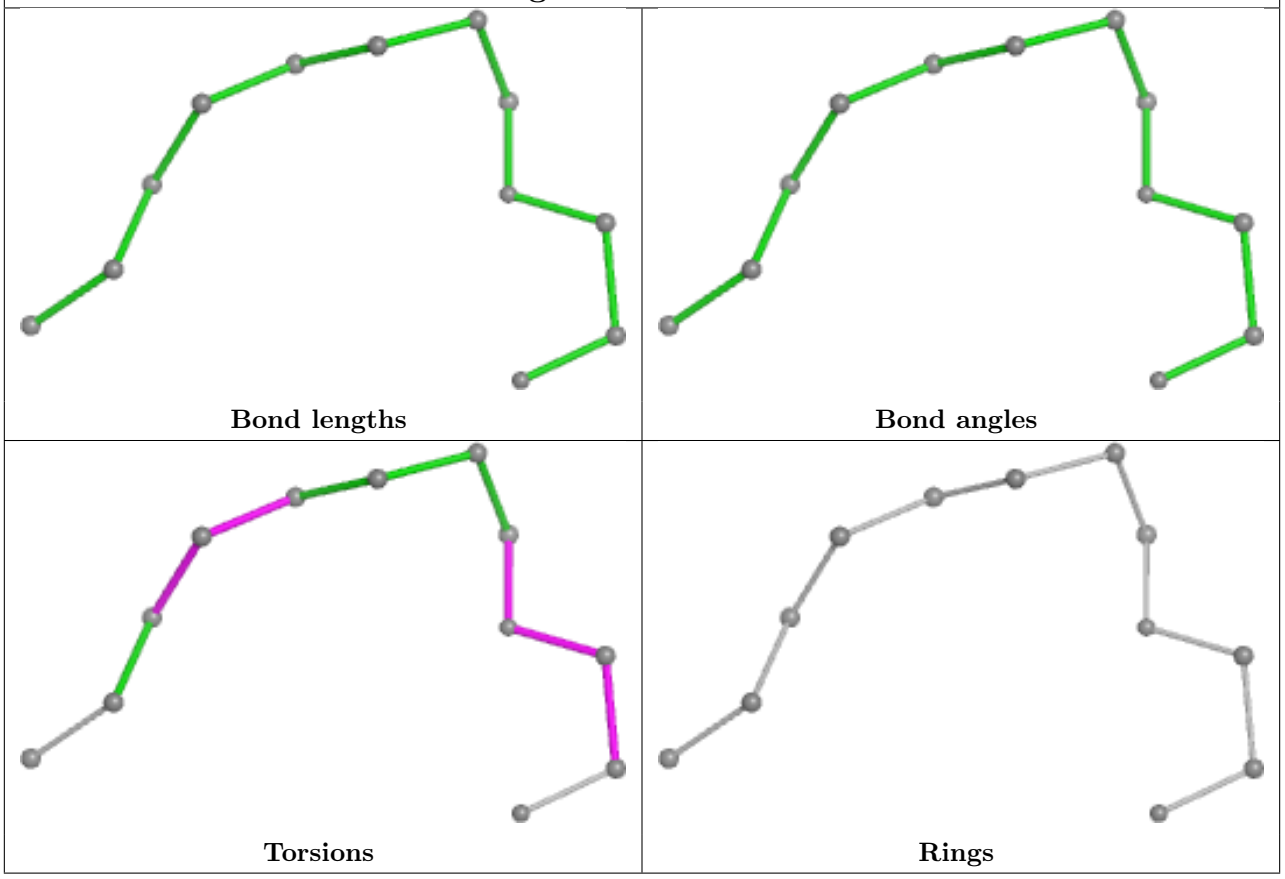


Torsions

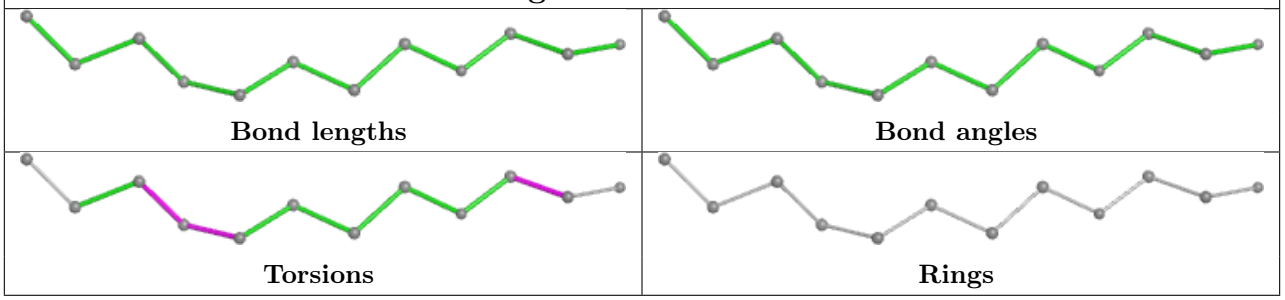


Rings

Ligand C8E B 808



