



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:39 PM UTC

PDB ID : 9EX3 / pdb_00009ex3
Title : Ferric-mycobactin receptor (FemA) in complex with dihydroaeruginoic acid
Authors : Moynie, L.
Deposited on : 2024-04-05
Resolution : 2.15 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

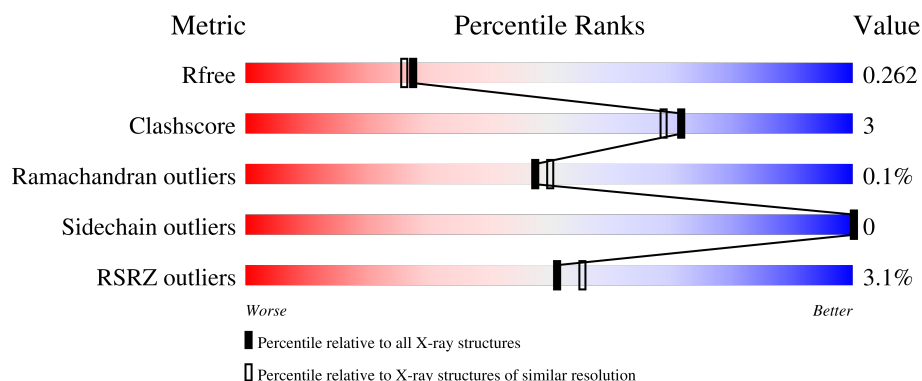
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 $\leq 5\%$. 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	
1	B	780	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11107 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.

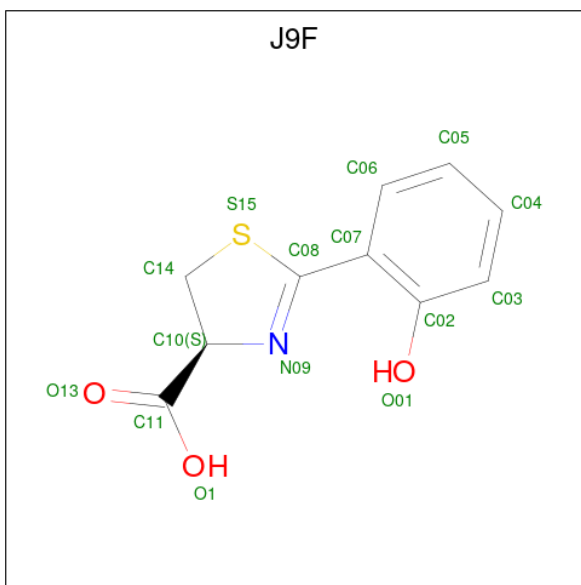
- Molecule 1 is a protein called Ferric-mycobactin receptor, FemA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	670	Total	C	N	O	S	0	2	0
			5159	3218	931	1001	9			
1	A	670	Total	C	N	O	S	0	1	0
			5148	3210	930	999	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 (4S)-2-(2-hydroxyphenyl)-4,5-dihydro-1,3-thiazole-4-carboxylic acid (CCD ID: J9F) (formula: C₁₀H₉NO₃S) (labeled as "Ligand of Interest" by depositor).



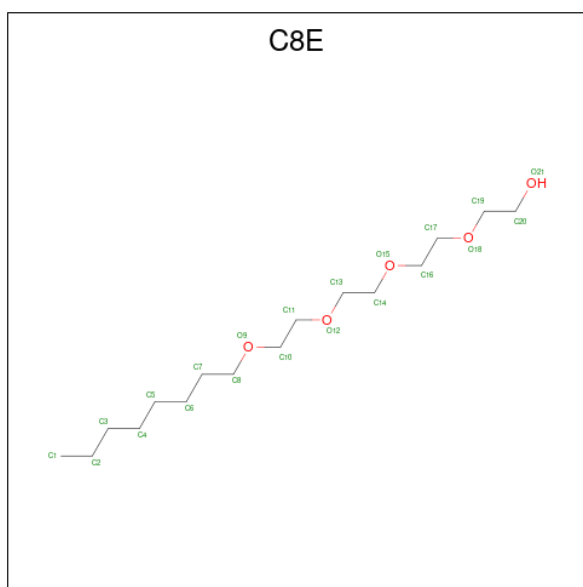
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			15	10	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			15	10	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			15	10	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			15	10	1	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



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

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	K	0	0
			1	1		
6	A	5	Total	K	0	0
			5	5		

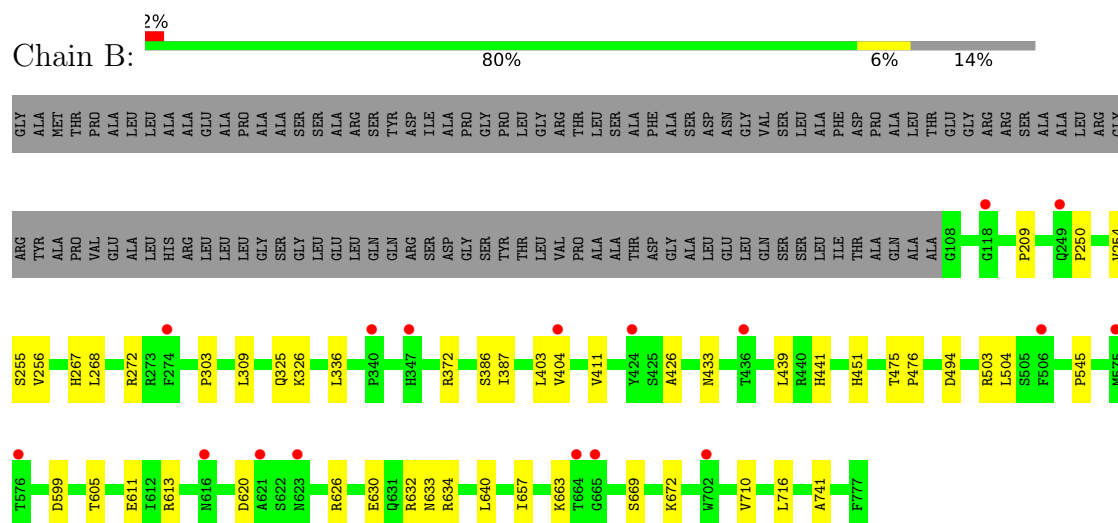
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	287	Total 287	O 287	0	0
7	A	319	Total 319	O 319	0	0

