



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2022 – 10:07 am BST

PDB ID : 7O0D
Title : monomeric acetyl-CoA synthase in open conformation with methanethiol moiety of CoA bound to nickel proximal
Authors : Kreibich, J.; Jeoung, J.H.; Dobbek, H.
Deposited on : 2021-03-26
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

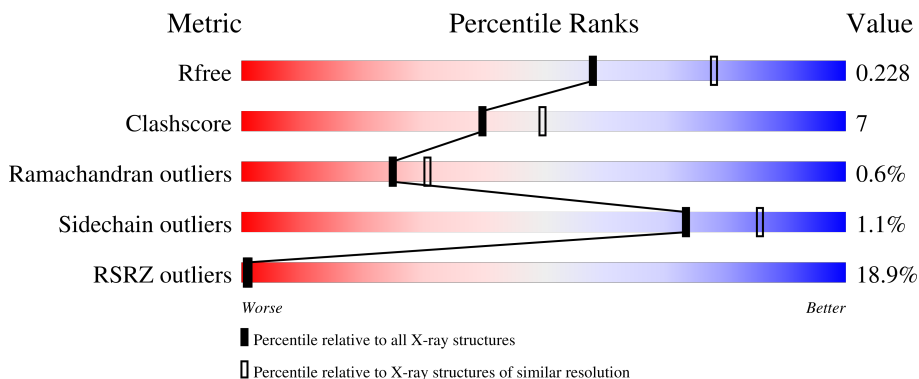
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	734	

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
8	SO4	A	811	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12226 atoms, of which 5965 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.

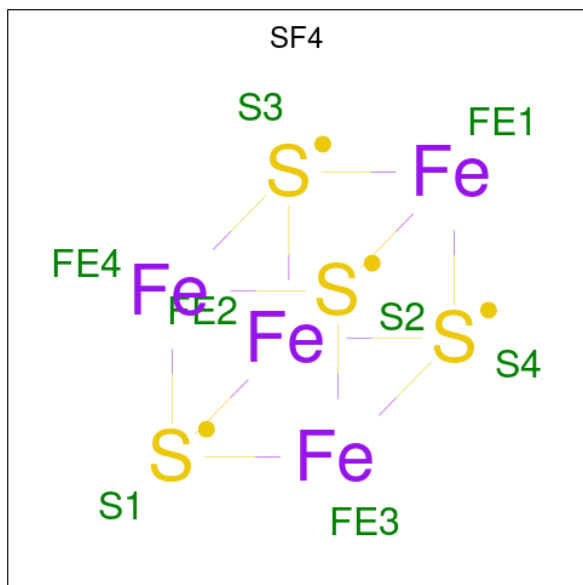
- Molecule 1 is a protein called CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	729	11509	3702	5743	965	1070	29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q3ACS4
A	0	ASN	-	expression tag	UNP Q3ACS4

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

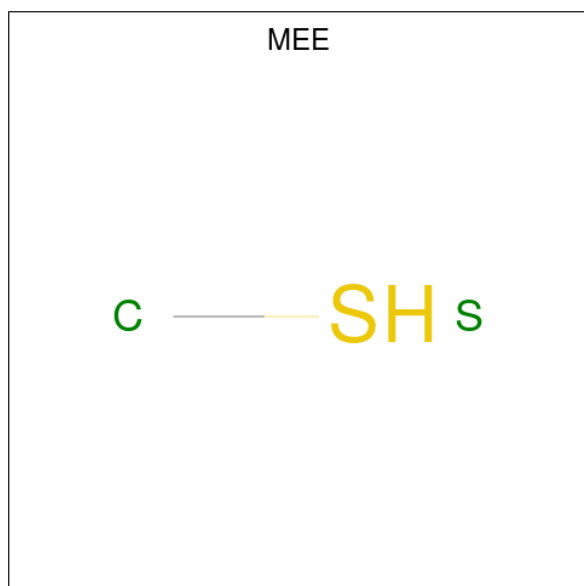


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

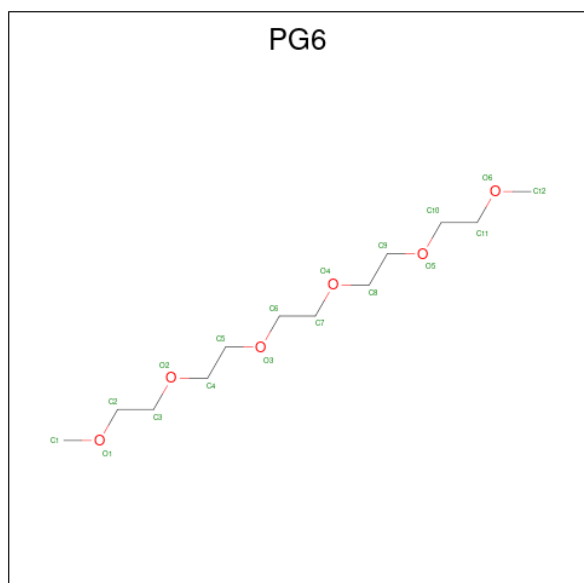
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ni	0	0
			2	2		

- Molecule 4 is METHANETHIOL (three-letter code: MEE) (formula: CH₄S) (labeled as "Ligand of Interest" by depositor).



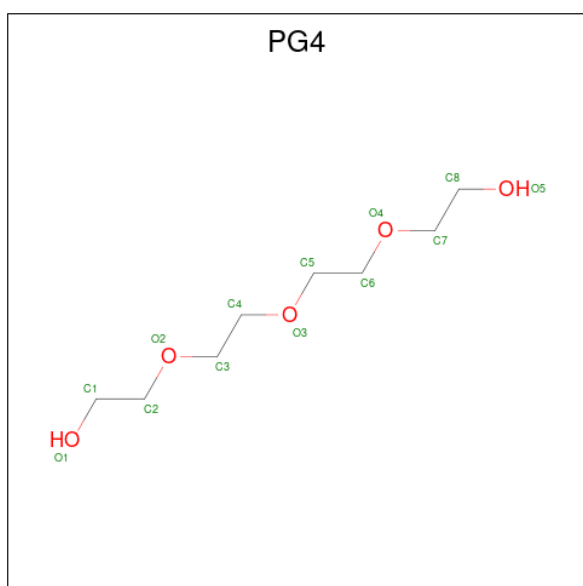
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	S	0	0
			5	1	3	1		

- Molecule 5 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: C₁₂H₂₆O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			44	12	26	6		
5	A	1	Total	C	H	O	0	0
			44	12	26	6		
5	A	1	Total	C	H	O	0	0
			44	12	26	6		
5	A	1	Total	C	H	O	0	0
			44	12	26	6		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			31	8	18	5		
6	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



