



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2022 – 10:08 am BST

PDB ID : 7NYP
Title : monomeric acetyl-CoA synthase in closed conformation
Authors : Kreibich, J.; Jeoung, J.H.; Dobbek, H.
Deposited on : 2021-03-23
Resolution : 2.10 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

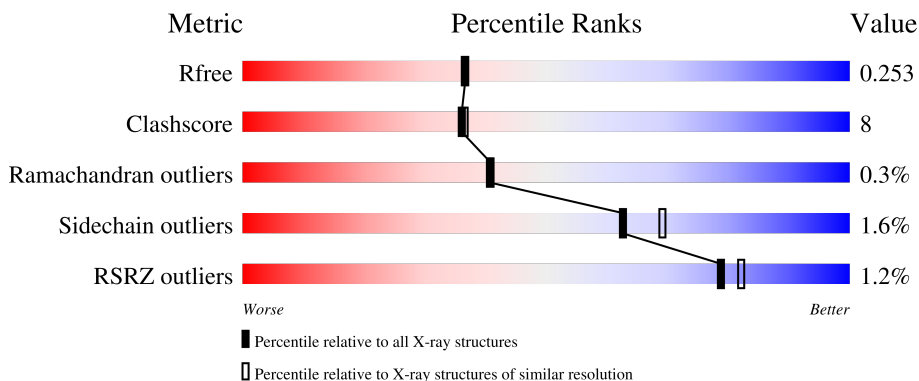
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


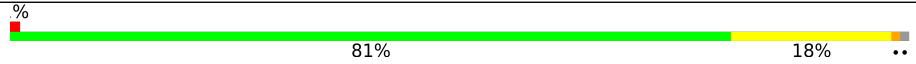
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	 85% 14% ..
1	B	734	 81% 18% ..

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
4	PEG	A	804	-	-	X	-
4	PEG	B	801	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24154 atoms, of which 11534 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	11510	3702	5744	965	1070	29	0	0	0
1	B	729	11512	3702	5746	965	1070	29	0	0	0

There are 4 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
B	-1	GLY	-	expression tag	UNP Q3ACS4
B	0	ASN	-	expression tag	UNP Q3ACS4

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



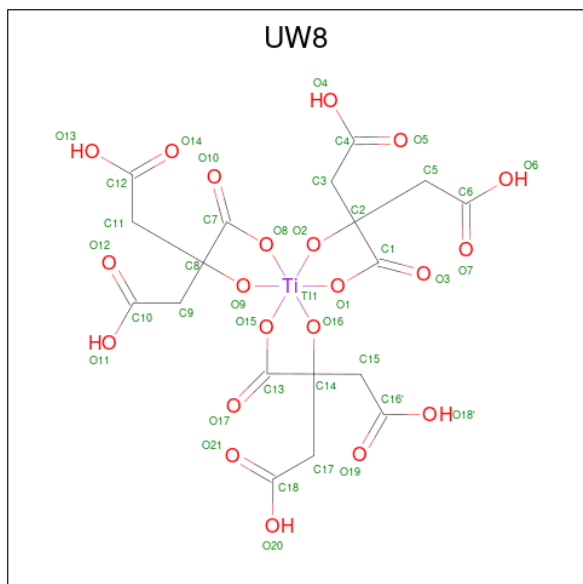
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is 2-[3,8,8,12,12-pentakis(2-hydroxy-2-oxoethyl)-2,7,11-tris(oxidanylidene)-1,4,6,9,10,13-hexaoxa-5 λ ^6-titanaspiro[4.4 \wedge {5}.4 \wedge {5}]tridecan-3-yl]ethanoic acid (three-letter code: UW8) (formula: C₁₈H₁₈O₂₁Ti).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	O	Ti	0	0
				52	18	12	21		
5	B	1	Total	C	H	O	Ti	0	0
				52	18	12	21		

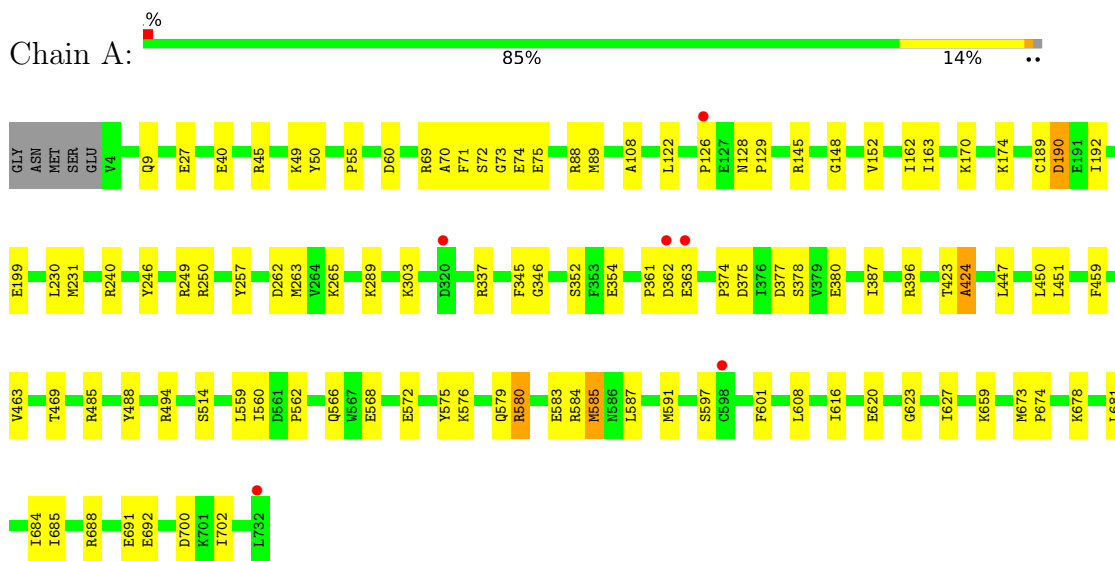
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	466	Total	O	0	0
				466		
6	B	508	Total	O	0	0
				508		