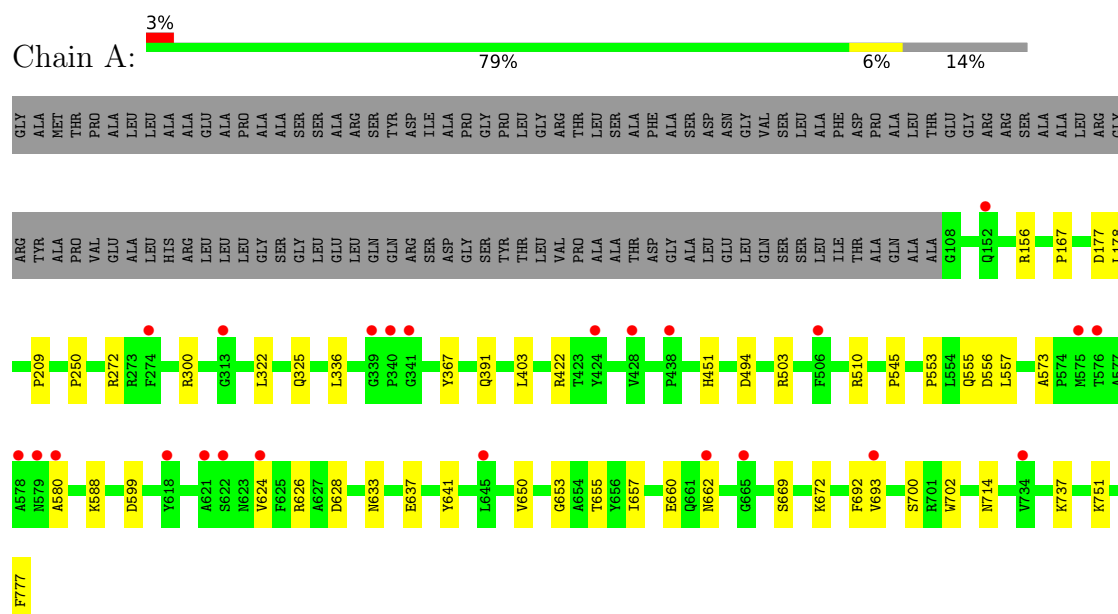
3 Residue-property plots [i](#)

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



- Molecule 1: Ferric-mycobactin receptor, FemA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.94Å 86.31Å 88.29Å 90.01° 61.63° 66.33°	Depositor
Resolution (Å)	44.07 – 2.15 44.07 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.8 (44.07-2.15) 96.2 (44.07-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.229 , 0.264 0.228 , 0.262	Depositor DCC
R_{free} test set	1964 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11107	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, J9F, EDO, FE, C8E

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	0.41	0/5254	0.55	0/7139
1	B	0.41	0/5269	0.57	0/7159
All	All	0.41	0/10523	0.56	0/14298

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	5148	0	5006	36	0
1	B	5159	0	5015	30	0
2	A	30	0	0	0	0
2	B	30	0	0	1	0
3	A	24	0	35	5	0
3	B	32	0	48	4	0
4	A	43	0	67	5	0
4	B	27	0	46	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	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	319	0	0	6	0
7	B	287	0	0	4	0
All	All	11107	0	10217	69	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 (69) 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:A:556:ASP:OD1	7:A:901:HOH:O	1.99	0.81
1:A:322:LEU:HB3	4:A:801:C8E:H51	1.69	0.74
1:B:325:GLN:NE2	7:B:903:HOH:O	2.21	0.74
1:B:439:LEU:HD11	1:B:504:LEU:HB3	1.68	0.73
1:A:325:GLN:NE2	7:A:903:HOH:O	2.22	0.70
1:B:387:ILE:HD12	1:B:426:ALA:HB2	1.74	0.68
1:B:599:ASP:OD2	7:B:901:HOH:O	2.12	0.67
1:B:250:PRO:HB3	1:B:272:ARG:HD3	1.79	0.65
2:B:806:J9F:O13	7:B:902:HOH:O	2.14	0.65
1:B:309:LEU:HB3	4:B:807:C8E:H12	1.80	0.63
1:B:710:VAL:HG12	1:B:716:LEU:HB2	1.81	0.63
1:A:553:PRO:HG2	1:A:557:LEU:HD23	1.83	0.61
1:B:256:VAL:HG23	4:B:811:C8E:H42	1.81	0.60
1:B:620:ASP:OD2	1:B:626:ARG:NH1	2.34	0.60
1:A:300:ARG:HH22	3:A:808:EDO:H11	1.68	0.57
1:B:267:HIS:ND1	3:B:802:EDO:H11	2.20	0.56
1:A:700:SER:OG	4:A:811:C8E:O21	2.24	0.56
1:B:336:LEU:HD11	1:B:403:LEU:HG	1.87	0.56
1:A:555:GLN:H	1:A:555:GLN:CD	2.14	0.54
1:B:404:VAL:HG21	1:B:411:VAL:HG23	1.88	0.54
1:B:663:LYS:NZ	7:B:908:HOH:O	2.38	0.53
1:B:630:GLU:HB2	1:B:663:LYS:HE2	1.90	0.53
1:A:702:TRP:HB2	4:A:811:C8E:H171	1.92	0.52
1:A:503:ARG:HD3	3:A:805:EDO:H11	1.91	0.52
1:B:633:ASN:HB3	1:B:657:ILE:HD11	1.92	0.52
1:A:451:HIS:ND1	1:A:494:ASP:OD2	2.41	0.52
1:A:156:ARG:O	3:A:808:EDO:H22	2.10	0.50
1:B:741:ALA:HB1	4:B:811:C8E:H101	1.93	0.50
1:B:254:VAL:HG22	1:B:268:LEU:HD22	1.92	0.50
1:A:391:GLN:OE1	1:A:422:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ARG:HG2	1:B:386:SER:OG	2.13	0.49
3:A:809:EDO:H12	7:A:914:HOH:O	2.12	0.48
1:A:751:LYS:HG3	7:A:1071:HOH:O	2.13	0.48
1:A:451:HIS:HD1	1:A:494:ASP:CG	2.21	0.48
1:B:475:THR:HB	1:B:476:PRO:HD2	1.96	0.48
1:A:556:ASP:HB3	1:A:599:ASP:O	2.14	0.48
1:B:255:SER:OG	3:B:802:EDO:H21	2.14	0.47
1:A:588:LYS:NZ	7:A:910:HOH:O	2.41	0.47
1:A:209:PRO:HG3	1:A:325:GLN:HG3	1.96	0.46
1:A:177:ASP:OD1	1:A:178:LEU:N	2.48	0.46
1:A:672:LYS:NZ	7:A:919:HOH:O	2.49	0.46
1:A:672:LYS:HB3	1:A:714:ASN:OD1	2.16	0.46
1:A:300:ARG:NH2	3:A:808:EDO:H11	2.29	0.45
1:A:660:GLU:HG2	1:A:662:ASN:HB3	1.97	0.45
1:B:605:THR:HG22	1:B:640:LEU:HD12	1.99	0.45
1:A:624:VAL:HG11	1:A:626:ARG:HH21	1.81	0.45
4:A:810:C8E:H132	4:A:810:C8E:H102	1.38	0.45
1:B:451:HIS:ND1	1:B:494:ASP:OD2	2.41	0.44
1:A:167:PRO:HG3	1:A:653:GLY:HA3	1.99	0.44
1:B:503:ARG:HD3	3:B:805:EDO:O2	2.16	0.44
1:A:637:GLU:HG2	1:A:655:THR:HG22	1.98	0.44
1:B:433:ASN:HA	1:B:441:HIS:O	2.17	0.44
1:A:669:SER:HA	1:A:672:LYS:HG3	2.00	0.44
1:B:209:PRO:HG3	1:B:325:GLN:HG3	2.00	0.44
1:B:613:ARG:HH21	1:B:632:ARG:CZ	2.30	0.43
1:B:267:HIS:CE1	3:B:802:EDO:H11	2.54	0.43
1:A:250:PRO:HB3	1:A:272:ARG:HD3	2.01	0.42
1:A:633:ASN:HB3	1:A:657:ILE:HD11	2.02	0.42
1:A:692:PHE:CD2	1:A:693:VAL:HG23	2.55	0.42
1:B:611:GLU:HB2	1:B:634:ARG:HG2	2.01	0.42
1:A:336:LEU:HD11	1:A:403:LEU:HG	2.02	0.42
1:A:737:LYS:HD2	1:A:777:PHE:CD1	2.54	0.42
1:B:669:SER:HA	1:B:672:LYS:HG3	2.02	0.41
1:A:573:ALA:HB3	1:A:580:ALA:O	2.20	0.41
1:A:367:TYR:HD2	4:A:801:C8E:H81	1.85	0.41
1:A:510:ARG:NH2	1:A:553:PRO:O	2.54	0.41
1:A:641:TYR:HA	1:A:650:VAL:O	2.21	0.41
1:B:303:PRO:HD2	1:B:326:LYS:O	2.20	0.40
1:A:626:ARG:HD2	1:A:628:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	669/780 (86%)	654 (98%)	14 (2%)	1 (0%)	48	50
1	B	670/780 (86%)	651 (97%)	18 (3%)	1 (0%)	48	50
All	All	1339/1560 (86%)	1305 (98%)	32 (2%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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	536/612 (88%)	536 (100%)	0	100	100
1	B	537/612 (88%)	537 (100%)	0	100	100
All	All	1073/1224 (88%)	1073 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	120	GLN
1	B	153	GLN