Ligand C8E A 801



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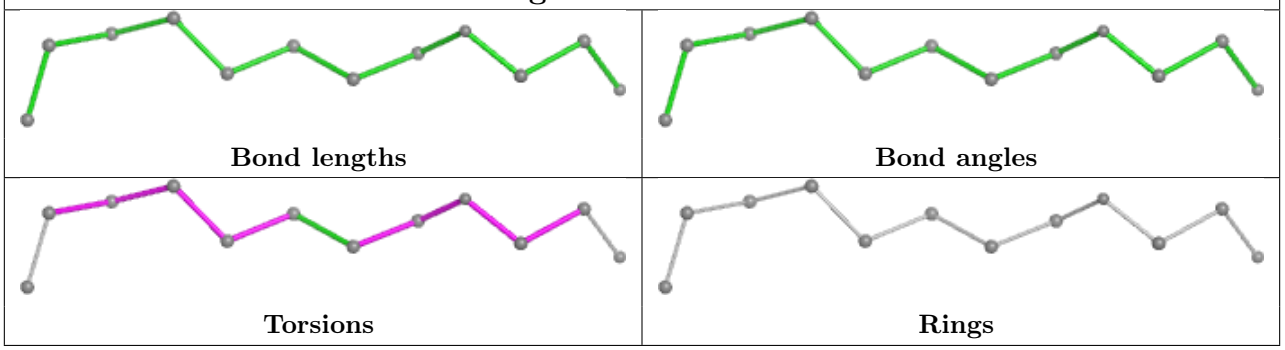