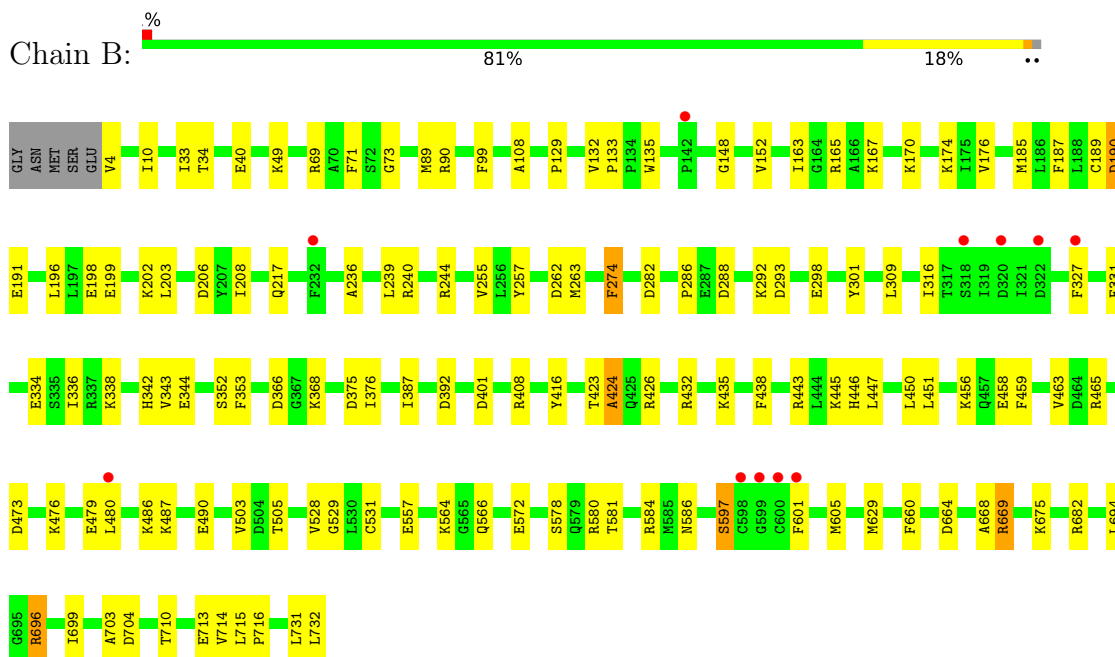
3 Residue-property plots

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



- Molecule 1: CO-methylating acetyl-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.95Å 99.48Å 238.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.43 – 2.10 46.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	82.0 (46.43-2.10) 65.0 (46.43-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.199 , 0.243 0.213 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.024	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	24154	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: UW8, SF4, NI, PEG

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	0.46	4/5900 (0.1%)	0.63	4/7988 (0.1%)
1	B	0.45	4/5900 (0.1%)	0.62	3/7988 (0.0%)
All	All	0.46	8/11800 (0.1%)	0.63	7/15976 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	PRO	N-CD	-13.89	1.28	1.47
1	A	361	PRO	N-CD	-9.18	1.34	1.47
1	B	129	PRO	N-CD	-8.86	1.35	1.47
1	A	126	PRO	N-CD	-5.20	1.40	1.47
1	A	597	SER	CA-CB	-5.20	1.45	1.52
1	B	531	CYS	CB-SG	-5.15	1.73	1.81
1	B	629	MET	C-O	-5.02	1.13	1.23
1	B	597	SER	CA-CB	-5.01	1.45	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ARG	NE-CZ-NH2	10.27	125.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	CB-CG-CD	-9.19	87.70	111.60
1	B	696	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	B	696	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	A	580	ARG	CG-CD-NE	6.28	124.99	111.80
1	A	396	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	B	174	LYS	CD-CE-NZ	-5.34	99.42	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	GLU	Sidechain
1	A	579	GLN	Sidechain
1	B	198	GLU	Sidechain