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Mol	Chain	Res	Type
1	B	154	GLN
1	B	165	ASN
1	B	190	GLN
1	B	347	HIS
1	B	616	ASN
1	B	661	GLN
1	A	152	GLN
1	A	249	GLN
1	A	260	GLN
1	A	285	ASN
1	A	344	HIS
1	A	347	HIS
1	A	661	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	J9F	A	807	5	16,16,16	0.50	0	19,22,22	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	810	-	3,3,3	0.49	0	2,2,2	0.55	0
3	EDO	B	804	-	3,3,3	0.44	0	2,2,2	0.52	0
3	EDO	B	809	-	3,3,3	0.53	0	2,2,2	0.10	0
3	EDO	B	812	6	3,3,3	0.40	0	2,2,2	0.44	0
3	EDO	A	808	-	3,3,3	0.39	0	2,2,2	0.05	0
4	C8E	B	811	-	14,14,20	0.36	0	13,13,19	0.57	0
3	EDO	A	806	-	3,3,3	0.44	0	2,2,2	0.44	0
3	EDO	B	803	-	3,3,3	0.40	0	2,2,2	0.48	0
4	C8E	A	810	-	14,14,20	0.34	0	13,13,19	0.55	0
4	C8E	B	807	-	11,11,20	0.36	0	10,10,19	0.55	0
4	C8E	A	801	-	14,14,20	0.33	0	13,13,19	0.68	0
3	EDO	A	809	6	3,3,3	0.44	0	2,2,2	0.50	0
3	EDO	B	802	-	3,3,3	0.43	0	2,2,2	0.18	0
3	EDO	B	805	-	3,3,3	0.36	0	2,2,2	0.65	0
2	J9F	B	806	5	16,16,16	0.51	0	19,22,22	0.90	0
2	J9F	A	802	5	16,16,16	0.65	0	19,22,22	1.49	4 (21%)
3	EDO	A	803	-	3,3,3	0.43	0	2,2,2	0.60	0
3	EDO	B	808	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	A	804	-	3,3,3	0.41	0	2,2,2	0.33	0
4	C8E	A	811	-	12,12,20	0.42	0	11,11,19	0.41	0
3	EDO	A	805	-	3,3,3	0.44	0	2,2,2	0.76	0
2	J9F	B	801	5	16,16,16	0.65	0	19,22,22	1.48	2 (10%)

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	J9F	A	807	5	-	4/8/17/17	0/2/2/2
3	EDO	B	810	-	-	1/1/1/1	-
3	EDO	B	804	-	-	0/1/1/1	-
3	EDO	B	809	-	-	0/1/1/1	-
3	EDO	B	812	6	-	0/1/1/1	-
3	EDO	A	808	-	-	1/1/1/1	-
4	C8E	B	811	-	-	7/12/12/18	-
3	EDO	A	806	-	-	0/1/1/1	-
3	EDO	B	803	-	-	0/1/1/1	-
4	C8E	A	810	-	-	6/12/12/18	-
4	C8E	B	807	-	-	2/9/9/18	-
4	C8E	A	801	-	-	5/12/12/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	809	6	-	0/1/1/1	-
3	EDO	B	802	-	-	0/1/1/1	-
3	EDO	B	805	-	-	1/1/1/1	-
2	J9F	B	806	5	-	4/8/17/17	0/2/2/2
2	J9F	A	802	5	-	4/8/17/17	0/2/2/2
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	B	808	-	-	0/1/1/1	-
3	EDO	A	804	-	-	1/1/1/1	-
4	C8E	A	811	-	-	7/10/10/18	-
3	EDO	A	805	-	-	0/1/1/1	-
2	J9F	B	801	5	-	4/8/17/17	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	J9F	C02-C07-C08	4.36	124.76	120.23
2	A	802	J9F	C02-C07-C08	3.92	124.30	120.23
2	B	801	J9F	C14-C10-N09	-3.25	104.12	110.03
2	A	802	J9F	C14-C10-N09	-3.08	104.43	110.03
2	A	802	J9F	C14-S15-C08	-2.70	86.84	89.40
2	A	807	J9F	C10-C14-S15	-2.56	100.69	105.74
2	A	802	J9F	C10-C14-S15	-2.27	101.28	105.74

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	J9F	C14-C10-C11-O13
2	B	801	J9F	C14-C10-C11-O1
2	B	806	J9F	N09-C10-C11-O13
2	B	806	J9F	C14-C10-C11-O13
2	B	806	J9F	C14-C10-C11-O1
2	A	802	J9F	C14-C10-C11-O13
2	A	802	J9F	C14-C10-C11-O1
2	A	807	J9F	N09-C10-C11-O13
2	A	807	J9F	C14-C10-C11-O13
2	A	807	J9F	C14-C10-C11-O1
4	A	810	C8E	C10-C11-O12-C13
4	A	811	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
4	A	801	C8E	O12-C13-C14-O15
4	A	810	C8E	O9-C10-C11-O12
4	A	810	C8E	C6-C7-C8-O9
4	A	811	C8E	O18-C19-C20-O21
4	A	810	C8E	C2-C3-C4-C5
4	B	811	C8E	C5-C6-C7-C8
4	B	811	C8E	C3-C4-C5-C6
4	B	811	C8E	C6-C7-C8-O9
4	B	811	C8E	C2-C3-C4-C5
4	A	810	C8E	O12-C13-C14-O15
4	B	807	C8E	C1-C2-C3-C4
4	A	801	C8E	C3-C4-C5-C6
4	A	811	C8E	C17-C16-O15-C14
2	B	801	J9F	N09-C10-C11-O1
2	A	802	J9F	N09-C10-C11-O13
2	A	807	J9F	N09-C10-C11-O1
4	A	811	C8E	C16-C17-O18-C19
4	A	811	C8E	C13-C14-O15-C16
4	B	811	C8E	C4-C5-C6-C7
4	A	801	C8E	C6-C7-C8-O9
4	A	810	C8E	C14-C13-O12-C11
4	B	807	C8E	C2-C3-C4-C5
4	A	801	C8E	C11-C10-O9-C8
3	A	804	EDO	O1-C1-C2-O2
4	B	811	C8E	C10-C11-O12-C13
4	A	811	C8E	C14-C13-O12-C11
4	A	801	C8E	C14-C13-O12-C11
2	B	801	J9F	N09-C10-C11-O13
2	B	806	J9F	N09-C10-C11-O1
2	A	802	J9F	N09-C10-C11-O1
4	B	811	C8E	C7-C8-O9-C10
3	B	810	EDO	O1-C1-C2-O2
3	A	808	EDO	O1-C1-C2-O2
3	B	805	EDO	O1-C1-C2-O2
4	A	811	C8E	O15-C16-C17-O18

There are no ring outliers.