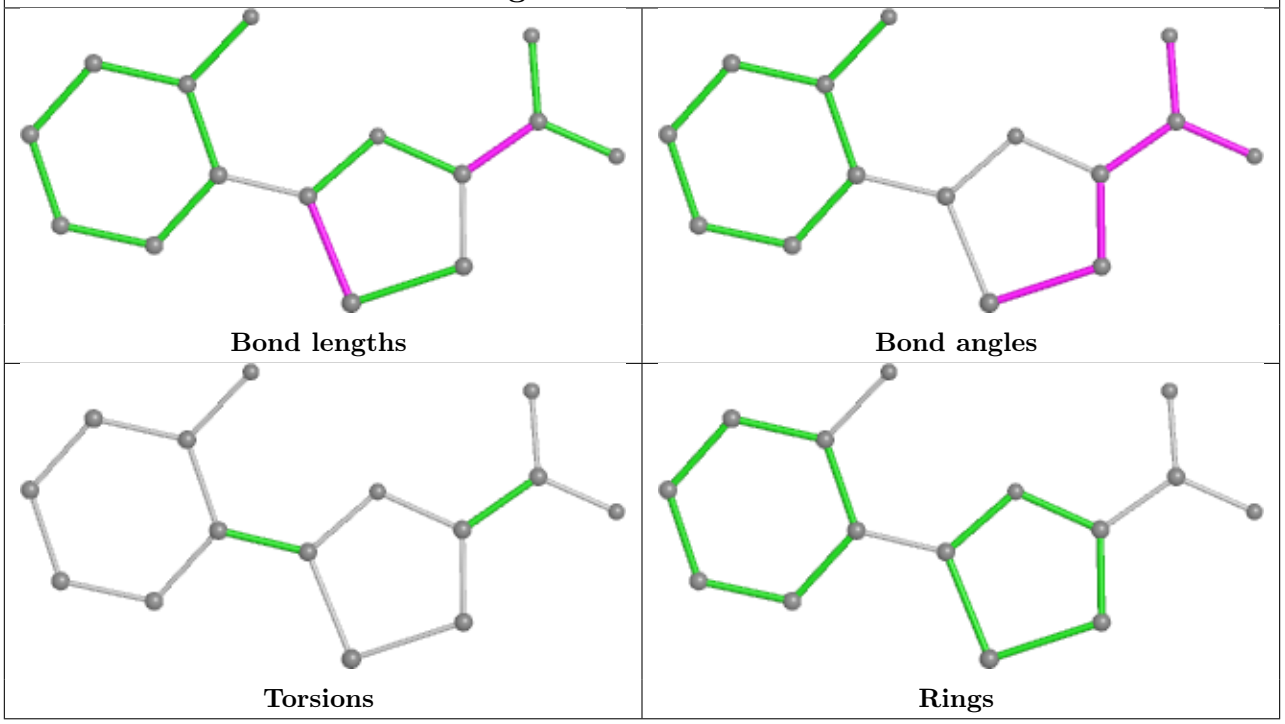
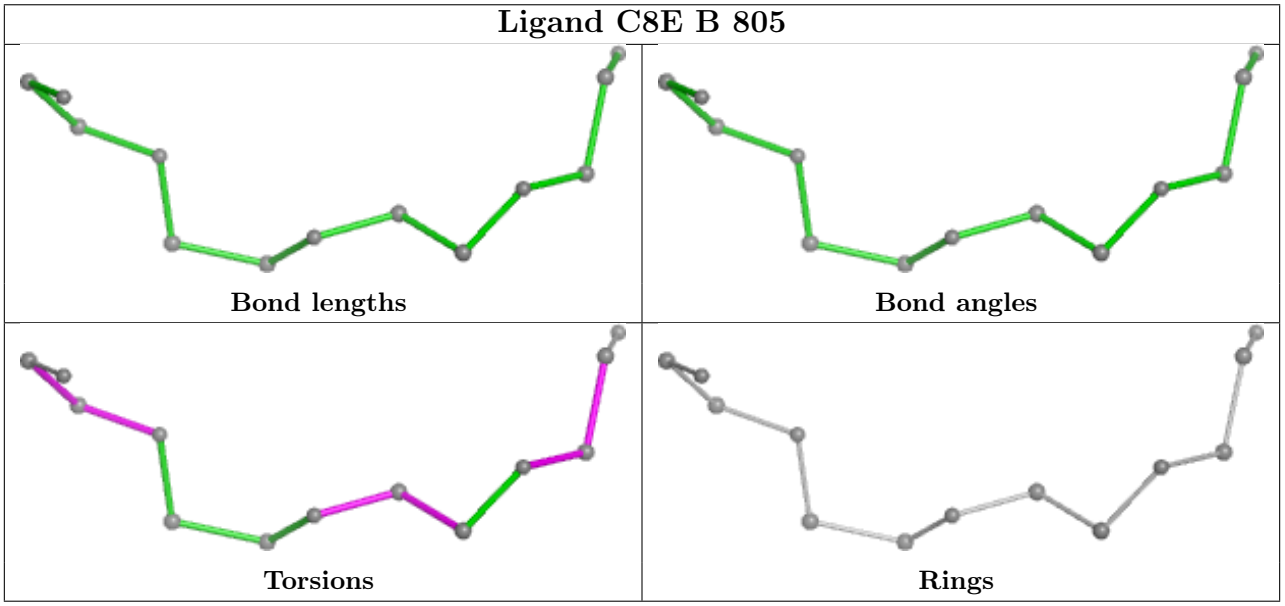
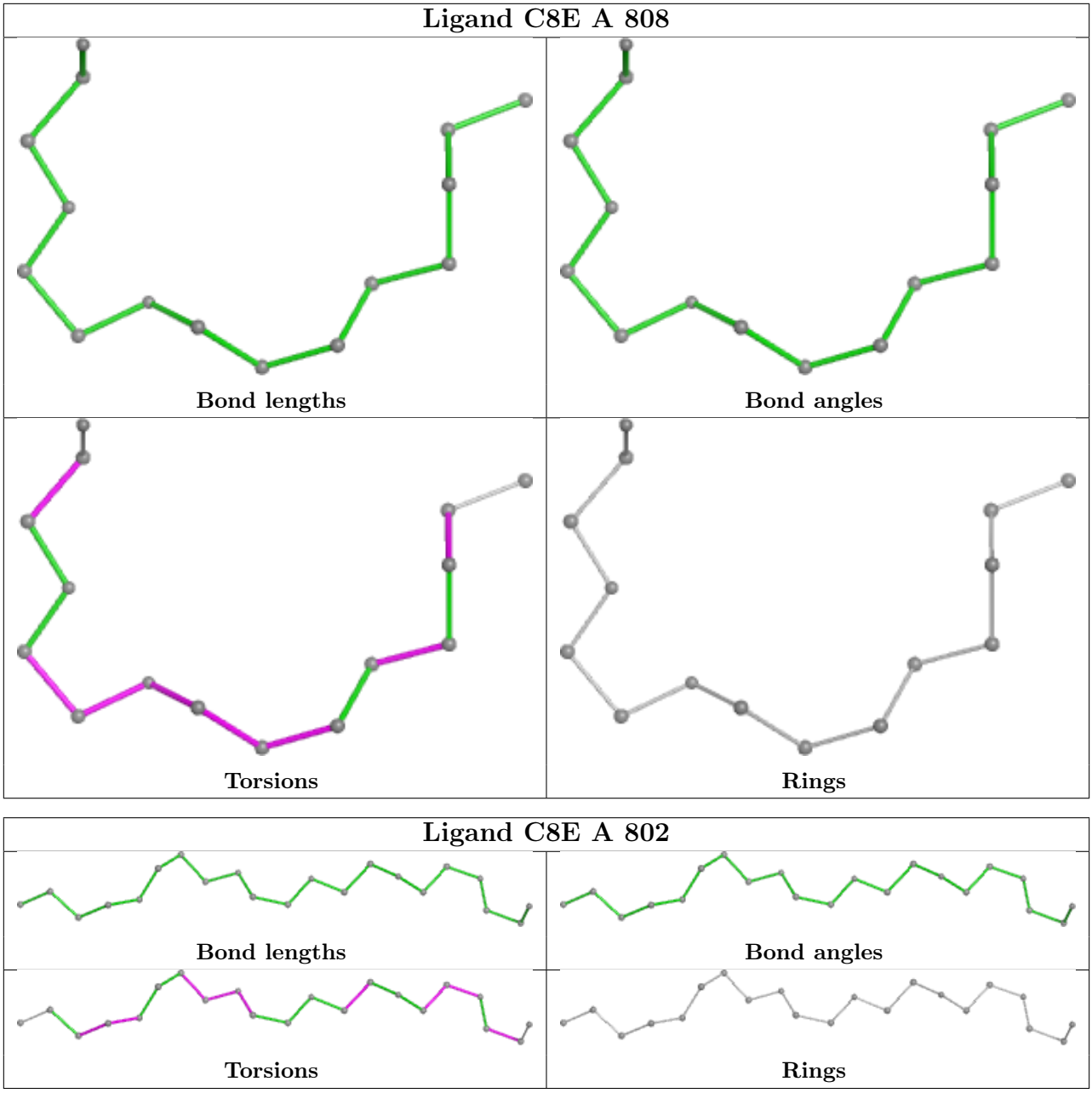