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	5766	5744	5744	76	0
1	B	5766	5746	5743	94	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	7	10	10	6	0
4	B	7	10	10	5	0
5	B	80	24	0	14	0
6	A	466	0	0	19	1
6	B	508	0	0	23	1
All	All	12620	11534	11507	184	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (184) 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)
4:B:801:PEG:H11	6:B:1222:HOH:O	1.38	1.20
1:A:380:GLU:OE1	6:A:901:HOH:O	1.65	1.12
1:B:572:GLU:OE1	6:B:902:HOH:O	1.75	1.05
1:A:700:ASP:OD1	6:A:902:HOH:O	1.80	1.00
1:A:337:ARG:NH2	6:A:904:HOH:O	1.92	0.99
1:B:135:TRP:CE3	6:B:1294:HOH:O	2.16	0.97
5:B:806:UW8:O14	6:B:903:HOH:O	1.83	0.95
1:B:282:ASP:OD2	6:B:904:HOH:O	1.86	0.93
1:A:459:PHE:O	1:A:463:VAL:HG22	1.70	0.92
1:A:75:GLU:OE2	6:A:903:HOH:O	1.91	0.88
1:A:623:GLY:N	6:A:906:HOH:O	2.04	0.86
1:B:327:PHE:CE1	1:B:450:LEU:HD11	2.15	0.82
1:B:682:ARG:NH2	6:B:909:HOH:O	2.12	0.80
1:A:591:MET:O	6:A:905:HOH:O	2.01	0.77
1:A:263:MET:HG2	6:A:1118:HOH:O	1.85	0.76
1:A:688:ARG:NH2	1:A:692:GLU:OE1	2.19	0.76
1:B:375:ASP:OD2	6:B:905:HOH:O	2.03	0.75
1:B:327:PHE:CZ	1:B:450:LEU:HD11	2.21	0.74
1:A:88:ARG:HG3	1:A:88:ARG:HH11	1.52	0.74
1:B:557:GLU:OE1	6:B:906:HOH:O	2.05	0.74
1:A:659:LYS:NZ	6:A:914:HOH:O	2.21	0.73
1:B:710:THR:OG1	1:B:713:GLU:HG3	1.89	0.73
1:B:327:PHE:CE1	1:B:450:LEU:HD21	2.24	0.72
1:B:165:ARG:HG3	1:B:165:ARG:HH11	1.53	0.72
1:B:368:LYS:NZ	6:B:918:HOH:O	2.21	0.71
1:B:336:ILE:O	1:B:432:ARG:NH1	2.25	0.69
1:B:206:ASP:OD1	6:B:907:HOH:O	2.11	0.68
1:B:191:GLU:OE2	6:B:908:HOH:O	2.11	0.67
1:B:185:MET:HG3	1:B:208:ILE:HG22	1.76	0.67
1:A:162:ILE:HG21	1:A:192:ILE:HD13	1.77	0.67
1:B:4:VAL:N	6:B:922:HOH:O	2.27	0.67
1:A:681:LEU:HB3	1:A:684:ILE:HD11	1.76	0.66
1:A:60:ASP:OD2	6:A:908:HOH:O	2.13	0.66
1:A:375:ASP:O	1:A:378:SER:OG	2.10	0.65
1:B:327:PHE:HE1	1:B:450:LEU:HD21	1.61	0.65
1:B:476:LYS:HD2	1:B:479:GLU:OE1	1.96	0.65
1:A:583:GLU:OE1	6:A:909:HOH:O	2.15	0.64
1:B:401:ASP:OD2	6:B:910:HOH:O	2.14	0.64
1:B:458:GLU:OE2	6:B:911:HOH:O	2.15	0.64
1:A:494:ARG:NH1	6:A:907:HOH:O	2.05	0.63
1:B:298:GLU:OE2	6:B:912:HOH:O	2.16	0.62
1:A:469:THR:OG1	6:A:910:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HE3	1:A:199:GLU:OE1	2.01	0.60
4:A:804:PEG:H11	4:A:804:PEG:H41	1.84	0.59
1:A:263:MET:CG	6:A:1118:HOH:O	2.46	0.59
5:B:806:UW8:O6	5:B:806:UW8:C1	2.50	0.58
1:A:354:GLU:OE2	6:A:911:HOH:O	2.17	0.58
1:B:605:MET:HE3	1:B:660:PHE:CE1	2.39	0.57
1:A:560:ILE:HD11	1:A:568:GLU:HG3	1.85	0.57
1:B:292:LYS:HE3	1:B:293:ASP:OD2	2.05	0.57
1:A:575:TYR:CZ	1:A:580:ARG:HD3	2.40	0.56
1:A:55:PRO:O	6:A:912:HOH:O	2.17	0.56
1:B:236:ALA:HB3	1:B:239:LEU:HD12	1.87	0.56
1:B:392:ASP:OD2	6:B:913:HOH:O	2.17	0.56
1:B:564:LYS:HE3	6:B:1141:HOH:O	2.05	0.56
1:A:163:ILE:HG22	1:A:189:CYS:HB3	1.88	0.56
1:B:675:LYS:HE3	1:B:704:ASP:OD2	2.06	0.56
1:B:473:ASP:OD1	6:B:914:HOH:O	2.18	0.55
1:B:566:GLN:OE1	1:B:584:ARG:NH1	2.36	0.55
1:B:34:THR:OG1	1:B:263:MET:CE	2.54	0.55
1:B:675:LYS:O	1:B:675:LYS:HD3	2.05	0.55
1:A:262:ASP:OD2	1:A:265:LYS:HD2	2.06	0.55
1:B:89:MET:HE2	1:B:108:ALA:HA	1.89	0.55
1:B:34:THR:OG1	1:B:263:MET:HE1	2.07	0.55
5:B:806:UW8:O6	5:B:806:UW8:O3	2.25	0.54
1:B:49:LYS:NZ	5:B:806:UW8:O15	2.39	0.54
1:B:89:MET:CE	1:B:108:ALA:HA	2.38	0.54
1:B:262:ASP:OD2	6:B:915:HOH:O	2.18	0.54
1:B:309:LEU:HD13	1:B:316:ILE:HD12	1.90	0.54
1:B:669:ARG:CD	1:B:731:LEU:HD11	2.38	0.54
1:B:696:ARG:HG3	1:B:696:ARG:NH2	2.21	0.54
1:A:88:ARG:HG3	1:A:88:ARG:NH1	2.14	0.54
4:A:804:PEG:H31	6:A:943:HOH:O	2.07	0.53
1:B:176:VAL:HG21	1:B:196:LEU:HD11	1.89	0.53
1:B:675:LYS:NZ	6:B:916:HOH:O	2.20	0.53
1:B:445:LYS:NZ	6:B:941:HOH:O	2.39	0.53
1:A:45:ARG:NH1	4:B:801:PEG:O4	2.40	0.52
1:B:217:GLN:HE22	4:B:801:PEG:H32	1.74	0.52
1:A:616:ILE:O	1:A:674:PRO:HD3	2.09	0.52
1:A:352:SER:HA	1:A:387:ILE:O	2.10	0.52
1:B:486:LYS:HE2	1:B:490:GLU:OE2	2.09	0.52
1:B:170:LYS:HD3	1:B:199:GLU:OE2	2.10	0.52
1:B:703:ALA:CB	1:B:714:VAL:HG13	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HE3	1:A:50:TYR:CZ	2.46	0.51
1:A:71:PHE:O	1:A:240:ARG:HB2	2.11	0.51
1:B:732:LEU:O	1:B:732:LEU:HG	2.11	0.51
1:B:301:TYR:OH	6:B:904:HOH:O	2.01	0.50
1:B:165:ARG:HG3	1:B:165:ARG:NH1	2.22	0.50
1:B:327:PHE:CE1	1:B:416:TYR:HB2	2.47	0.50