11 monomers are involved in 18 short contacts:

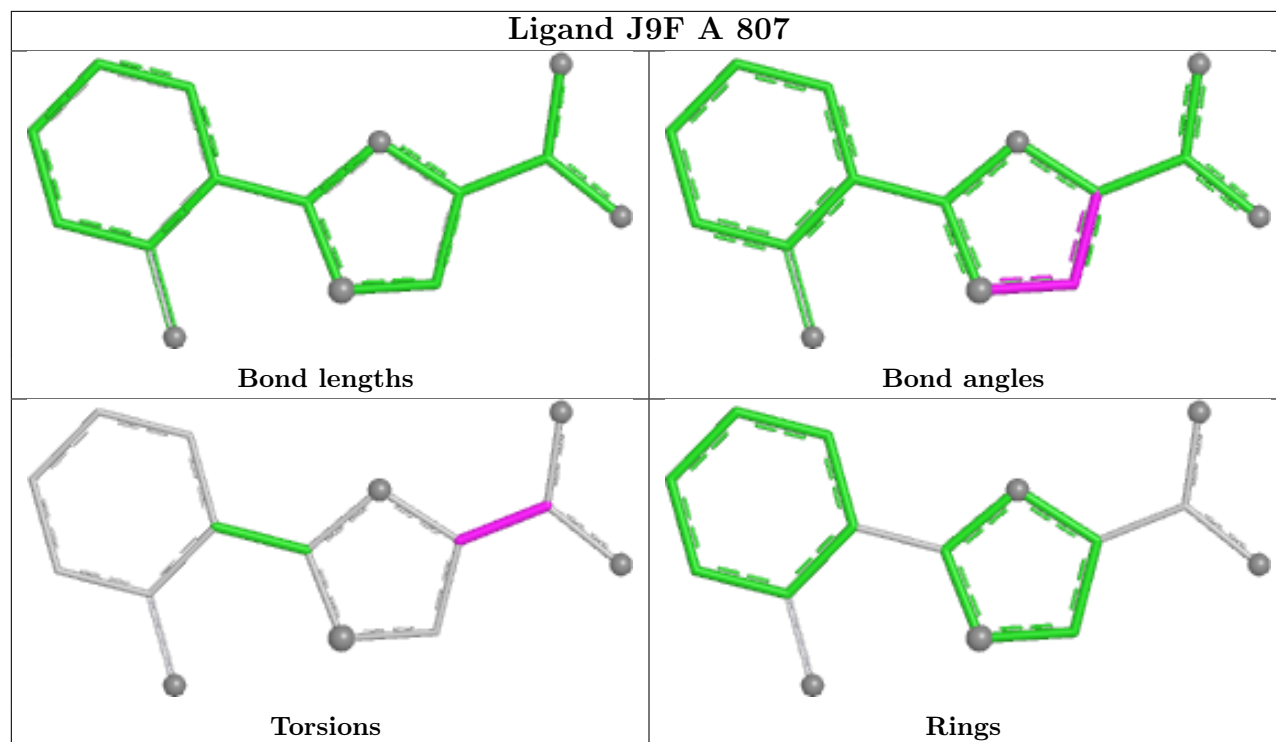
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	808	EDO	3	0
4	B	811	C8E	2	0