Ligand A1H49 B 802



Ligand C8E B 805





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	674/780 (86%)	0.64	69 (10%) 13 13	14, 31, 54, 76	2 (0%)
1	B	674/780 (86%)	0.53	59 (8%) 17 18	13, 30, 52, 73	5 (0%)
All	All	1348/1560 (86%)	0.58	128 (9%) 15 15	13, 30, 53, 76	7 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	PHE	5.4
1	B	107	ALA	5.0
1	A	577	ALA	4.7
1	B	621	ALA	4.7
1	A	107	ALA	4.5
1	B	506	PHE	4.5
1	A	576	THR	4.5
1	A	624	VAL	4.3
1	A	621	ALA	4.3
1	A	340	PRO	4.3
1	B	575	MET	4.2
1	A	575	MET	4.2
1	B	340	PRO	4.2
1	B	578	ALA	4.2
1	A	439	LEU	4.1
1	A	578	ALA	4.1
1	A	668	ALA	4.1
1	B	665	GLY	4.0
1	A	583	VAL	3.9
1	A	580	ALA	3.9
1	A	438	PRO	3.9
1	B	439	LEU	3.8
1	A	665	GLY	3.8
1	B	693	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	581	GLY	3.6
1	A	104	ALA	3.6
1	B	343	THR	3.6
1	A	693	VAL	3.6
1	B	735	ALA	3.5
1	B	574	PRO	3.5
1	B	624	VAL	3.5
1	B	344	HIS	3.5
1	A	574	PRO	3.5
1	B	438	PRO	3.5
1	B	533	ALA	3.4
1	A	735	ALA	3.4
1	A	339	GLY	3.4
1	A	739	LEU	3.4
1	A	667	PRO	3.3
1	B	577	ALA	3.2
1	A	734	VAL	3.2
1	A	616	ASN	3.2
1	B	623	ASN	3.1
1	A	623	ASN	3.1
1	B	530	THR	3.1
1	B	576	THR	3.1
1	A	541	HIS	3.1
1	B	668	ALA	3.0
1	A	533	ALA	3.0
1	A	543	TRP	3.0
1	B	622	SER	3.0
1	B	616[A]	ASN	3.0
1	A	618	TYR	3.0
1	A	435	ASP	3.0
1	B	734	VAL	2.9
1	A	622	SER	2.9
1	B	435	ASP	2.9
1	A	555	GLN	2.9
1	A	600	LEU	2.8
1	B	104	ALA	2.8
1	A	662	ASN	2.8
1	A	408	GLY	2.8
1	A	434	PHE	2.8
1	B	534	ARG	2.8
1	B	600	LEU	2.7
1	B	573	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	530	THR	2.7
1	A	619	THR	2.7
1	A	666	ASP	2.7
1	B	347	HIS	2.7
1	A	737	LYS	2.7
1	B	618	TYR	2.7
1	B	339	GLY	2.7
1	B	437	GLY	2.7
1	B	603	PHE	2.6
1	A	341	GLY	2.6
1	A	344	HIS	2.6
1	A	436	THR	2.6
1	B	692	PHE	2.6
1	A	106	ALA	2.6
1	A	627	ALA	2.6
1	A	603	PHE	2.5
1	A	702	TRP	2.5
1	A	509	ASP	2.5
1	B	583	VAL	2.5
1	B	584	LEU	2.4
1	B	663	LYS	2.4
1	A	379	ASP	2.4
1	B	702	TRP	2.4
1	A	573	ALA	2.4
1	B	736	GLY	2.4
1	B	424	TYR	2.4
1	A	108	GLY	2.3
1	B	777	PHE	2.3
1	A	347	HIS	2.3
1	A	105	GLN	2.3
1	A	276	GLU	2.3
1	B	619	THR	2.3
1	A	664	THR	2.3
1	B	582	GLN	2.3
1	B	620	ASP	2.3
1	B	638	LEU	2.3
1	B	645	LEU	2.3
1	A	645	LEU	2.3
1	B	601	GLY	2.2
1	B	543	TRP	2.2
1	A	648	VAL	2.2
1	A	625	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	519	ARG	2.2
1	A	582	GLN	2.2
1	B	662	ASN	2.2
1	A	684[A]	LEU	2.2
1	B	375	TYR	2.2
1	B	341	GLY	2.1
1	A	777	PHE	2.1
1	A	312	ARG	2.1
1	B	656[A]	TYR	2.1
1	A	663	LYS	2.1
1	A	437	GLY	2.1
1	B	581	GLY	2.1
1	B	739	LEU	2.0
1	B	751	LYS	2.0
1	A	407	GLN	2.0
1	B	613	ARG	2.0
1	B	580	ALA	2.0
1	A	508	GLU	2.0
1	B	691	PRO	2.0
1	A	692	PHE	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
5	P2D	A	807	7/7	0.67	0.24	43,47,52,52	0
5	P2D	B	807	7/7	0.72	0.22	44,46,54,55	0
2	C8E	A	808	15/21	0.75	0.22	43,51,62,67	0