1:B:682:ARG:HG3	1:B:699:ILE:HD13	1.92	0.50
1:A:45:ARG:NH2	4:B:801:PEG:O4	2.41	0.50
5:B:806:UW8:C4	5:B:806:UW8:O16	2.60	0.49
1:A:447:LEU:O	1:A:451:LEU:HG	2.12	0.49
1:B:459:PHE:O	1:B:463:VAL:HG22	2.13	0.49
1:B:445:LYS:HG3	1:B:446:HIS:N	2.28	0.49
1:A:250:ARG:NH1	1:A:514:SER:O	2.43	0.49
1:A:262:ASP:HB2	4:A:804:PEG:H32	1.95	0.49
1:B:664:ASP:O	1:B:669:ARG:NE	2.42	0.49
1:A:122:LEU:HD23	6:A:912:HOH:O	2.13	0.49
5:B:805:UW8:O17	5:B:805:UW8:C16'	2.56	0.48
1:B:342:HIS:HB2	1:B:435:LYS:HA	1.96	0.48
1:A:684:ILE:HG13	1:A:685:ILE:N	2.29	0.47
1:A:575:TYR:CE1	1:A:580:ARG:HB3	2.49	0.47
1:B:10:ILE:HG12	1:B:10:ILE:O	2.15	0.47
1:B:40:GLU:OE2	6:B:917:HOH:O	2.20	0.47
5:B:806:UW8:O16	5:B:806:UW8:O4	2.32	0.47
1:A:374:PRO:HB2	1:A:378:SER:OG	2.15	0.46
1:B:33:ILE:HG23	1:B:90:ARG:HH12	1.80	0.46
1:B:189:CYS:O	1:B:190:ASP:HB2	2.15	0.46
1:A:362:ASP:OD1	1:A:362:ASP:N	2.45	0.46
1:B:352:SER:HA	1:B:387:ILE:O	2.15	0.46
1:A:423:THR:O	1:A:424:ALA:HB3	2.16	0.46
1:A:681:LEU:O	1:A:684:ILE:HG13	2.15	0.46
5:B:805:UW8:O1	5:B:805:UW8:C18	2.63	0.46
1:B:202:LYS:O	1:B:203:LEU:HD23	2.15	0.46
1:A:263:MET:HE2	1:A:263:MET:HB2	1.86	0.46
1:A:450:LEU:HD22	1:A:451:LEU:HD23	1.97	0.46
1:A:27:GLU:OE2	1:A:289:LYS:HE3	2.17	0.45
1:A:89:MET:CE	1:A:108:ALA:HA	2.46	0.45
1:A:485:ARG:HA	1:A:488:TYR:CD2	2.51	0.45
1:A:608:LEU:HD21	1:A:627:ILE:HB	1.98	0.45
1:A:72:SER:OG	1:A:74:GLU:OE1	2.18	0.45
1:A:263:MET:H	4:A:804:PEG:H41	1.82	0.45
1:A:688:ARG:NH1	1:A:691:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:PHE:HA	1:B:426:ARG:O	2.17	0.45
5:B:805:UW8:O11	5:B:805:UW8:C7	2.64	0.45
1:A:199:GLU:O	6:A:915:HOH:O	2.21	0.45
1:A:346:GLY:CA	1:A:352:SER:HB3	2.47	0.45
1:B:327:PHE:CZ	1:B:416:TYR:HB2	2.51	0.45
1:A:162:ILE:CG2	1:A:192:ILE:HD13	2.45	0.45
1:B:338:LYS:NZ	5:B:805:UW8:O17	2.50	0.45
1:B:423:THR:O	1:B:424:ALA:HB3	2.17	0.45
1:B:605:MET:HE3	1:B:660:PHE:HE1	1.80	0.45
1:A:303:LYS:HD3	1:A:303:LYS:HA	1.66	0.45
1:B:148:GLY:O	1:B:152:VAL:HG13	2.17	0.45
1:B:217:GLN:NE2	4:B:801:PEG:H32	2.32	0.45
1:A:450:LEU:C	1:A:450:LEU:HD23	2.38	0.44
1:A:673:MET:HE2	1:A:678:LYS:HG3	1.98	0.44
1:B:71:PHE:O	1:B:240:ARG:HB2	2.18	0.44
1:B:327:PHE:CE1	1:B:450:LEU:CD1	2.96	0.44
1:A:620:GLU:OE2	6:A:913:HOH:O	2.21	0.44
1:A:678:LYS:HE3	1:A:702:ILE:HB	2.00	0.44
1:B:715:LEU:HB3	1:B:716:PRO:HD3	1.99	0.44
1:A:263:MET:HE2	4:A:804:PEG:H11	1.98	0.44
1:A:450:LEU:CD2	1:A:451:LEU:HD23	2.48	0.43
1:A:673:MET:HE2	1:A:678:LYS:CG	2.48	0.43
4:A:804:PEG:H11	4:A:804:PEG:C4	2.44	0.43
5:B:806:UW8:O19	5:B:806:UW8:C13	2.63	0.43
1:A:346:GLY:HA2	1:A:352:SER:HB3	2.00	0.43
1:B:338:LYS:NZ	5:B:805:UW8:C13	2.81	0.43
1:B:343:VAL:HG22	1:B:344:GLU:N	2.33	0.43
1:B:668:ALA:HB2	1:B:694:LEU:HD11	2.00	0.43
1:B:331:PHE:O	1:B:334:GLU:HG2	2.19	0.43
1:B:366:ASP:HB2	1:B:465:ARG:HG2	2.01	0.42
1:B:578:SER:O	1:B:581:THR:OG1	2.30	0.42
1:A:559:LEU:HD11	1:A:562:PRO:N	2.35	0.42
1:B:244:ARG:HD3	1:B:274:PHE:CZ	2.54	0.42
1:B:263:MET:HB3	1:B:263:MET:HE2	1.77	0.42
1:B:528:VAL:HG22	1:B:529:GLY:N	2.35	0.42
1:B:476:LYS:O	1:B:480:LEU:HG	2.19	0.42
1:B:366:ASP:OD1	1:B:456:LYS:HE2	2.20	0.42
1:B:286:PRO:HB2	1:B:288:ASP:OD1	2.20	0.42
1:B:566:GLN:HB2	1:B:586:ASN:OD1	2.20	0.42
1:A:70:ALA:HB2	1:A:230:LEU:HD11	2.00	0.42
1:A:566:GLN:OE1	1:A:584:ARG:NH1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:806:UW8:O16	5:B:806:UW8:C3	2.67	0.42
1:B:167:LYS:HD3	1:B:301:TYR:CE1	2.54	0.41
1:A:246:TYR:CE2	1:A:250:ARG:HD2	2.56	0.41
1:B:69:ARG:O	1:B:73:GLY:HA2	2.21	0.41
1:B:132:VAL:HG23	1:B:133:PRO:HD2	2.02	0.41
1:A:88:ARG:HH11	1:A:88:ARG:CG	2.26	0.41
1:B:163:ILE:HD12	1:B:255:VAL:HG13	2.01	0.41
1:B:376:ILE:HD12	1:B:438:PHE:HD1	1.86	0.41
1:A:69:ARG:O	1:A:73:GLY:HA2	2.20	0.41
1:A:189:CYS:O	1:A:190:ASP:HB2	2.21	0.41
1:A:572:GLU:O	1:A:576:LYS:HG2	2.21	0.41
1:B:447:LEU:O	1:B:451:LEU:HG	2.21	0.41
1:A:576:LYS:HA	1:A:576:LYS:HD2	1.69	0.41
1:A:585:MET:HE3	1:A:587:LEU:HA	2.03	0.41
1:B:185:MET:HE3	1:B:187:PHE:HZ	1.85	0.41
1:B:338:LYS:NZ	5:B:805:UW8:O15	2.49	0.40
1:B:503:VAL:HG12	1:B:505:THR:H	1.86	0.40
1:A:145:ARG:NH1	1:A:231:MET:HG2	2.35	0.40
1:A:148:GLY:O	1:A:152:VAL:HG13	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1196:HOH:O	6:B:1051:HOH:O[3_455]	2.11	0.09