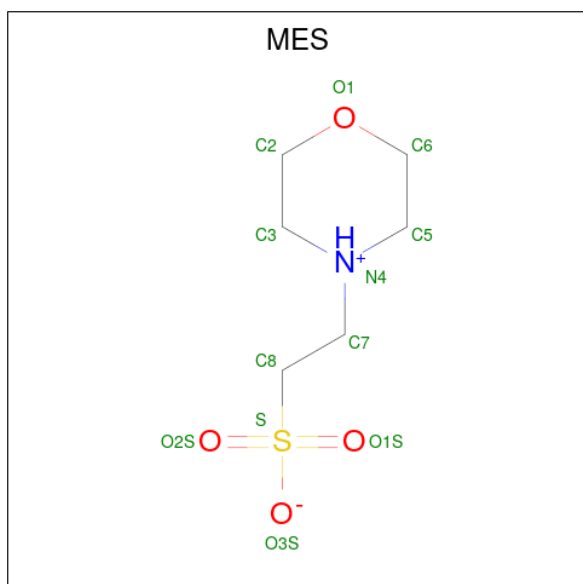
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	17	4	10	3	0	0
7	A	1	17	4	10	3	0	0
7	A	1	17	4	10	3	0	0
7	A	1	17	4	10	3	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
9	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
9	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

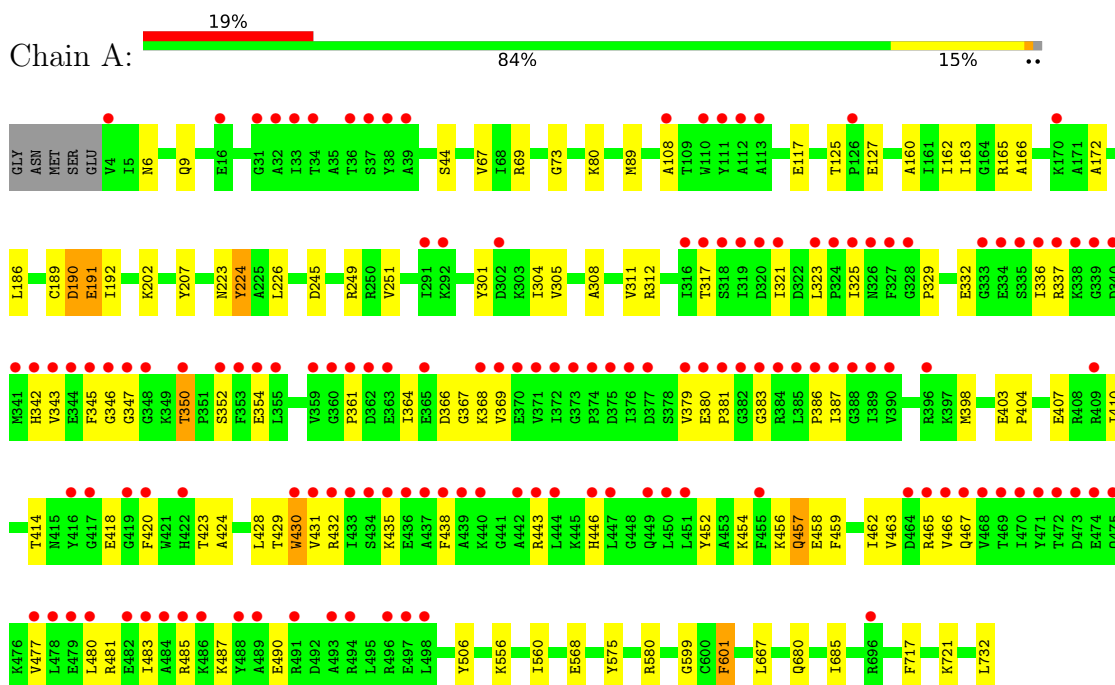
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	291	Total 291	O 291	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: CO-methylating acetyl-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	199.34Å 199.34Å 168.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.88 – 2.30 48.88 – 2.22	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.88-2.30) 83.1 (48.88-2.22)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.196 , 0.222 0.205 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12226	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, SO4, NI, PEG, PG6, PG4, MEE, MES

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	0.28	0/5900	0.53	0/7988

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5766	5743	5744	79	0
2	A	8	0	0	0	0
3	A	2	0	0	0	0
4	A	2	3	0	0	0
5	A	72	104	104	3	0
6	A	26	36	36	1	0
7	A	28	40	40	3	0
8	A	30	0	0	3	0
9	A	36	39	39	2	0
10	A	291	0	0	10	0
All	All	6261	5965	5963	87	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 7.