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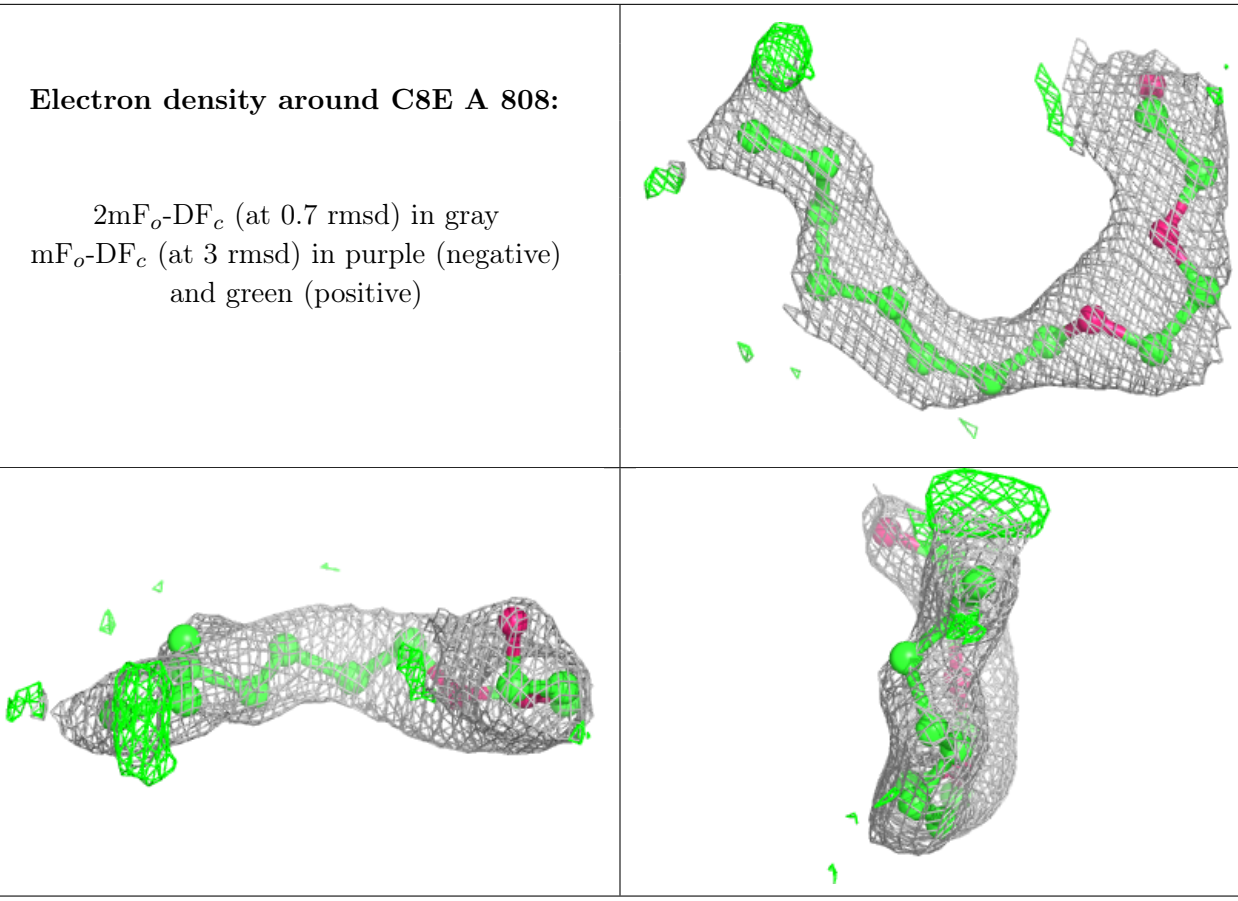
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	C8E	B	808	12/21	0.80	0.20	38,45,59,65	0
7	K	B	812	1/1	0.81	0.45	56,56,56,56	0
2	C8E	B	801	12/21	0.83	0.16	31,38,48,50	0
2	C8E	B	805	13/21	0.84	0.15	30,42,47,48	0
3	A1H49	A	804	15/15	0.85	0.14	31,38,43,54	15
2	C8E	A	802	21/21	0.85	0.15	34,42,50,53	0
4	EDO	A	806	4/4	0.86	0.14	39,40,45,46	0
2	C8E	B	804	15/21	0.86	0.15	32,38,44,48	0
7	K	B	811	1/1	0.87	0.36	55,55,55,55	0
3	A1H49	B	803	15/15	0.89	0.12	31,36,41,52	15
4	EDO	B	806	4/4	0.90	0.14	26,31,34,36	0
7	K	B	815	1/1	0.90	0.45	57,57,57,57	0
7	K	A	815	1/1	0.90	0.24	69,69,69,69	0
7	K	A	816	1/1	0.90	0.28	56,56,56,56	0
2	C8E	A	801	12/21	0.91	0.13	24,30,36,44	0
4	EDO	A	805	4/4	0.91	0.10	25,32,34,40	0
7	K	A	812	1/1	0.93	0.32	50,50,50,50	0
7	K	A	817	1/1	0.93	0.39	51,51,51,51	0
7	K	A	814	1/1	0.94	0.36	56,56,56,56	0
3	A1H49	A	803	15/15	0.94	0.10	26,30,36,37	15
7	K	B	814	1/1	0.94	0.18	57,57,57,57	0
7	K	A	813	1/1	0.94	0.37	54,54,54,54	0
3	A1H49	B	802	15/15	0.95	0.09	27,32,36,37	15
7	K	A	810	1/1	0.95	0.17	55,55,55,55	0
7	K	B	813	1/1	0.97	0.41	49,49,49,49	0
7	K	B	810	1/1	0.97	0.35	50,50,50,50	0
7	K	A	811	1/1	0.97	0.28	49,49,49,49	0
6	FE	B	809	1/1	0.99	0.03	29,29,29,29	1
6	FE	A	809	1/1	0.99	0.03	30,30,30,30	1

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.