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%)	710 (98%)	15 (2%)	2 (0%)	41 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	727/734 (99%)	711 (98%)	14 (2%)	2 (0%)	41	41
All	All	1454/1468 (99%)	1421 (98%)	29 (2%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	ALA
1	B	190	ASP
1	A	190	ASP
1	B	424	ALA

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%)	601 (98%)	10 (2%)	62	69
1	B	611/615 (99%)	601 (98%)	10 (2%)	62	69
All	All	1222/1230 (99%)	1202 (98%)	20 (2%)	62	69

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	40	GLU
1	A	128	ASN
1	A	174	LYS
1	A	249	ARG
1	A	257	TYR
1	A	345	PHE
1	A	377	ASP
1	A	585	MET
1	A	601	PHE
1	B	99	PHE
1	B	257	TYR

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Mol	Chain	Res	Type
1	B	274	PHE
1	B	408	ARG
1	B	443	ARG
1	B	487	LYS
1	B	580	ARG
1	B	597	SER
1	B	601	PHE
1	B	669	ARG

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	449	GLN
1	B	306	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
3	SF4	B	804	1	0,12,12	-	-	-		
5	UW8	B	805	-	24,42,42	4.87	8 (33%)	33,72,72	4.64	19 (57%)
5	UW8	B	806	-	24,42,42	5.59	8 (33%)	33,72,72	3.76	17 (51%)
4	PEG	B	801	-	6,6,6	0.51	0	5,5,5	0.37	0
3	SF4	A	803	1	0,12,12	-	-	-		
4	PEG	A	804	-	6,6,6	0.47	0	5,5,5	0.32	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
5	UW8	B	805	-	-	12/18/93/93	0/3/3/3
3	SF4	B	804	1	-	-	0/6/5/5
5	UW8	B	806	-	-	13/18/93/93	0/3/3/3
4	PEG	B	801	-	-	2/4/4/4	-
3	SF4	A	803	1	-	-	0/6/5/5
4	PEG	A	804	-	-	4/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	806	UW8	O15-C13	15.09	1.44	1.28
5	B	806	UW8	O1-C1	15.06	1.44	1.28
5	B	806	UW8	O8-C7	14.69	1.44	1.28
5	B	805	UW8	O1-C1	14.55	1.44	1.28
5	B	805	UW8	O15-C13	13.69	1.43	1.28
5	B	805	UW8	O8-C7	11.07	1.40	1.28
5	B	806	UW8	O9-C8	5.00	1.46	1.41
5	B	806	UW8	O16-C14	4.56	1.45	1.41
5	B	805	UW8	O9-TI1	-2.94	1.83	1.87
5	B	806	UW8	C2-C1	-2.66	1.49	1.54
5	B	805	UW8	C15-C14	-2.51	1.51	1.55
5	B	805	UW8	O16-C14	2.49	1.43	1.41
5	B	806	UW8	O16-TI1	2.37	1.90	1.87
5	B	805	UW8	C11-C8	-2.31	1.51	1.55
5	B	805	UW8	C9-C8	-2.08	1.51	1.55
5	B	806	UW8	C8-C7	-2.06	1.50	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	805	UW8	O16-C14-C15	-13.94	91.43	110.07
5	B	805	UW8	C14-C15-C16'	-12.03	97.53	115.47
5	B	805	UW8	O9-C8-C9	-10.31	96.28	110.07
5	B	806	UW8	O16-C14-C13	-9.54	101.75	107.28
5	B	806	UW8	O2-C2-C1	-9.12	102.00	107.28
5	B	806	UW8	C14-C15-C16'	-8.70	102.50	115.47
5	B	806	UW8	O2-C2-C5	6.14	118.28	110.07
5	B	805	UW8	O8-C7-O10	-6.04	118.48	124.30
5	B	806	UW8	O16-C14-C17	5.92	117.98	110.07
5	B	805	UW8	O15-C13-O17	-5.81	118.70	124.30
5	B	805	UW8	O16-C14-C13	5.70	110.58	107.28
5	B	806	UW8	O2-C2-C3	-5.61	102.56	110.07
5	B	805	UW8	O9-C8-C7	5.49	110.46	107.28
5	B	805	UW8	O2-C2-C3	-4.75	103.72	110.07
5	B	805	UW8	O1-C1-O3	-4.60	119.87	124.30
5	B	806	UW8	C2-C3-C4	-4.01	109.49	115.47
5	B	806	UW8	O15-C13-O17	-3.70	120.73	124.30
5	B	806	UW8	O8-C7-O10	-3.63	120.81	124.30
5	B	806	UW8	C14-C17-C18	3.57	120.79	115.47
5	B	806	UW8	C8-C9-C10	-3.42	110.37	115.47
5	B	805	UW8	O2-C2-C1	-3.37	105.33	107.28
5	B	805	UW8	O10-C7-C8	3.00	130.40	122.41
5	B	805	UW8	O16-C14-C17	2.91	113.96	110.07
5	B	805	UW8	C2-C3-C4	-2.91	111.13	115.47
5	B	805	UW8	O8-C7-C8	-2.83	111.02	113.91
5	B	806	UW8	C3-C2-C1	2.68	117.62	110.52
5	B	806	UW8	O16-C14-C15	-2.45	106.80	110.07
5	B	806	UW8	O1-C1-O3	-2.32	122.06	124.30
5	B	805	UW8	C17-C14-C15	2.28	115.58	109.69
5	B	805	UW8	C15-C14-C13	2.26	116.49	110.52
5	B	806	UW8	O9-C8-C7	-2.17	106.02	107.28
5	B	806	UW8	C5-C2-C1	-2.13	104.88	110.52
5	B	805	UW8	C11-C8-C9	2.13	115.21	109.69
5	B	806	UW8	C8-C11-C12	2.12	118.63	115.47
5	B	805	UW8	O2-C2-C5	2.09	112.86	110.07
5	B	805	UW8	O17-C13-C14	2.05	127.87	122.41