All (87) 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)
9:A:818:MES:O2S	10:A:901:HOH:O	1.93	0.86
1:A:336:ILE:HD11	1:A:432:ARG:HB3	1.60	0.82
1:A:321:ILE:HG22	1:A:323:LEU:HD23	1.66	0.77
1:A:680:GLN:NE2	10:A:909:HOH:O	2.17	0.77
8:A:811:SO4:O3	10:A:902:HOH:O	2.02	0.77
9:A:821:MES:O3S	10:A:903:HOH:O	2.04	0.75
1:A:398:MET:HA	1:A:462:ILE:HD11	1.68	0.74
1:A:160:ALA:HB3	1:A:186:LEU:CD2	2.19	0.72
8:A:811:SO4:O4	10:A:904:HOH:O	2.04	0.72
1:A:165:ARG:HB3	1:A:191:GLU:HG3	1.72	0.70
7:A:808:PEG:O4	10:A:905:HOH:O	2.08	0.70
7:A:822:PEG:O4	10:A:906:HOH:O	2.11	0.68
1:A:480:LEU:HD13	1:A:483:ILE:HD12	1.79	0.64
1:A:160:ALA:HB3	1:A:186:LEU:HD22	1.80	0.64
6:A:810:PG4:O1	10:A:908:HOH:O	2.13	0.63
1:A:407:GLU:O	1:A:410:ILE:HG12	1.98	0.63
8:A:816:SO4:O1	10:A:907:HOH:O	2.12	0.62
1:A:575:TYR:CZ	1:A:580:ARG:HG3	2.39	0.57
1:A:342:HIS:CD2	1:A:381:PRO:HA	2.41	0.56
1:A:202:LYS:NZ	1:A:207:TYR:OH	2.37	0.55
1:A:732:LEU:HD23	10:A:969:HOH:O	2.06	0.55
1:A:354:GLU:CD	1:A:410:ILE:HD11	2.26	0.55
1:A:429:THR:HG23	1:A:429:THR:O	2.07	0.55
1:A:438:PHE:CD1	1:A:438:PHE:O	2.59	0.54
1:A:380:GLU:HG3	1:A:381:PRO:HD2	1.89	0.54
1:A:162:ILE:HG21	1:A:192:ILE:HD13	1.89	0.53
1:A:452:TYR:CE2	1:A:466:VAL:HG13	2.44	0.53
1:A:481:ARG:O	1:A:485:ARG:HG2	2.10	0.51
1:A:343:VAL:HG12	1:A:345:PHE:CE1	2.46	0.51
1:A:379:VAL:HG21	1:A:383:GLY:HA3	1.91	0.51
1:A:345:PHE:HB2	1:A:431:VAL:HB	1.92	0.51
1:A:459:PHE:O	1:A:463:VAL:HG22	2.11	0.51
1:A:44:SER:OG	5:A:805:PG6:H122	2.11	0.51
1:A:346:GLY:H	1:A:350:THR:HG23	1.77	0.50
1:A:398:MET:CA	1:A:462:ILE:HD11	2.38	0.50
1:A:117:GLU:OE1	5:A:809:PG6:H123	2.12	0.49
1:A:308:ALA:O	1:A:311:VAL:HG12	2.11	0.49
1:A:342:HIS:ND1	1:A:435:LYS:HA	2.27	0.49
1:A:67:VAL:HG22	1:A:226:LEU:HD12	1.95	0.49
1:A:323:LEU:HD13	1:A:446:HIS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HD11	1:A:418:GLU:HB2	1.95	0.48
1:A:457:GLN:HG2	1:A:458:GLU:N	2.29	0.48
1:A:717:PHE:O	1:A:721:LYS:HG2	2.13	0.48
1:A:452:TYR:CD2	1:A:466:VAL:HG13	2.49	0.47
1:A:6:ASN:O	1:A:9:GLN:HG3	2.15	0.47
1:A:189:CYS:O	1:A:190:ASP:HB2	2.15	0.47
1:A:456:LYS:HD3	1:A:466:VAL:HG12	1.97	0.46
1:A:352:SER:HA	1:A:387:ILE:O	2.15	0.46
1:A:223:ASN:OD1	1:A:224:TYR:N	2.49	0.46
1:A:423:THR:O	1:A:424:ALA:HB3	2.16	0.46
1:A:44:SER:HA	5:A:805:PG6:H102	1.98	0.45
1:A:166:ALA:HB3	1:A:172:ALA:HB2	1.97	0.45
1:A:325:ILE:HD11	1:A:418:GLU:OE1	2.16	0.45
1:A:347:GLY:HA3	1:A:430:TRP:CE2	2.51	0.45
1:A:428:LEU:O	1:A:428:LEU:HG	2.16	0.45
1:A:329:PRO:O	1:A:332:GLU:HG3	2.17	0.45
1:A:245:ASP:O	1:A:249:ARG:HB2	2.17	0.45
1:A:506:TYR:OH	1:A:556:LYS:HE2	2.17	0.44
1:A:317:THR:HB	1:A:457:GLN:HG3	2.00	0.44
1:A:301:TYR:O	1:A:304:ILE:HG22	2.17	0.44
1:A:601:PHE:HD1	1:A:601:PHE:O	2.00	0.43
1:A:732:LEU:HD23	1:A:732:LEU:H	1.81	0.43
1:A:346:GLY:N	1:A:350:THR:HG23	2.33	0.43
1:A:367:GLY:O	1:A:369:VAL:HG23	2.18	0.43
1:A:69:ARG:O	1:A:73:GLY:HA2	2.18	0.43
1:A:454:LYS:HD3	1:A:457:GLN:NE2	2.34	0.43
1:A:304:ILE:HG23	1:A:305:VAL:N	2.34	0.43
1:A:366:ASP:HB2	1:A:465:ARG:HG3	2.00	0.43
1:A:163:ILE:HG22	1:A:189:CYS:HB3	2.01	0.43
1:A:368:LYS:HB3	1:A:467:GLN:HB2	2.00	0.42
1:A:336:ILE:O	1:A:336:ILE:HG13	2.19	0.42
1:A:560:ILE:HD11	1:A:568:GLU:HG3	2.01	0.42
1:A:732:LEU:HG	7:A:820:PEG:H12	2.02	0.42
1:A:364:ILE:HG12	1:A:467:GLN:HG2	2.01	0.41
1:A:667:LEU:HD21	1:A:685:ILE:HG23	2.03	0.41
1:A:89:MET:SD	1:A:108:ALA:HA	2.60	0.41
1:A:487:LYS:HD3	1:A:490:GLU:OE2	2.19	0.41
1:A:414:THR:O	1:A:420:PHE:HB2	2.20	0.41
1:A:251:VAL:O	1:A:312:ARG:NH2	2.52	0.41
1:A:386:PRO:HB2	1:A:477:VAL:HG11	2.03	0.41
1:A:343:VAL:HG12	1:A:345:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:THR:OG1	1:A:127:GLU:HG3	2.21	0.41
1:A:337:ARG:NE	1:A:337:ARG:HA	2.35	0.41
1:A:352:SER:HB2	1:A:429:THR:HG23	2.03	0.40
1:A:457:GLN:CG	1:A:458:GLU:N	2.84	0.40
1:A:403:GLU:HB2	1:A:404:PRO:HD3	2.02	0.40
1:A:6:ASN:OD1	1:A:9:GLN:HG3	2.22	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	727/734 (99%)	701 (96%)	22 (3%)	4 (1%)	25 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ASP
1	A	430	TRP
1	A	599	GLY
1	A	361	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	611/615 (99%)	604 (99%)	7 (1%)	73 86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	191	GLU
1	A	224	TYR
1	A	350	THR
1	A	443	ARG
1	A	457	GLN
1	A	601	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	$\# Z > 2$
9	MES	A	818	-	12,12,12	1.73	3 (25%)	14,16,16	2.13	5 (35%)
9	MES	A	817	-	12,12,12	1.66	3 (25%)	14,16,16	1.99	5 (35%)
5	PG6	A	823	-	17,17,17	0.53	0	16,16,16	0.64	0
7	PEG	A	822	-	6,6,6	0.48	0	5,5,5	0.28	0
8	SO4	A	812	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SF4	A	801	1	0,12,12	-	-	-	-	-
8	SO4	A	816	-	4,4,4	0.13	0	6,6,6	0.06	0
7	PEG	A	808	-	6,6,6	0.47	0	5,5,5	0.33	0
9	MES	A	821	-	12,12,12	1.69	2 (16%)	14,16,16	1.95	4 (28%)
8	SO4	A	813	-	4,4,4	0.14	0	6,6,6	0.05	0
7	PEG	A	807	-	6,6,6	0.49	0	5,5,5	0.29	0
8	SO4	A	814	-	4,4,4	0.15	0	6,6,6	0.08	0
5	PG6	A	805	-	17,17,17	0.53	0	16,16,16	0.41	0
5	PG6	A	809	-	17,17,17	0.52	0	16,16,16	0.24	0
6	PG4	A	810	-	12,12,12	0.53	0	11,11,11	0.22	0
7	PEG	A	820	-	6,6,6	0.49	0	5,5,5	0.27	0
5	PG6	A	819	-	17,17,17	0.51	0	16,16,16	0.37	0
4	MEE	A	804	3	0,1,1	-	-	-	-	-
8	SO4	A	811	-	4,4,4	0.14	0	6,6,6	0.11	0
6	PG4	A	806	-	12,12,12	0.53	0	11,11,11	0.26	0
8	SO4	A	815	-	4,4,4	0.13	0	6,6,6	0.08	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
9	MES	A	818	-	-	1/6/14/14	0/1/1/1
7	PEG	A	808	-	-	2/4/4/4	-
9	MES	A	817	-	-	1/6/14/14	0/1/1/1
6	PG4	A	810	-	-	2/10/10/10	-
5	PG6	A	823	-	-	9/15/15/15	-
7	PEG	A	807	-	-	2/4/4/4	-
7	PEG	A	820	-	-	3/4/4/4	-
9	MES	A	821	-	-	3/6/14/14	0/1/1/1
7	PEG	A	822	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG6	A	819	-	-	9/15/15/15	-
6	PG4	A	806	-	-	4/10/10/10	-
2	SF4	A	801	1	-	-	0/6/5/5
5	PG6	A	805	-	-	9/15/15/15	-
5	PG6	A	809	-	-	4/15/15/15	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	818	MES	C8-S	4.30	1.83	1.77
9	A	821	MES	C8-S	4.23	1.83	1.77
9	A	817	MES	C8-S	3.95	1.83	1.77
9	A	817	MES	O1S-S	2.43	1.52	1.45
9	A	821	MES	O2S-S	2.25	1.51	1.45
9	A	818	MES	O2S-S	2.25	1.51	1.45
9	A	817	MES	O2S-S	2.15	1.51	1.45
9	A	818	MES	O1S-S	2.11	1.51	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	817	MES	O3S-S-O1S	-3.97	101.58	111.27
9	A	818	MES	O3S-S-O2S	-3.90	101.74	111.27
9	A	821	MES	O3S-S-O2S	-3.77	102.05	111.27
9	A	817	MES	O3S-S-C8	3.74	111.82	105.77
9	A	821	MES	O2S-S-C8	3.72	111.39	106.92
9	A	818	MES	O3S-S-C8	3.50	111.42	105.77
9	A	821	MES	O3S-S-C8	3.49	111.42	105.77
9	A	818	MES	O2S-S-C8	3.34	110.93	106.92
9	A	818	MES	O1S-S-C8	3.04	110.57	106.92
9	A	817	MES	O1S-S-C8	2.86	110.35	106.92
9	A	817	MES	O2S-S-C8	2.53	109.97	106.92
9	A	818	MES	C6-C5-N4	2.29	113.58	110.10
9	A	817	MES	C6-C5-N4	2.29	113.57	110.10
9	A	821	MES	O1S-S-C8	2.06	109.40	106.92