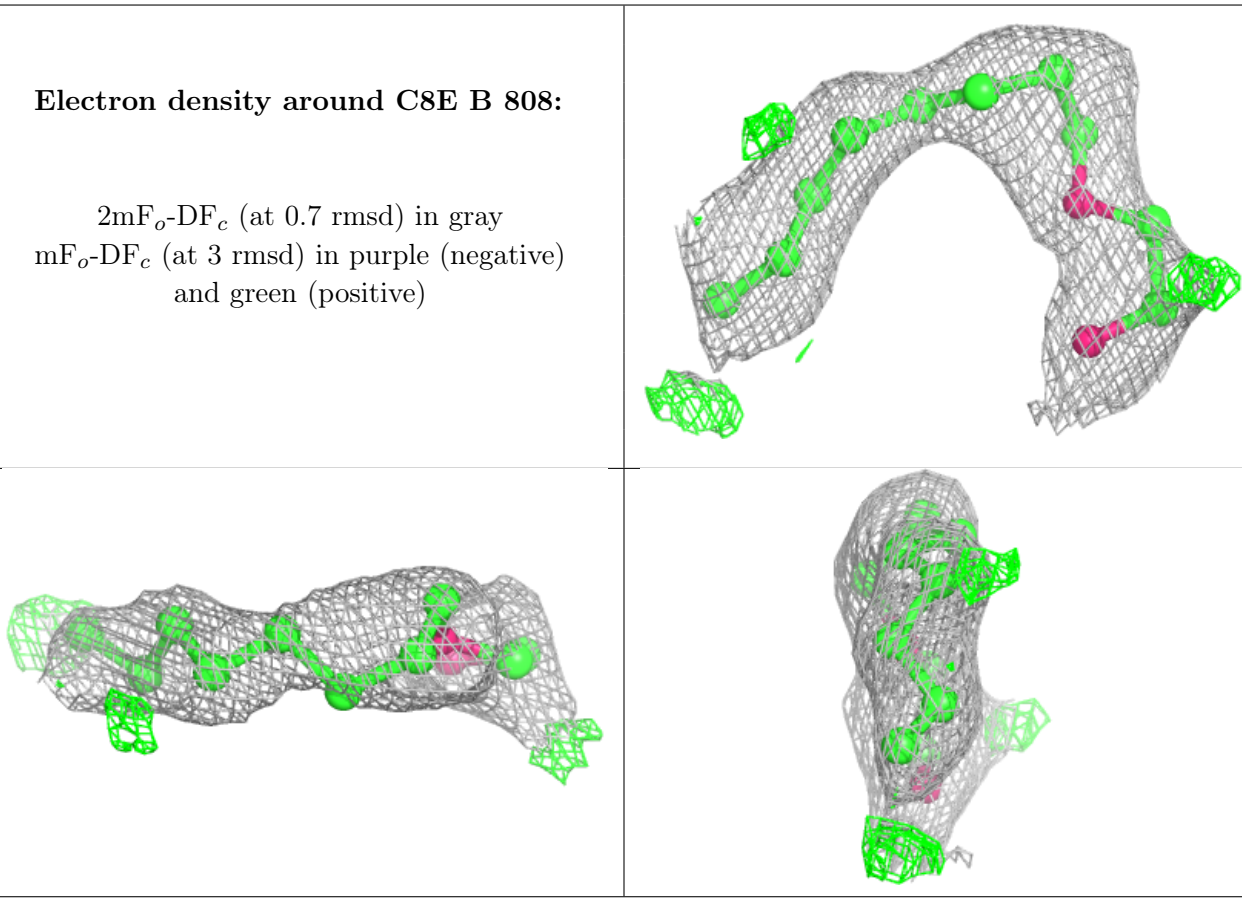
Electron density around C8E A 808:

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



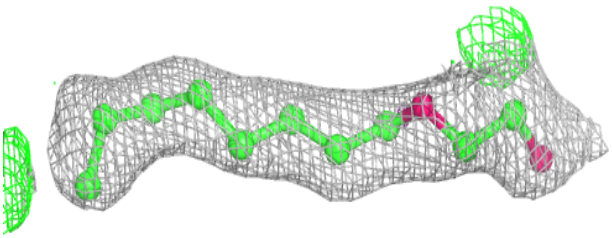
Electron density around C8E B 808:

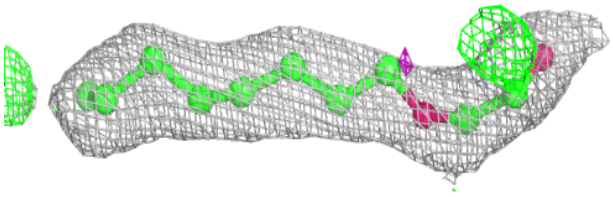
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

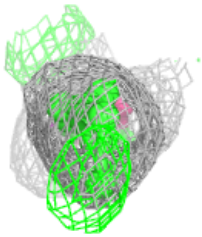


Electron density around C8E B 801:

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

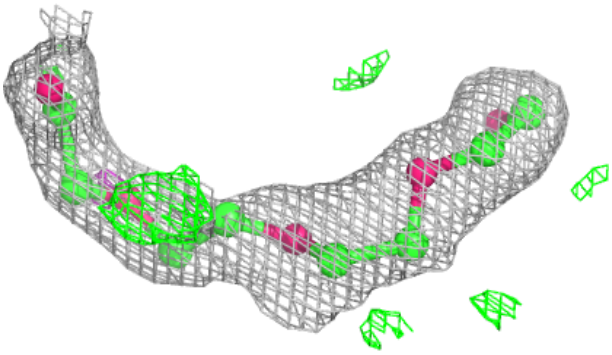


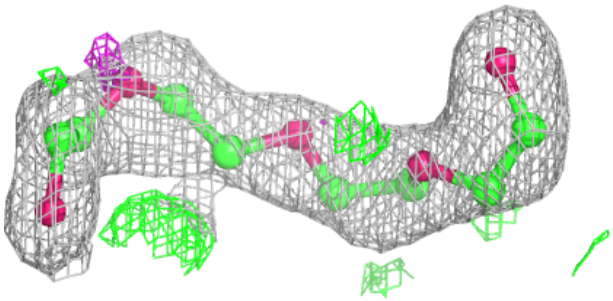


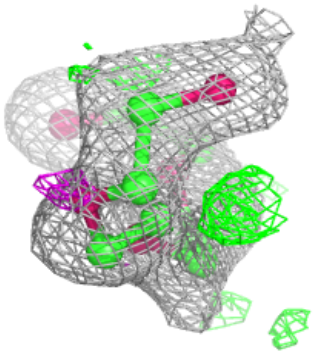


Electron density around C8E B 805:

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

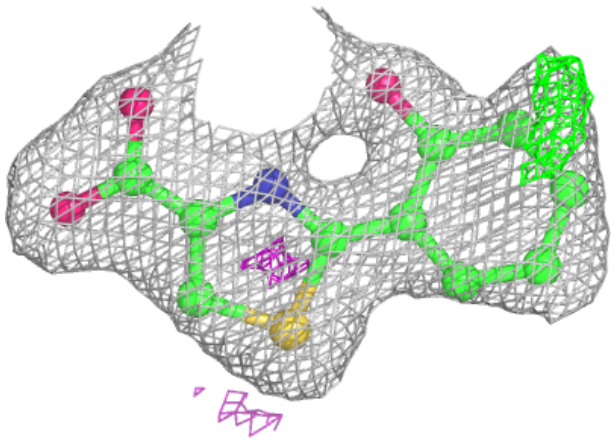


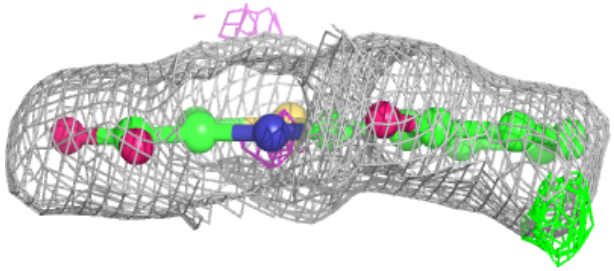


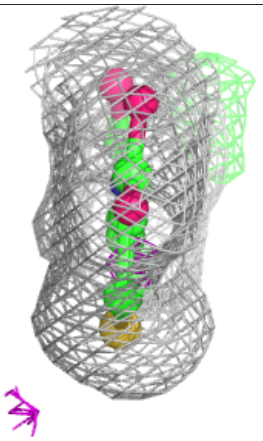


Electron density around A1H49 A 804:

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

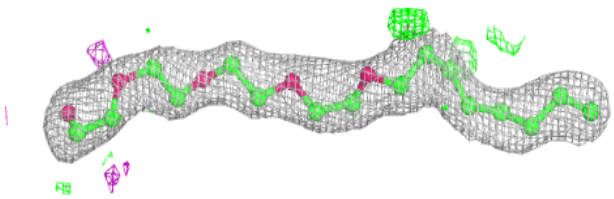


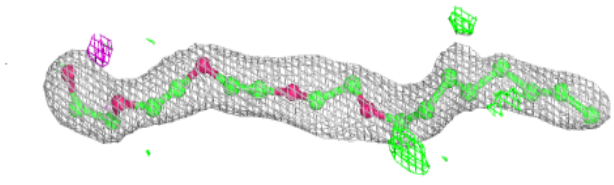


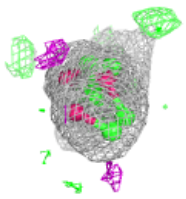


Electron density around C8E A 802:

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

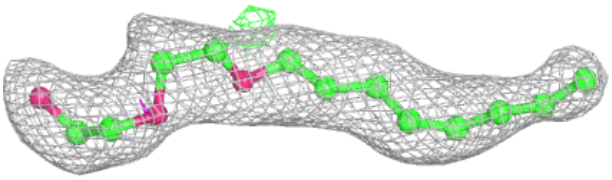


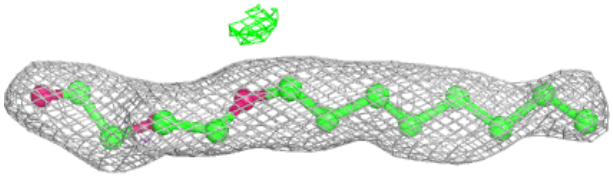


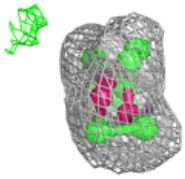


Electron density around C8E B 804:

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

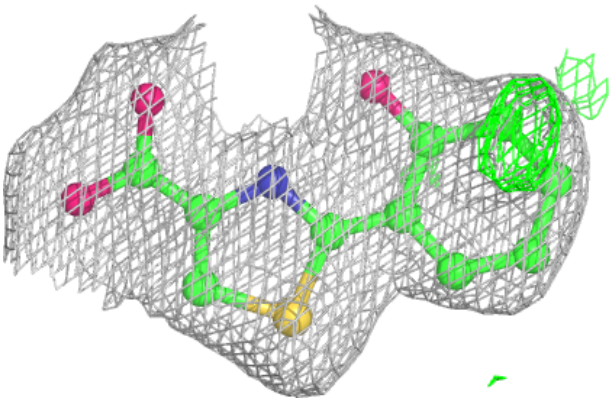


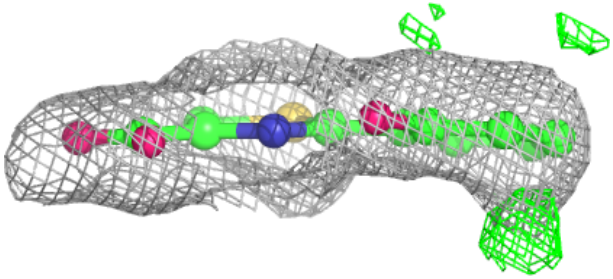


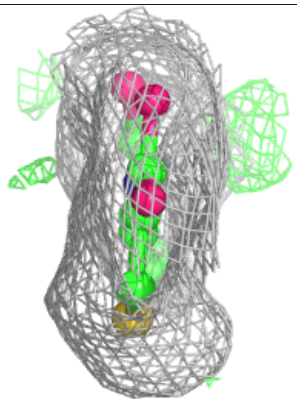


Electron density around A1H49 B 803:

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

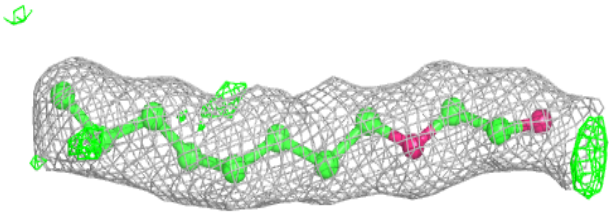


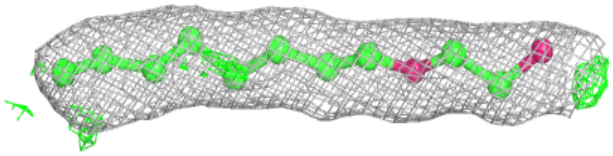


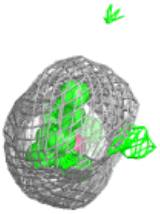


Electron density around C8E A 801:

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

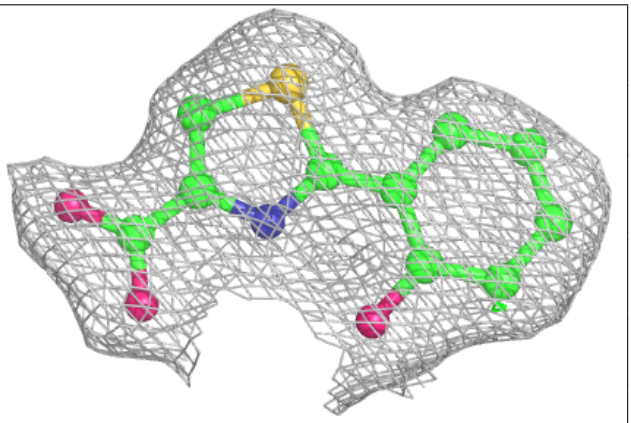


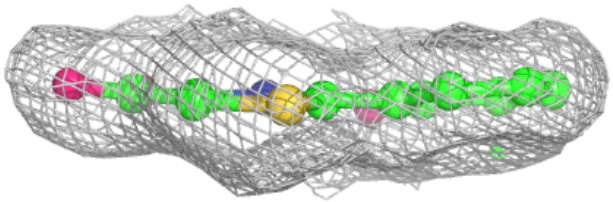


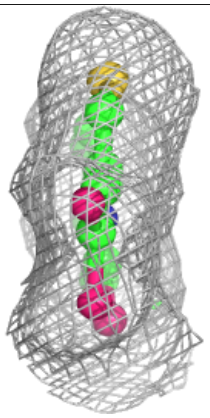


Electron density around A1H49 A 803:

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

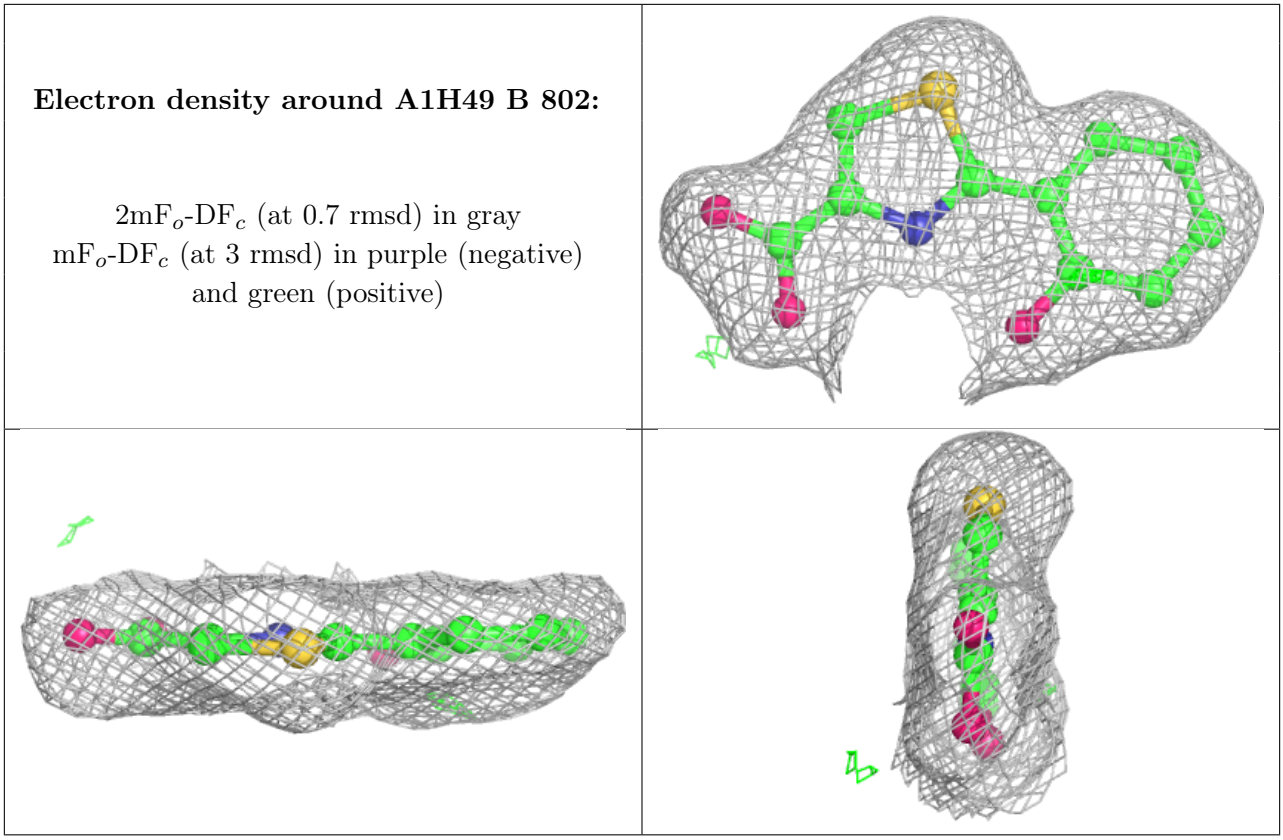






Electron density around A1H49 B 802:

$2mF_o$-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.