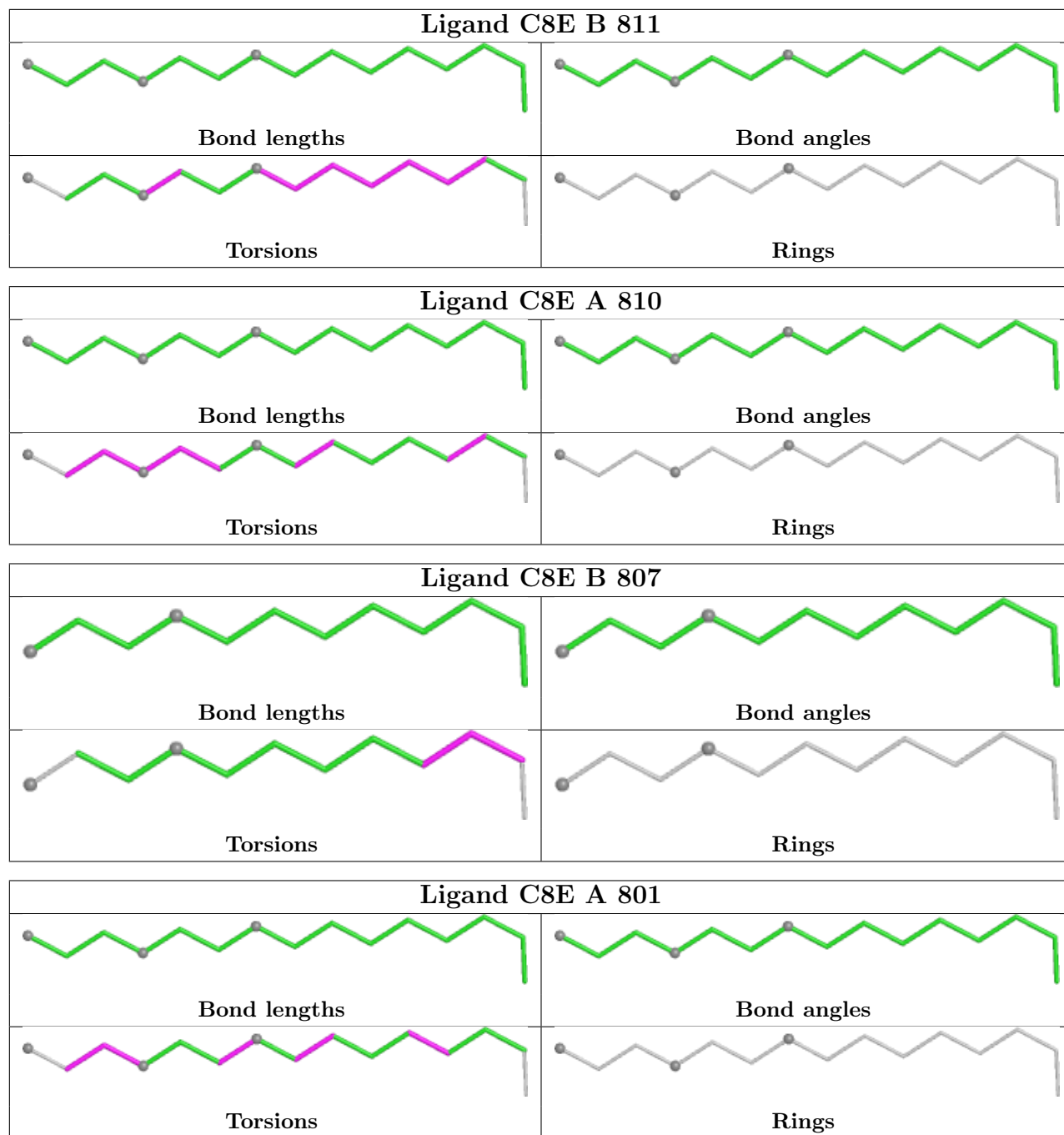
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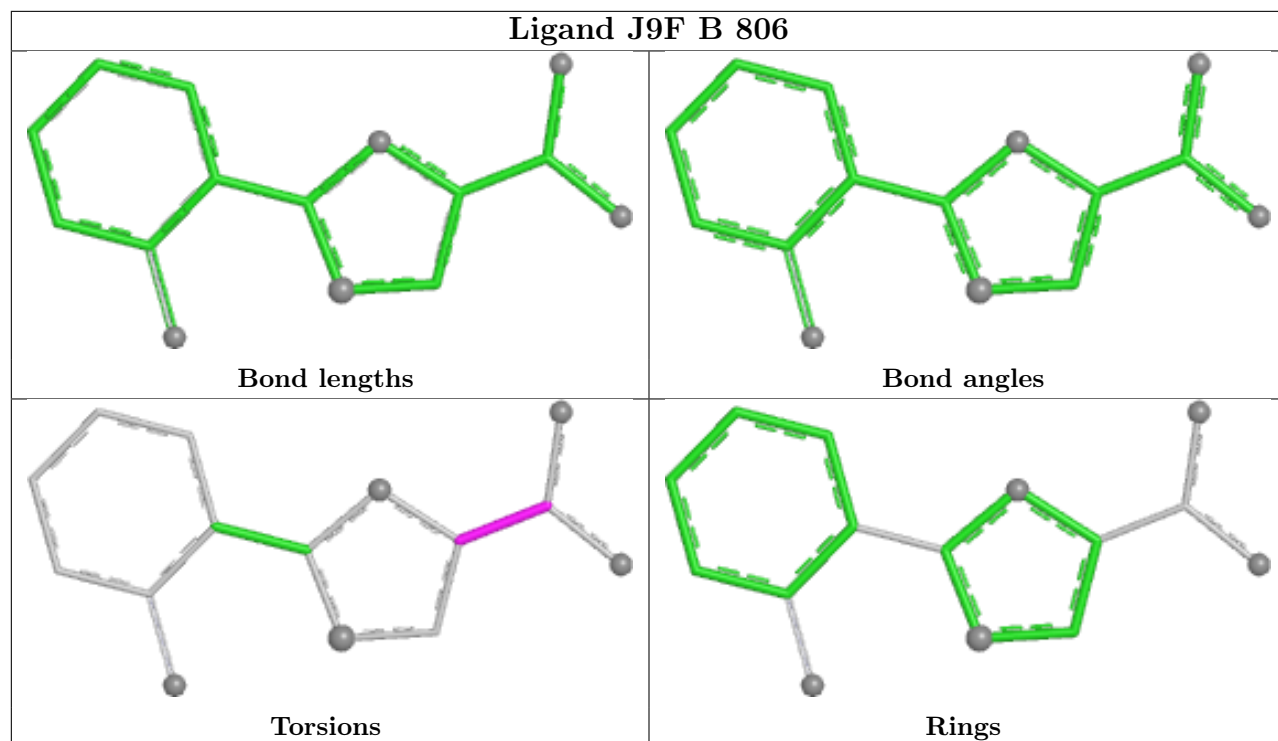
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	810	C8E	1	0
4	B	807	C8E	1	0
4	A	801	C8E	2	0
3	A	809	EDO	1	0
3	B	802	EDO	3	0
3	B	805	EDO	1	0
2	B	806	J9F	1	0
4	A	811	C8E	2	0
3	A	805	EDO	1	0