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	805	UW8	O2-C2-C3-C4
5	B	805	UW8	O2-C2-C5-C6

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Mol	Chain	Res	Type	Atoms
5	B	805	UW8	C12-C11-C8-C7
5	B	805	UW8	C12-C11-C8-C9
5	B	805	UW8	C12-C11-C8-O9
5	B	805	UW8	O16-C14-C15-C16'
5	B	806	UW8	O2-C2-C3-C4
5	B	806	UW8	C1-C2-C3-C4
5	B	806	UW8	C7-C8-C9-C10
5	B	806	UW8	C11-C8-C9-C10
5	B	806	UW8	O9-C8-C9-C10
5	B	806	UW8	C12-C11-C8-C7
5	B	806	UW8	C12-C11-C8-C9
5	B	806	UW8	C12-C11-C8-O9
5	B	806	UW8	C13-C14-C15-C16'
5	B	806	UW8	O16-C14-C15-C16'
5	B	805	UW8	C5-C2-C3-C4
5	B	805	UW8	C3-C2-C5-C6
5	B	806	UW8	C5-C2-C3-C4
5	B	806	UW8	C17-C14-C15-C16'
5	B	805	UW8	C1-C2-C3-C4
5	B	805	UW8	C1-C2-C5-C6
4	A	804	PEG	C1-C2-O2-C3
4	B	801	PEG	O2-C3-C4-O4
5	B	805	UW8	C17-C14-C15-C16'
5	B	806	UW8	C1-C2-C5-C6
4	A	804	PEG	O1-C1-C2-O2
5	B	805	UW8	O9-C8-C9-C10
4	A	804	PEG	O2-C3-C4-O4
4	A	804	PEG	C4-C3-O2-C2
4	B	801	PEG	C1-C2-O2-C3

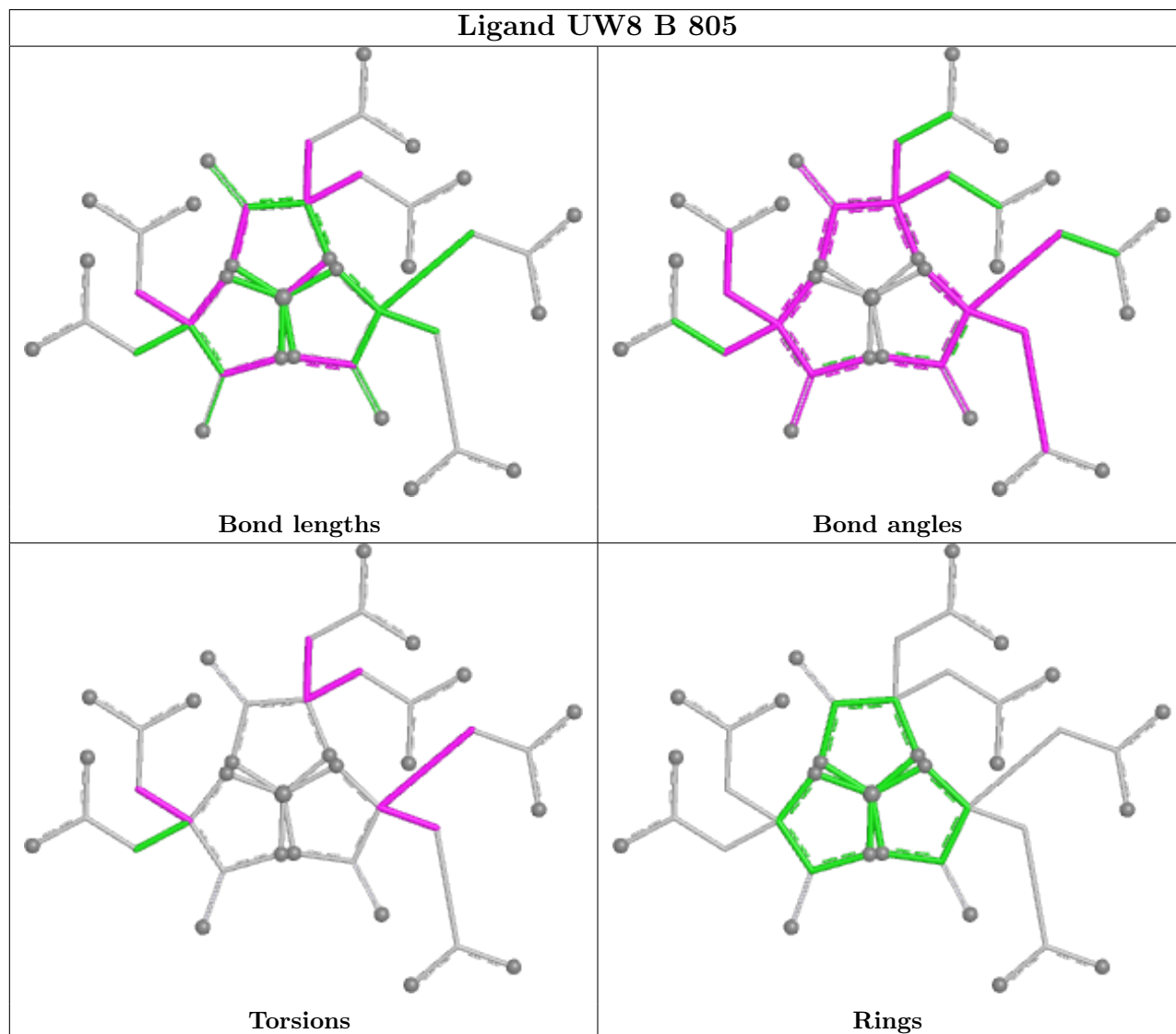
There are no ring outliers.