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	817	MES	N4-C7-C8-S
9	A	821	MES	C7-C8-S-O1S
5	A	805	PG6	O4-C8-C9-O5
5	A	819	PG6	O2-C4-C5-O3
5	A	805	PG6	O3-C6-C7-O4
6	A	806	PG4	O2-C3-C4-O3
5	A	805	PG6	C3-C2-O1-C1
9	A	821	MES	C7-C8-S-O3S
6	A	806	PG4	O1-C1-C2-O2
7	A	807	PEG	O2-C3-C4-O4
5	A	823	PG6	C3-C2-O1-C1
5	A	823	PG6	O4-C8-C9-O5
5	A	809	PG6	O2-C4-C5-O3
5	A	819	PG6	O1-C2-C3-O2
9	A	818	MES	C7-C8-S-O3S
7	A	822	PEG	O1-C1-C2-O2
5	A	805	PG6	O5-C10-C11-O6
7	A	820	PEG	O2-C3-C4-O4
5	A	823	PG6	C5-C4-O2-C3
6	A	806	PG4	C8-C7-O4-C6
5	A	819	PG6	C5-C4-O2-C3
5	A	819	PG6	C6-C7-O4-C8
5	A	819	PG6	C9-C8-O4-C7
5	A	809	PG6	O5-C10-C11-O6
7	A	807	PEG	O1-C1-C2-O2
5	A	823	PG6	C6-C7-O4-C8
7	A	808	PEG	C1-C2-O2-C3
7	A	820	PEG	C4-C3-O2-C2
9	A	821	MES	C7-C8-S-O2S
5	A	805	PG6	C4-C5-O3-C6
5	A	805	PG6	C10-C11-O6-C12
5	A	819	PG6	O3-C6-C7-O4
5	A	823	PG6	C7-C6-O3-C5
5	A	823	PG6	O1-C2-C3-O2
5	A	809	PG6	C3-C2-O1-C1
7	A	822	PEG	O2-C3-C4-O4
5	A	805	PG6	C11-C10-O5-C9
5	A	823	PG6	C9-C8-O4-C7
5	A	805	PG6	O1-C2-C3-O2
6	A	810	PG4	C5-C6-O4-C7
5	A	805	PG6	C9-C8-O4-C7
5	A	819	PG6	C11-C10-O5-C9
5	A	809	PG6	O1-C2-C3-O2