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

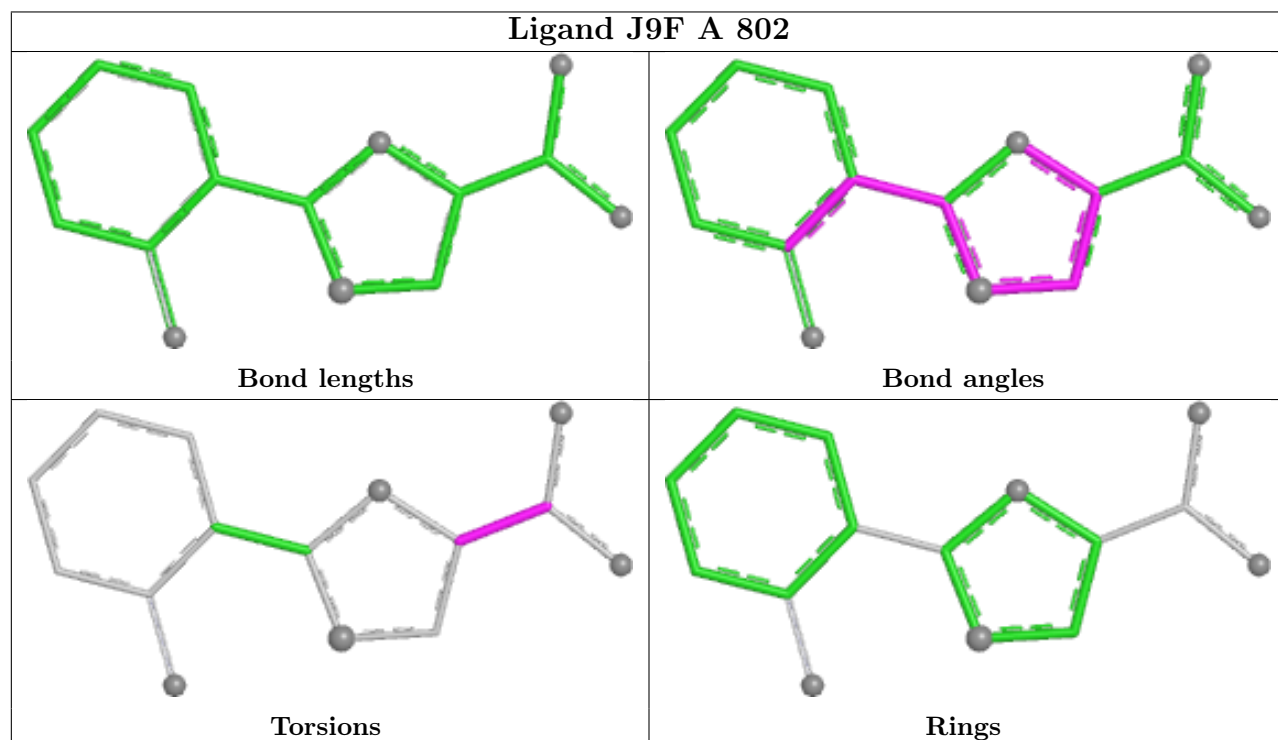




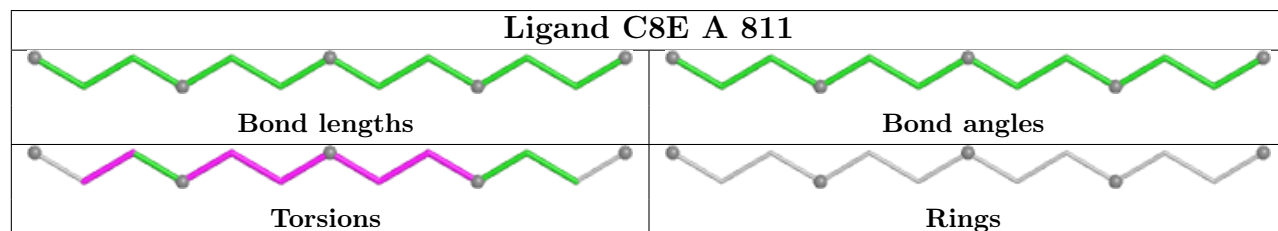
Ligand J9F B 806

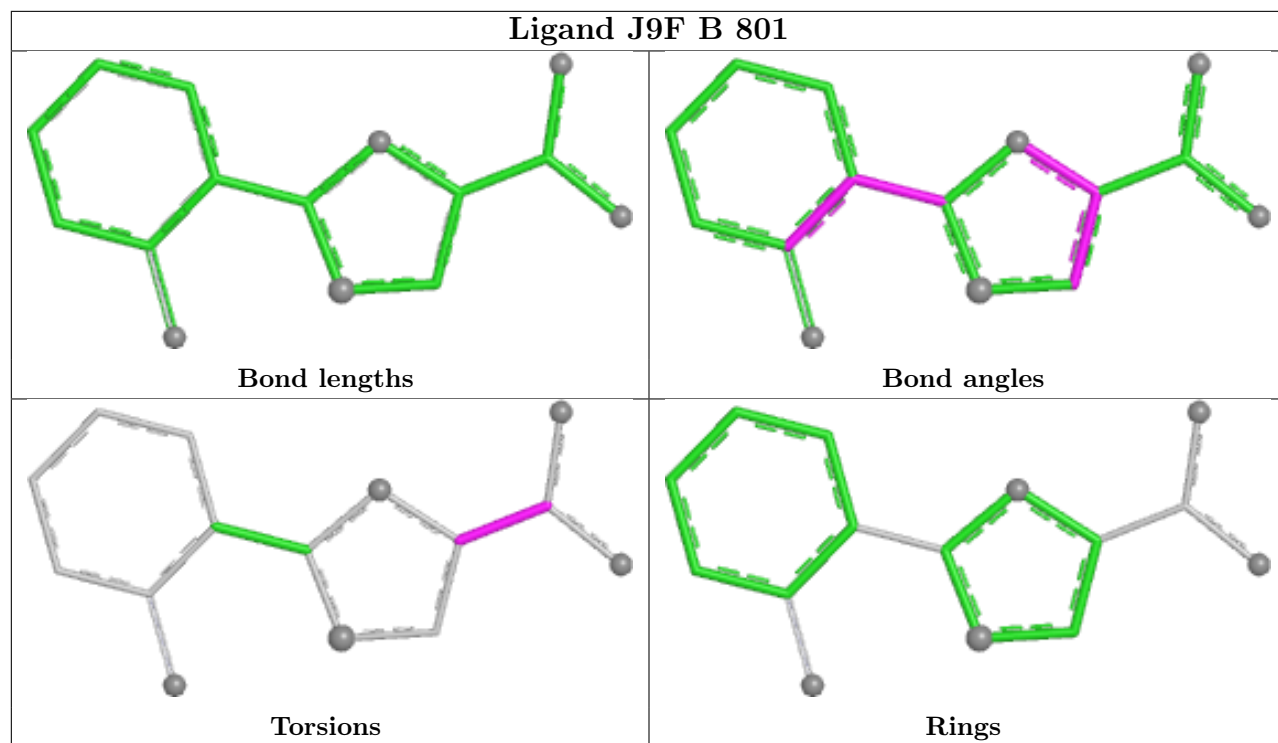


Ligand J9F A 802



Ligand C8E A 811





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	670/780 (85%)	0.23	24 (3%)	46 50	14, 28, 51, 70	1 (0%)
1	B	670/780 (85%)	0.20	17 (2%)	58 62	12, 28, 50, 65	2 (0%)
All	All	1340/1560 (85%)	0.22	41 (3%)	51 55	12, 28, 51, 70	3 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	TYR	4.7
1	B	621	ALA	4.0
1	A	621	ALA	3.8
1	A	428[A]	VAL	3.5
1	B	347	HIS	3.3
1	A	506	PHE	3.3
1	A	578	ALA	3.1
1	A	693	VAL	3.1
1	A	339	GLY	3.1
1	A	580	ALA	3.1
1	B	118	GLY	3.0
1	B	616	ASN	2.7
1	A	340	PRO	2.7
1	A	313	GLY	2.6
1	A	341	GLY	2.6
1	A	576	THR	2.5
1	B	249	GLN	2.4
1	B	664	THR	2.4
1	A	662	ASN	2.4
1	A	622	SER	2.4
1	A	618	TYR	2.3
1	B	274	PHE	2.3
1	B	506	PHE	2.3
1	A	665	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	404	VAL	2.3
1	B	665	GLY	2.3
1	A	152	GLN	2.2
1	A	274	PHE	2.2
1	A	438	PRO	2.2
1	A	645	LEU	2.2
1	B	702	TRP	2.2
1	A	579	ASN	2.2
1	A	575	MET	2.2
1	B	623	ASN	2.1
1	B	340	PRO	2.1
1	A	624	VAL	2.1
1	A	424	TYR	2.1
1	A	734	VAL	2.1
1	B	436	THR	2.1
1	B	576	THR	2.1
1	B	575	MET	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 oligosaccharides 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, 95th 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
4	C8E	A	810	15/21	0.79	0.14	31,39,47,60	0
4	C8E	B	807	12/21	0.84	0.13	32,39,48,49	0
4	C8E	B	811	15/21	0.84	0.11	30,35,46,50	0
3	EDO	B	803	4/4	0.84	0.22	31,39,41,41	0
4	C8E	A	811	13/21	0.84	0.12	34,42,49,49	0
6	K	A	816	1/1	0.84	0.24	58,58,58,58	0