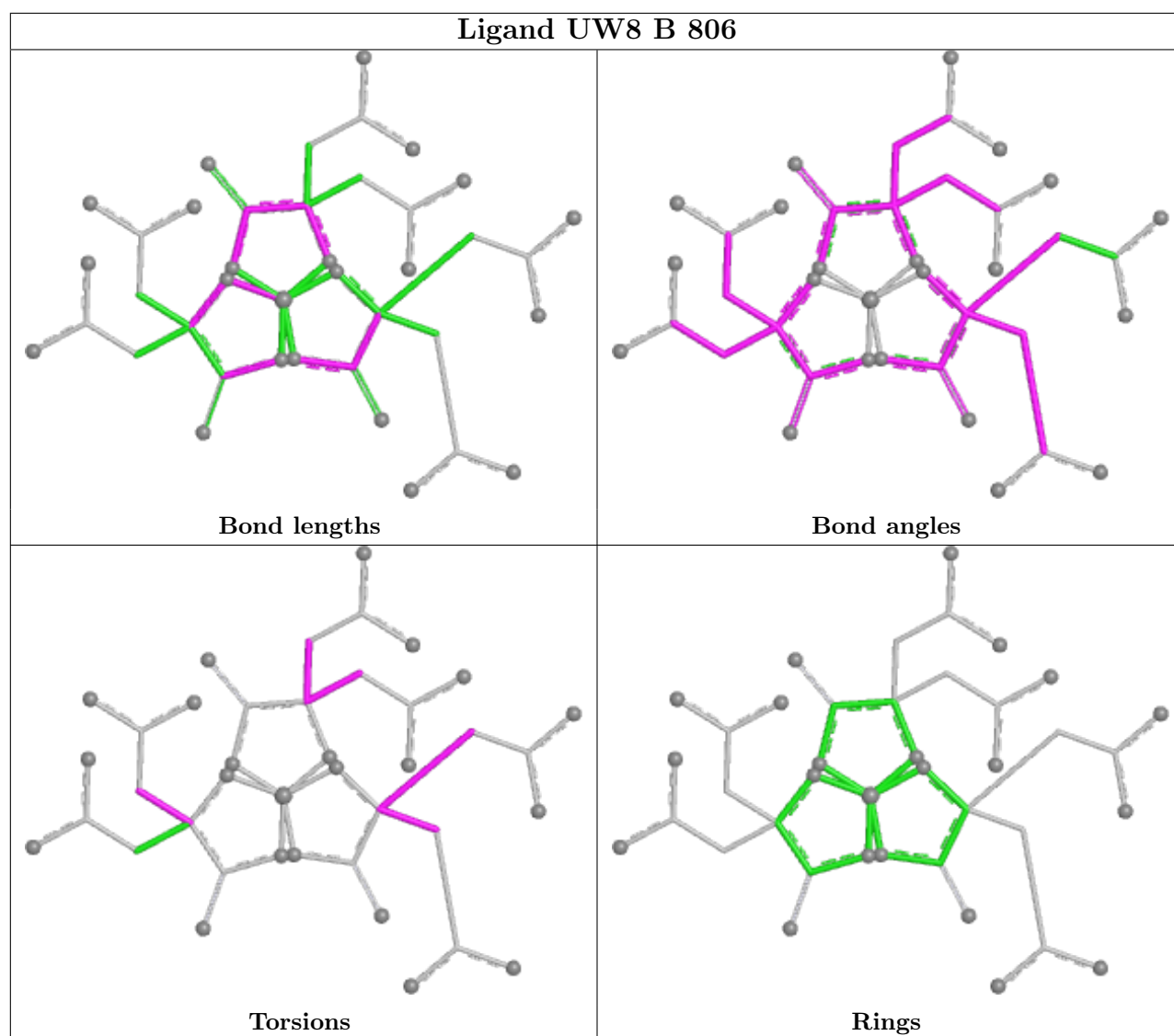
4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	805	UW8	6	0
5	B	806	UW8	8	0
4	B	801	PEG	5	0
4	A	804	PEG	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.23	6 (0%) 86 88	22, 35, 60, 114	0
1	B	729/734 (99%)	-0.14	11 (1%) 73 77	20, 34, 57, 105	0
All	All	1458/1468 (99%)	-0.18	17 (1%) 79 82	20, 34, 59, 114	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	ASP	4.3
1	B	600	CYS	3.6
1	B	480	LEU	3.1
1	A	732	LEU	3.1
1	B	318	SER	3.0
1	B	320	ASP	2.9
1	B	598	CYS	2.6
1	A	126	PRO	2.6
1	A	363	GLU	2.5
1	A	362	ASP	2.3
1	B	601	PHE	2.2
1	B	599	GLY	2.2
1	B	142	PRO	2.2
1	B	232	PHE	2.1
1	B	322	ASP	2.1
1	A	598	CYS	2.1
1	B	327	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](#)