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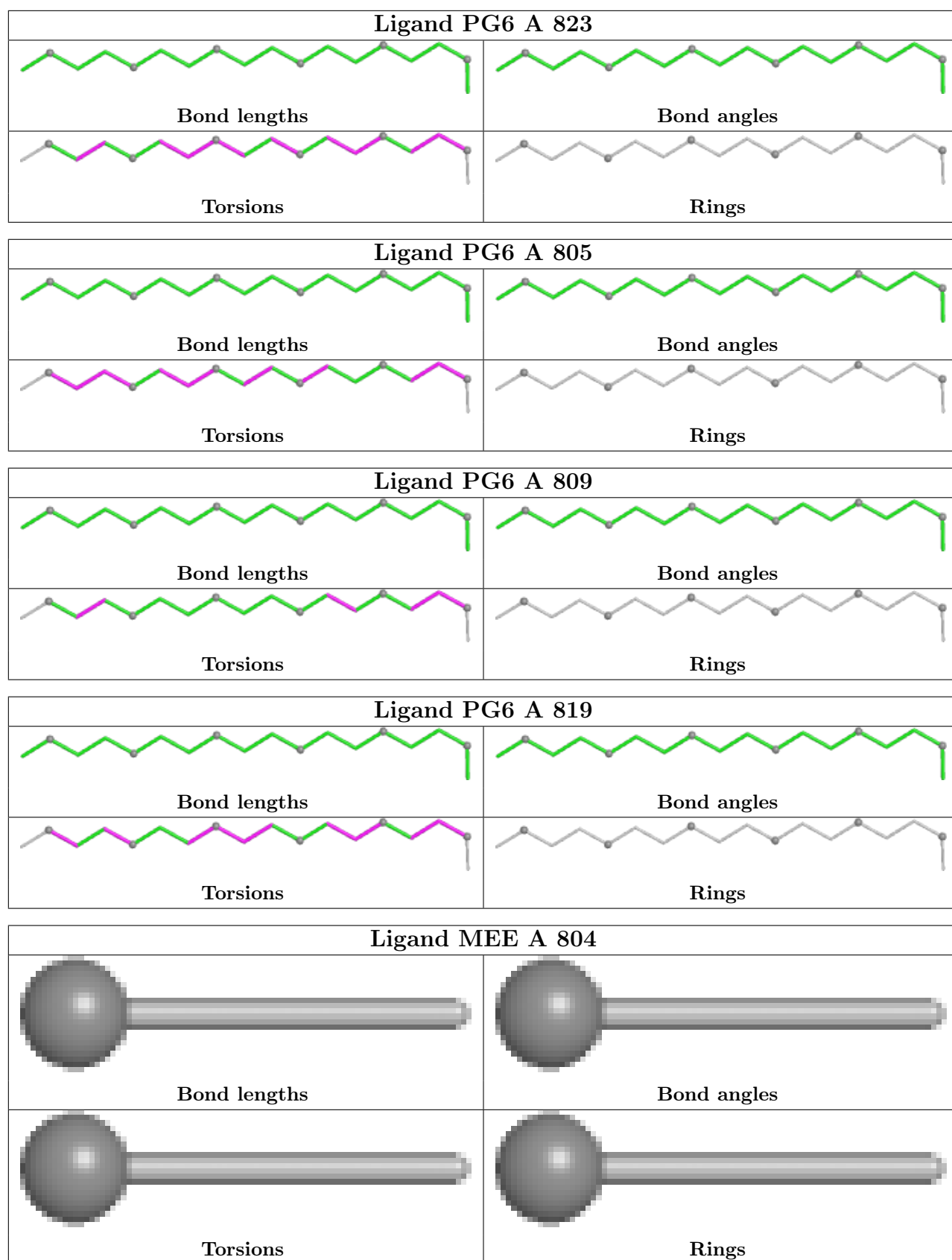
Mol	Chain	Res	Type	Atoms
5	A	819	PG6	C3-C2-O1-C1
6	A	806	PG4	O3-C5-C6-O4
7	A	820	PEG	O1-C1-C2-O2
5	A	819	PG6	C10-C11-O6-C12
5	A	823	PG6	O5-C10-C11-O6
6	A	810	PG4	C6-C5-O3-C4
5	A	823	PG6	O2-C4-C5-O3
7	A	808	PEG	C4-C3-O2-C2

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	818	MES	1	0
7	A	822	PEG	1	0
8	A	816	SO4	1	0
7	A	808	PEG	1	0
9	A	821	MES	1	0
5	A	805	PG6	2	0
5	A	809	PG6	1	0
6	A	810	PG4	1	0
7	A	820	PEG	1	0
8	A	811	SO4	2	0

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



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	729/734 (99%)	1.11	138 (18%) 1 1	33, 61, 166, 206	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	430	TRP	12.7
1	A	339	GLY	12.4
1	A	439	ALA	12.3
1	A	385	LEU	11.9
1	A	345	PHE	11.2
1	A	383	GLY	10.3
1	A	433	ILE	10.1
1	A	376	ILE	10.1
1	A	437	ALA	9.8
1	A	471	TYR	9.6
1	A	446	HIS	9.4
1	A	344	GLU	9.1
1	A	432	ARG	9.0
1	A	338	LYS	8.6
1	A	382	GLY	8.5
1	A	387	ILE	8.4
1	A	434	SER	8.4
1	A	343	VAL	8.1
1	A	381	PRO	8.0
1	A	431	VAL	7.9
1	A	320	ASP	7.5
1	A	478	LEU	7.4
1	A	361	PRO	7.4
1	A	493	ALA	7.3
1	A	341	MET	7.2
1	A	435	LYS	7.2
1	A	348	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	420	PHE	6.5
1	A	443	ARG	6.1
1	A	317	THR	6.0
1	A	470	ILE	6.0
1	A	442	ALA	5.9
1	A	362	ASP	5.9
1	A	336	ILE	5.9
1	A	386	PRO	5.8
1	A	472	THR	5.7
1	A	417	GLY	5.7
1	A	449	GLN	5.7
1	A	467	GLN	5.6
1	A	489	ALA	5.6
1	A	340	ASP	5.4
1	A	347	GLY	5.4
1	A	484	ALA	5.4
1	A	346	GLY	5.1
1	A	438	PHE	5.1
1	A	342	HIS	5.1
1	A	377	ASP	5.1
1	A	468	VAL	5.0
1	A	469	THR	4.9
1	A	494	ARG	4.9
1	A	444	LEU	4.9
1	A	380	GLU	4.9
1	A	374	PRO	4.8
1	A	370	GLU	4.8
1	A	372	ILE	4.8
1	A	371	VAL	4.7
1	A	466	VAL	4.7
1	A	396	ARG	4.7
1	A	696	ARG	4.7
1	A	318	SER	4.5
1	A	482	GLU	4.5
1	A	480	LEU	4.5
1	A	440	LYS	4.4
1	A	419	GLY	4.4
1	A	327	PHE	4.3
1	A	4	VAL	4.3
1	A	474	GLU	4.2
1	A	365	GLU	4.1
1	A	388	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	352	SER	4.1
1	A	465	ARG	4.0
1	A	497	GLU	4.0
1	A	323	LEU	4.0
1	A	496	ARG	4.0
1	A	316	ILE	4.0
1	A	488	TYR	3.9
1	A	447	LEU	3.8
1	A	473	ASP	3.7
1	A	369	VAL	3.7
1	A	355	LEU	3.7
1	A	337	ARG	3.7
1	A	324	PRO	3.6
1	A	319	ILE	3.6
1	A	455	PHE	3.6
1	A	379	VAL	3.6
1	A	353	PHE	3.5
1	A	389	ILE	3.5
1	A	486	LYS	3.5
1	A	325	ILE	3.4
1	A	450	LEU	3.3
1	A	483	ILE	3.3
1	A	416	TYR	3.2
1	A	334	GLU	3.2
1	A	477	VAL	3.2
1	A	359	VAL	3.1
1	A	32	ALA	3.1
1	A	384	ARG	3.1
1	A	292	LYS	3.1
1	A	31	GLY	3.0
1	A	373	GLY	3.0
1	A	350	THR	3.0
1	A	326	ASN	3.0
1	A	38	TYR	2.9
1	A	291	ILE	2.9
1	A	112	ALA	2.8
1	A	126	PRO	2.8
1	A	16	GLU	2.8
1	A	328	GLY	2.8
1	A	360	GLY	2.8
1	A	36	THR	2.8
1	A	33	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	390	VAL	2.7
1	A	498	LEU	2.6
1	A	170	LYS	2.6
1	A	37	SER	2.5
1	A	321	ILE	2.5
1	A	409	ARG	2.5
1	A	335	SER	2.5
1	A	368	LYS	2.5
1	A	110	TRP	2.5
1	A	111	TYR	2.4
1	A	34	THR	2.4
1	A	491	ARG	2.3
1	A	354	GLU	2.3
1	A	375	ASP	2.2
1	A	436	GLU	2.2
1	A	302	ASP	2.2
1	A	39	ALA	2.2
1	A	485	ARG	2.2
1	A	363	GLU	2.1
1	A	108	ALA	2.1
1	A	451	LEU	2.1
1	A	422	HIS	2.1
1	A	464	ASP	2.1
1	A	333	GLY	2.1
1	A	113	ALA	2.1
1	A	479	GLU	2.0
1	A	475	GLN	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,