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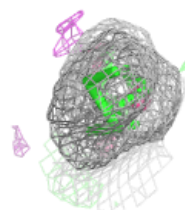
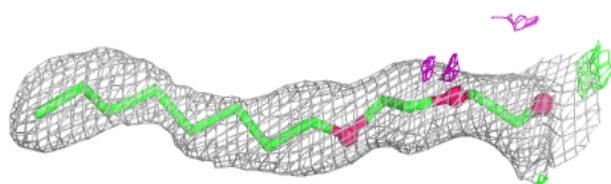
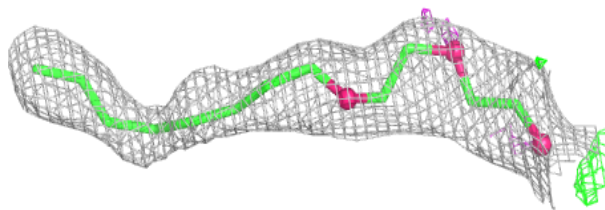
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	C8E	A	801	15/21	0.86	0.12	26,35,47,48	0
3	EDO	B	808	4/4	0.87	0.15	29,32,34,41	0
3	EDO	A	805	4/4	0.87	0.14	27,30,32,34	0
6	K	B	814	1/1	0.88	0.30	52,52,52,52	0
3	EDO	B	802	4/4	0.88	0.15	29,32,34,37	0
3	EDO	B	805	4/4	0.89	0.13	33,36,42,42	0
3	EDO	A	809	4/4	0.90	0.13	26,30,32,38	0
3	EDO	B	809	4/4	0.90	0.10	32,34,35,35	0
2	J9F	B	806	15/15	0.91	0.11	26,31,41,42	0
6	K	A	813	1/1	0.92	0.33	50,50,50,50	0
6	K	A	817	1/1	0.92	0.25	51,51,51,51	0
3	EDO	A	804	4/4	0.93	0.08	31,32,37,42	0
2	J9F	A	807	15/15	0.93	0.10	27,30,43,48	0
6	K	A	814	1/1	0.93	0.12	53,53,53,53	0
2	J9F	B	801	15/15	0.93	0.09	24,28,35,36	0
3	EDO	B	810	4/4	0.93	0.13	28,29,31,32	0
3	EDO	B	804	4/4	0.94	0.09	26,26,30,33	0
2	J9F	A	802	15/15	0.94	0.07	16,27,31,31	0
3	EDO	A	803	4/4	0.95	0.08	24,29,29,30	0
3	EDO	A	808	4/4	0.96	0.12	23,24,27,29	0
3	EDO	B	812	4/4	0.96	0.07	25,29,32,38	0
3	EDO	A	806	4/4	0.97	0.06	26,27,30,30	0
6	K	A	815	1/1	0.97	0.07	48,48,48,48	0
5	FE	B	813	1/1	0.99	0.02	31,31,31,31	0
5	FE	A	812	1/1	1.00	0.01	28,28,28,28	0

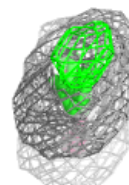
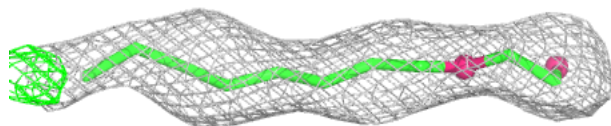
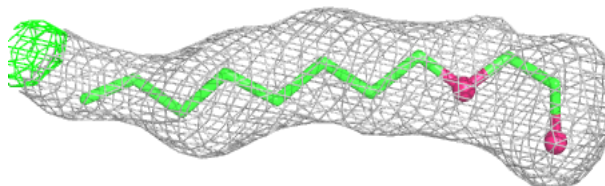
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 810:

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

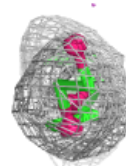
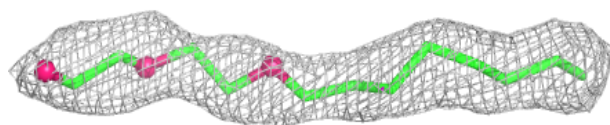
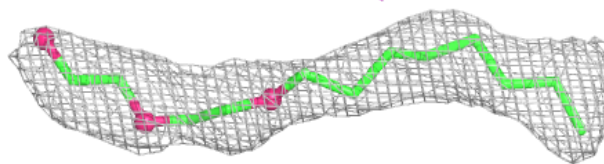
**Electron density around C8E B 807:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



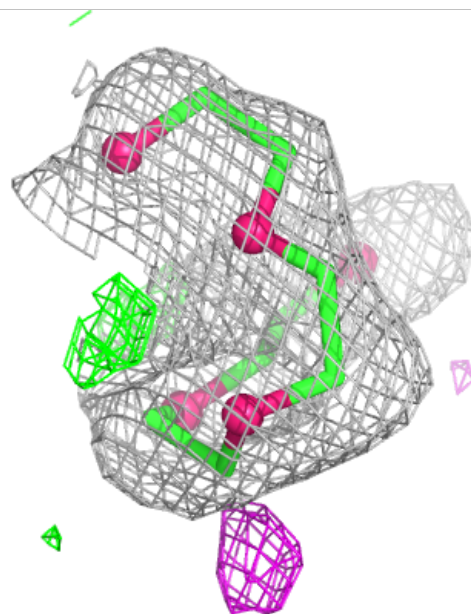
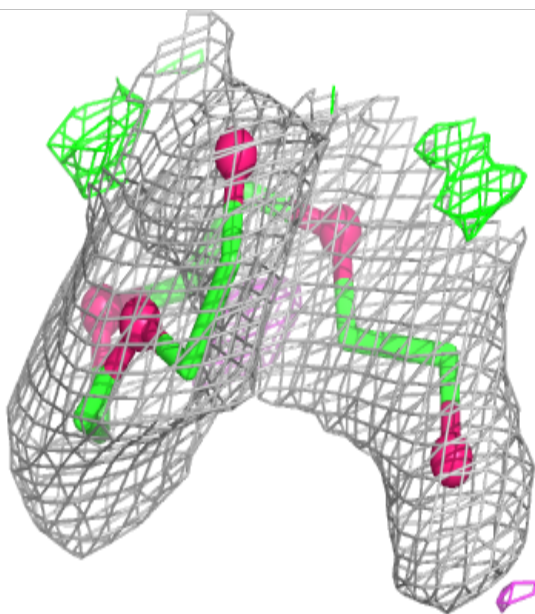
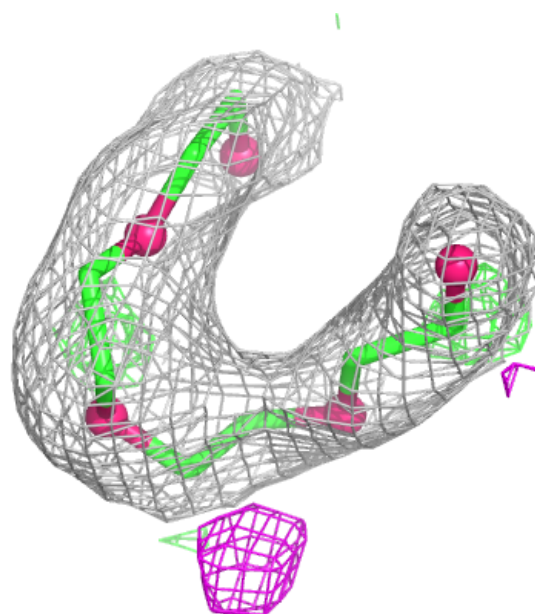
Electron density around C8E B 811:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



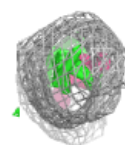
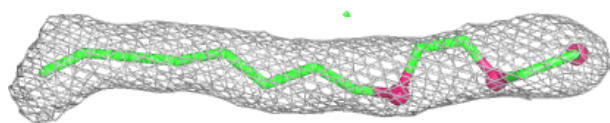
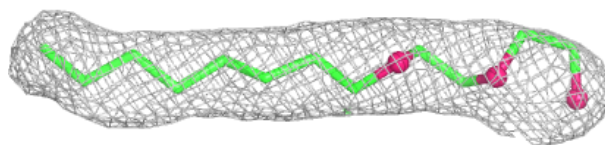
Electron density around C8E A 811:

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



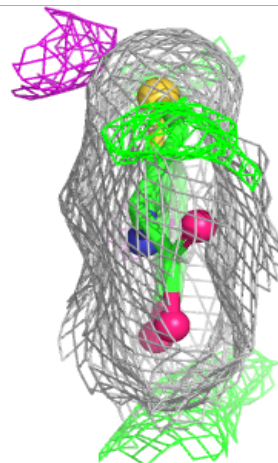
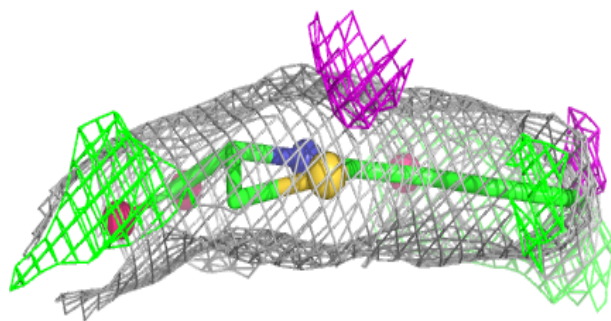
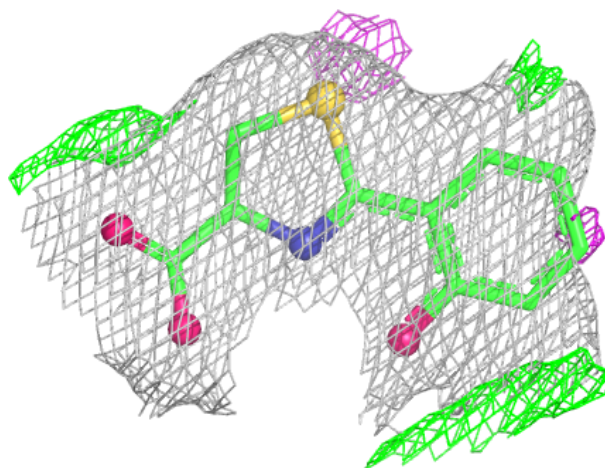
Electron density around C8E A 801:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



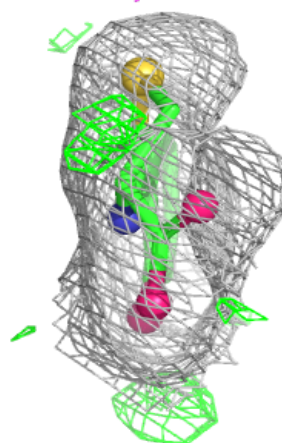
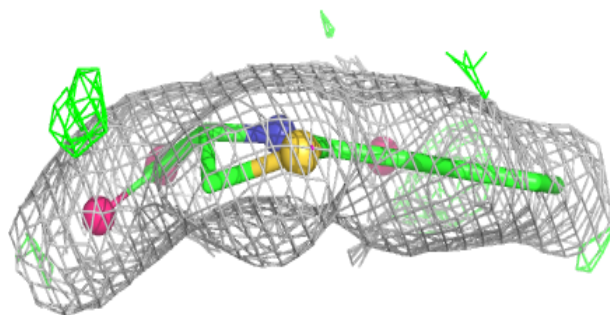
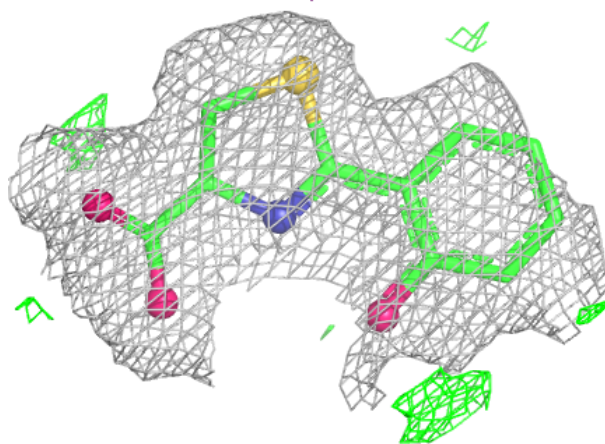
Electron density around J9F B 806:

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and green (positive)



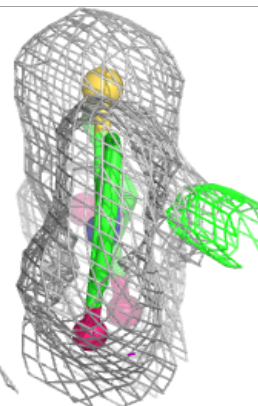
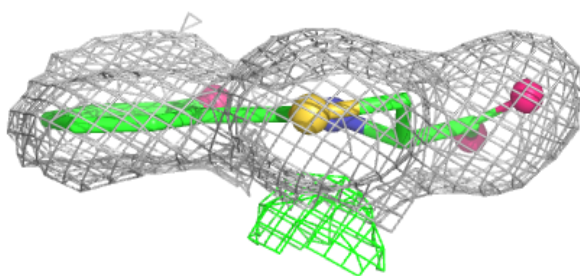
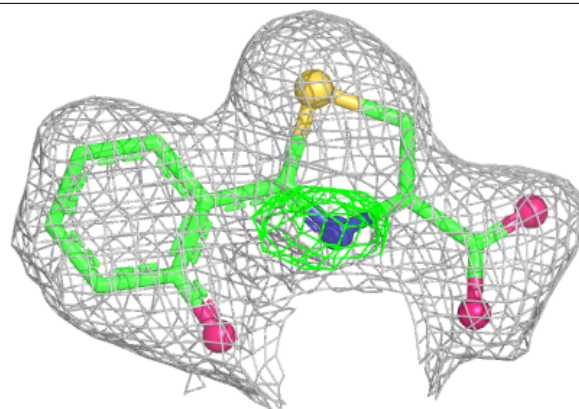
Electron density around J9F A 807:

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

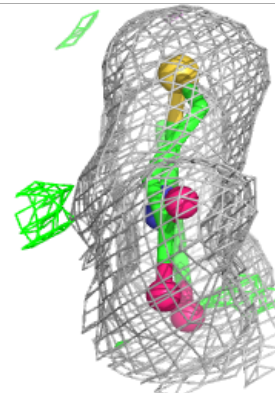
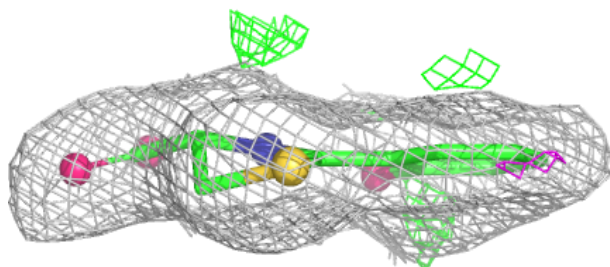
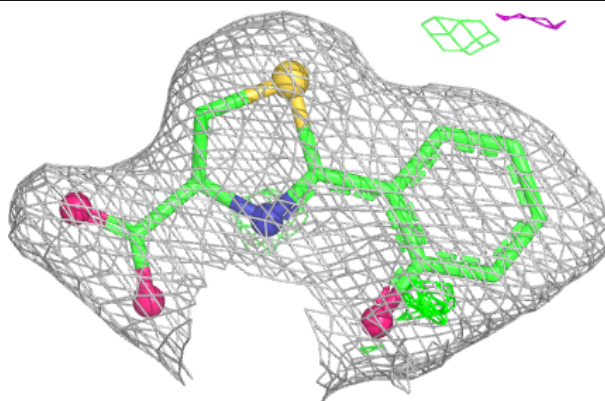


Electron density around J9F B 801:

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

**Electron density around J9F 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.