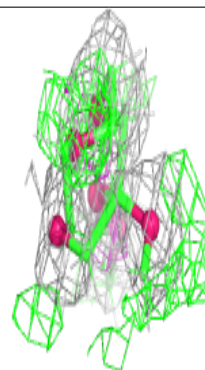
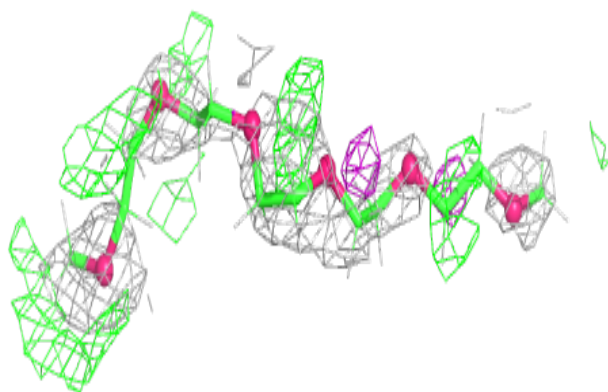
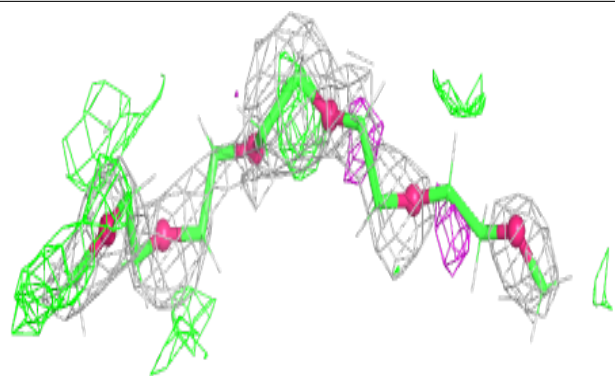
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PEG	A	822	7/7	0.66	0.17	78,94,101,104	17
7	PEG	A	820	7/7	0.69	0.19	62,83,100,100	0
5	PG6	A	823	18/18	0.73	0.38	37,55,70,72	44
5	PG6	A	819	18/18	0.77	0.24	52,68,82,87	44
6	PG4	A	806	13/13	0.81	0.12	72,88,100,102	0
8	SO4	A	813	5/5	0.86	0.24	48,56,57,65	5
8	SO4	A	814	5/5	0.88	0.19	111,112,114,116	0
8	SO4	A	816	5/5	0.88	0.25	55,65,75,80	5
9	MES	A	818	12/12	0.89	0.20	74,99,119,122	25
5	PG6	A	809	18/18	0.91	0.14	56,72,92,96	0
9	MES	A	817	12/12	0.91	0.17	62,82,97,102	0
7	PEG	A	808	7/7	0.91	0.13	51,68,89,89	0
6	PG4	A	810	13/13	0.92	0.12	49,59,73,75	0
7	PEG	A	807	7/7	0.92	0.15	51,61,69,83	17
8	SO4	A	815	5/5	0.93	0.18	71,72,79,88	5
5	PG6	A	805	18/18	0.93	0.18	40,62,85,90	0
9	MES	A	821	12/12	0.93	0.25	52,69,88,90	25
4	MEE	A	804	2/2	0.94	0.17	61,68,74,74	0
8	SO4	A	812	5/5	0.95	0.16	58,78,80,82	5
8	SO4	A	811	5/5	0.98	0.11	43,43,48,50	5
2	SF4	A	801	8/8	0.99	0.14	40,41,44,44	0
3	NI	A	803	1/1	0.99	0.19	39,39,39,39	0
3	NI	A	802	1/1	1.00	0.16	51,51,51,51	0

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

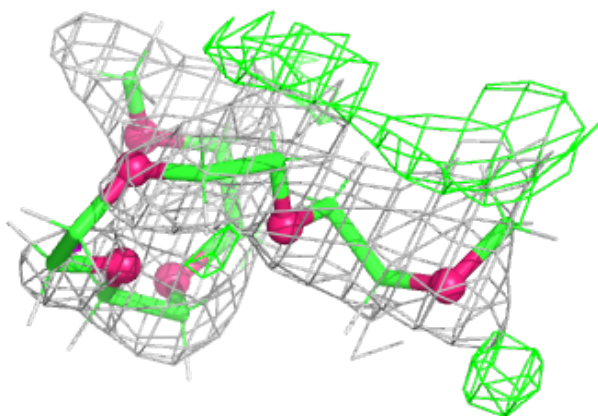
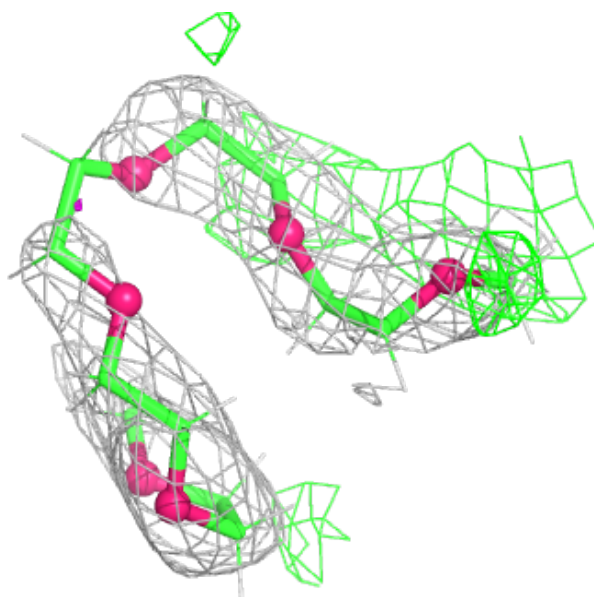
Electron density around PG6 A 823:

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



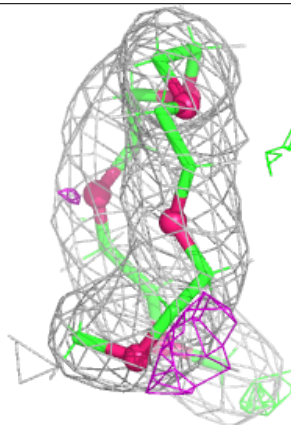
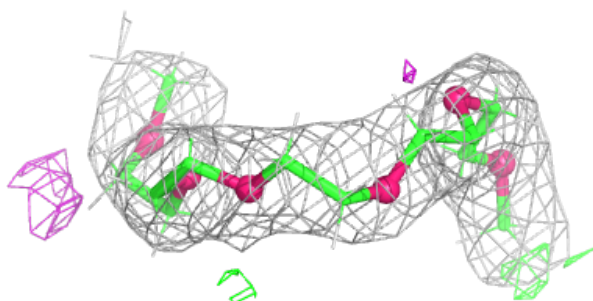
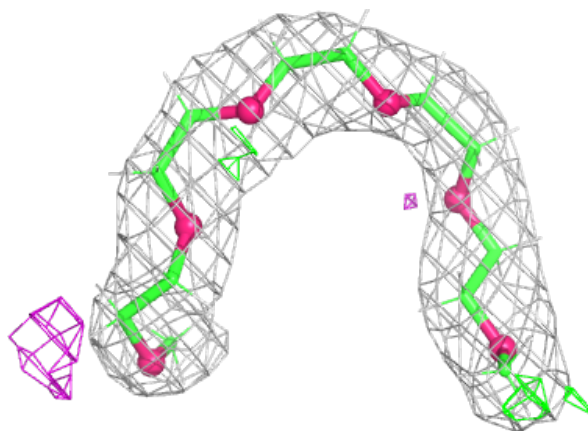
Electron density around PG6 A 819:

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



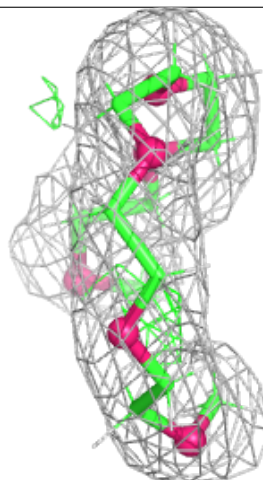
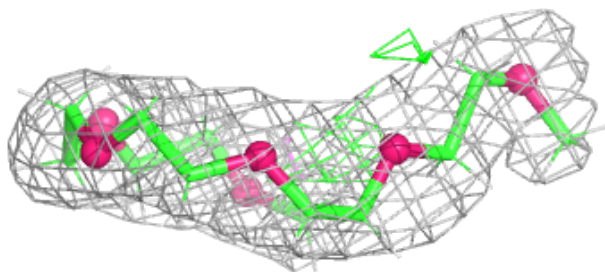
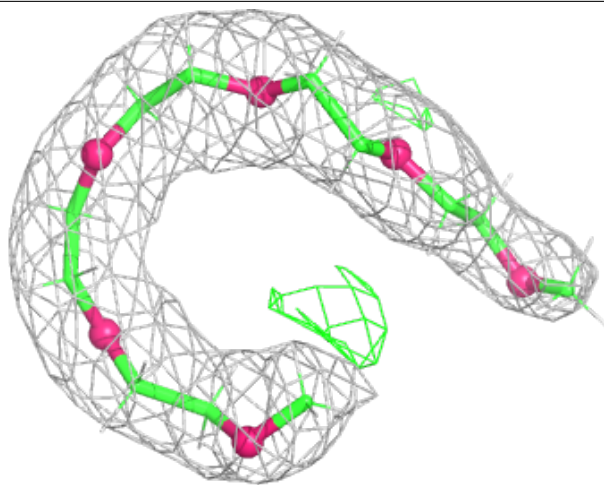
Electron density around PG6 A 809:

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



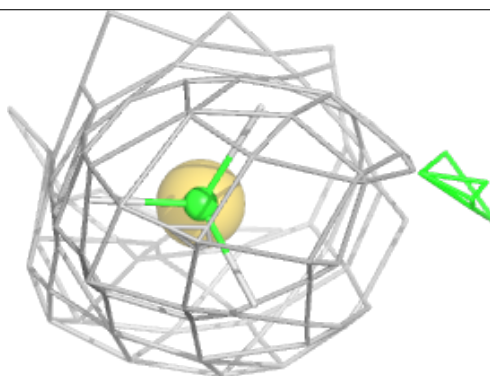
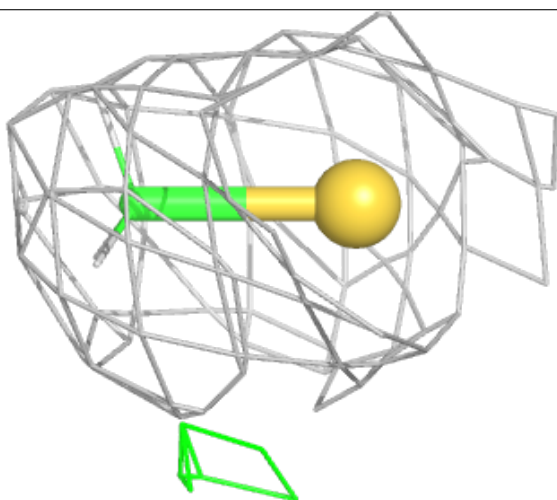
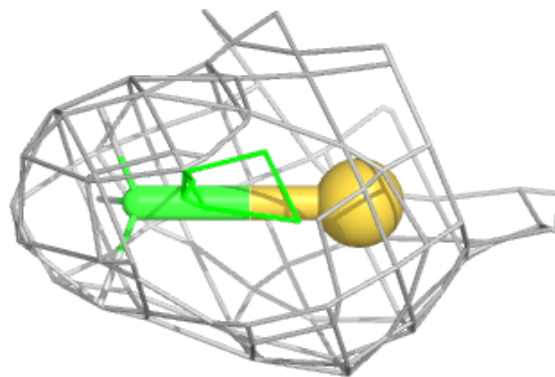
Electron density around PG6 A 805:

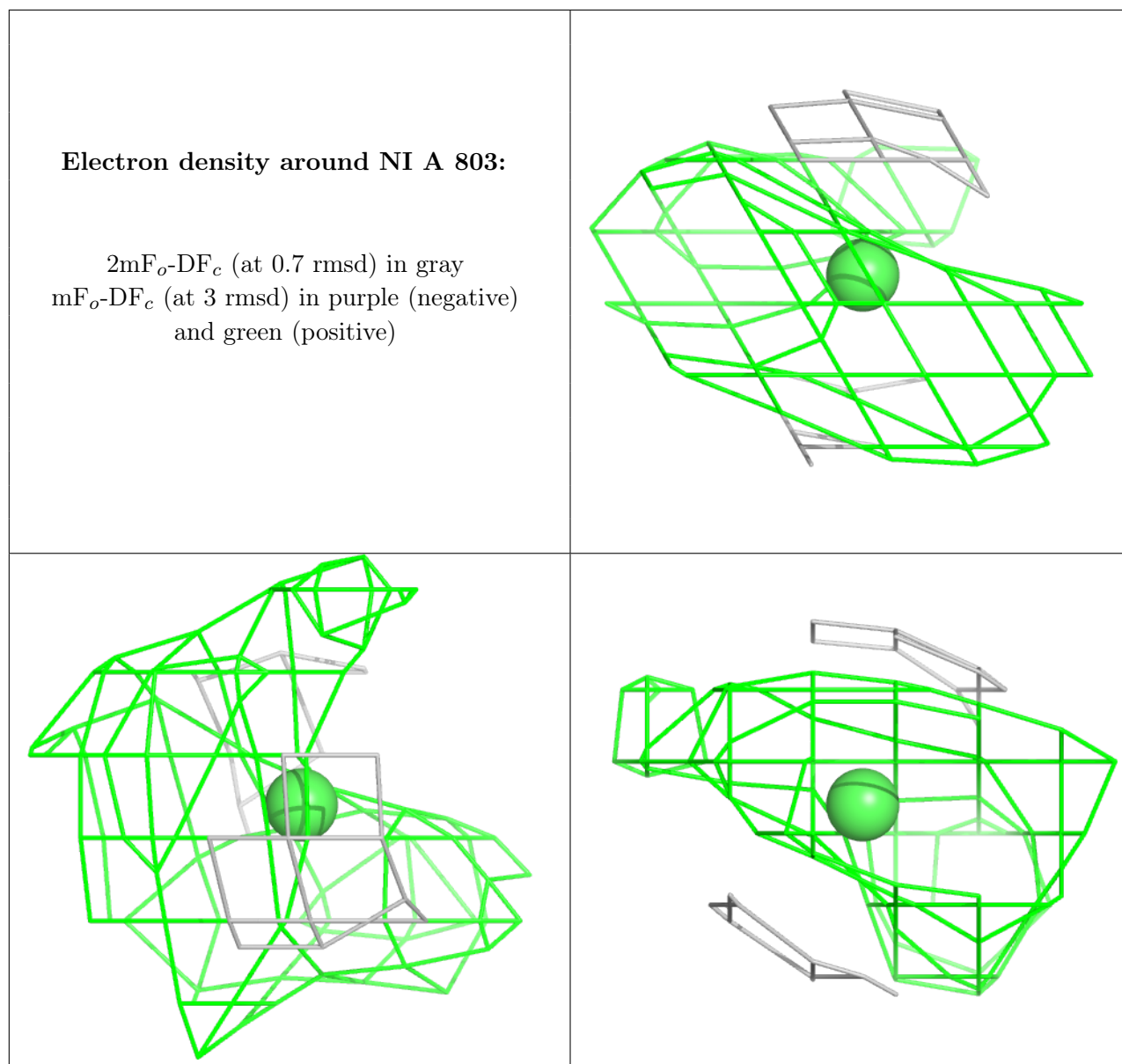
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

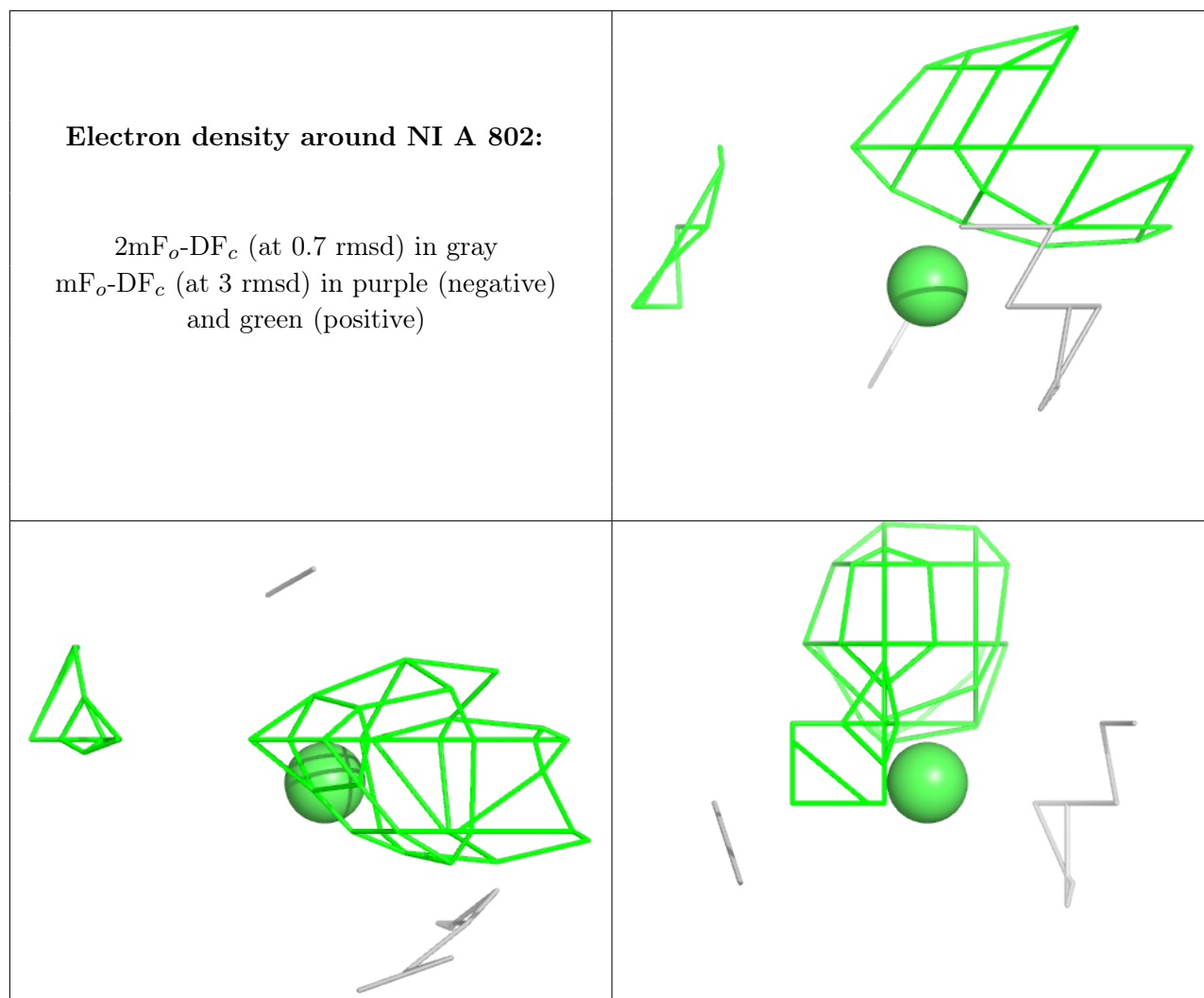


Electron density around MEE A 804:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.