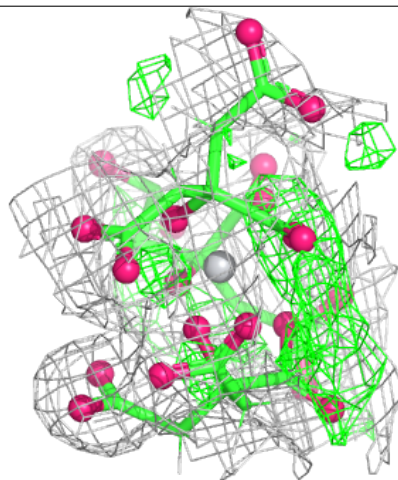
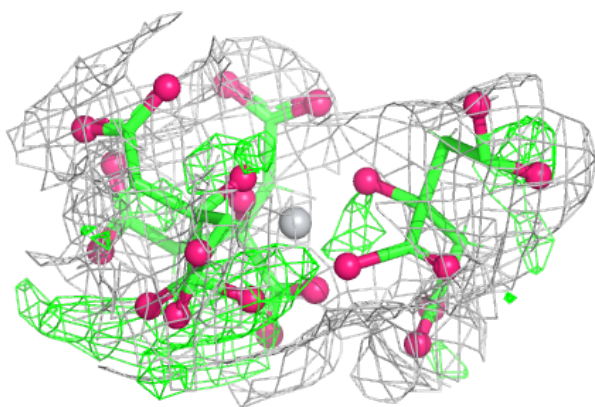
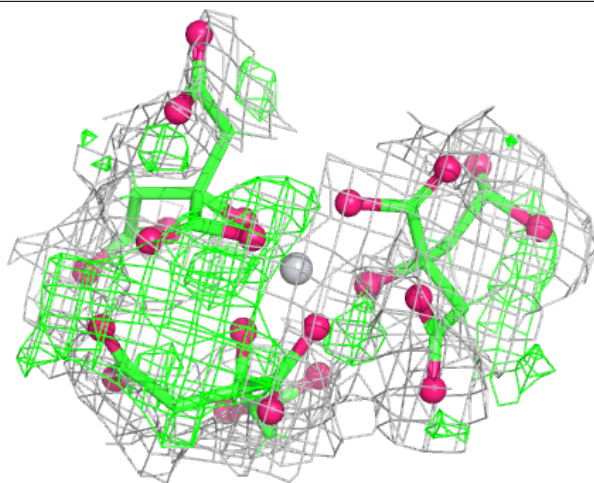
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEG	A	804	7/7	0.73	0.30	41,59,77,77	0
5	UW8	B	805	40/40	0.78	0.18	83,103,127,129	0
5	UW8	B	806	40/40	0.83	0.18	71,99,126,133	0
4	PEG	B	801	7/7	0.84	0.42	32,46,62,62	0
2	NI	A	801	1/1	0.97	0.13	27,27,27,27	0
2	NI	A	802	1/1	0.98	0.20	27,27,27,27	0
2	NI	B	802	1/1	0.98	0.17	29,29,29,29	0
3	SF4	A	803	8/8	0.98	0.15	25,28,30,30	0
3	SF4	B	804	8/8	0.98	0.16	23,27,28,29	0
2	NI	B	803	1/1	0.99	0.17	20,20,20,20	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.

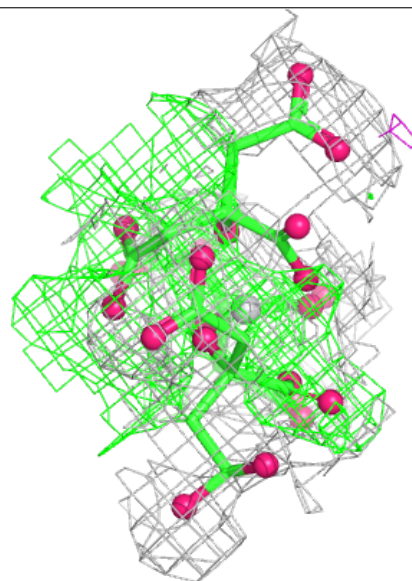
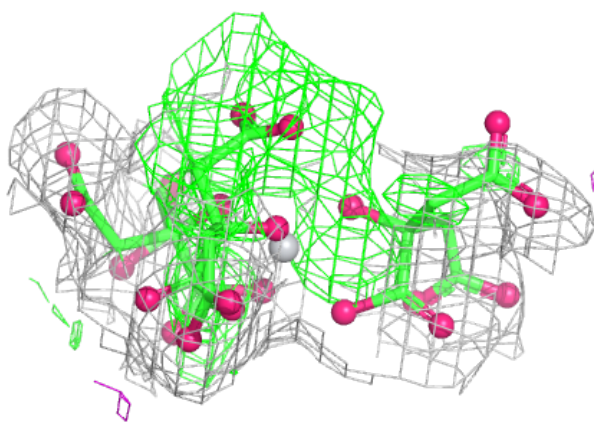
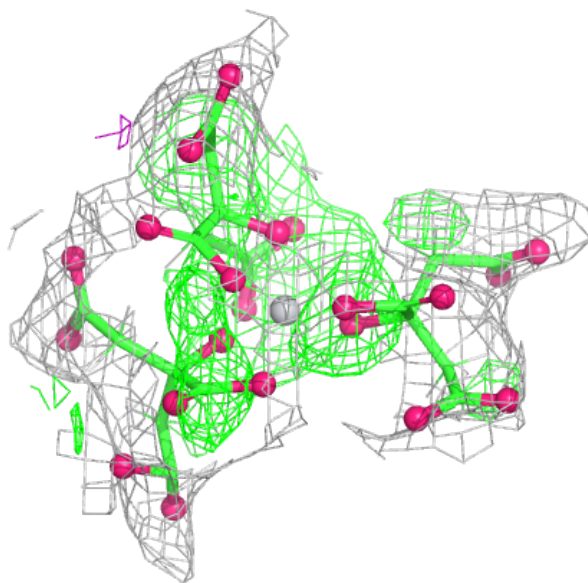
Electron density around UW8 B 805:

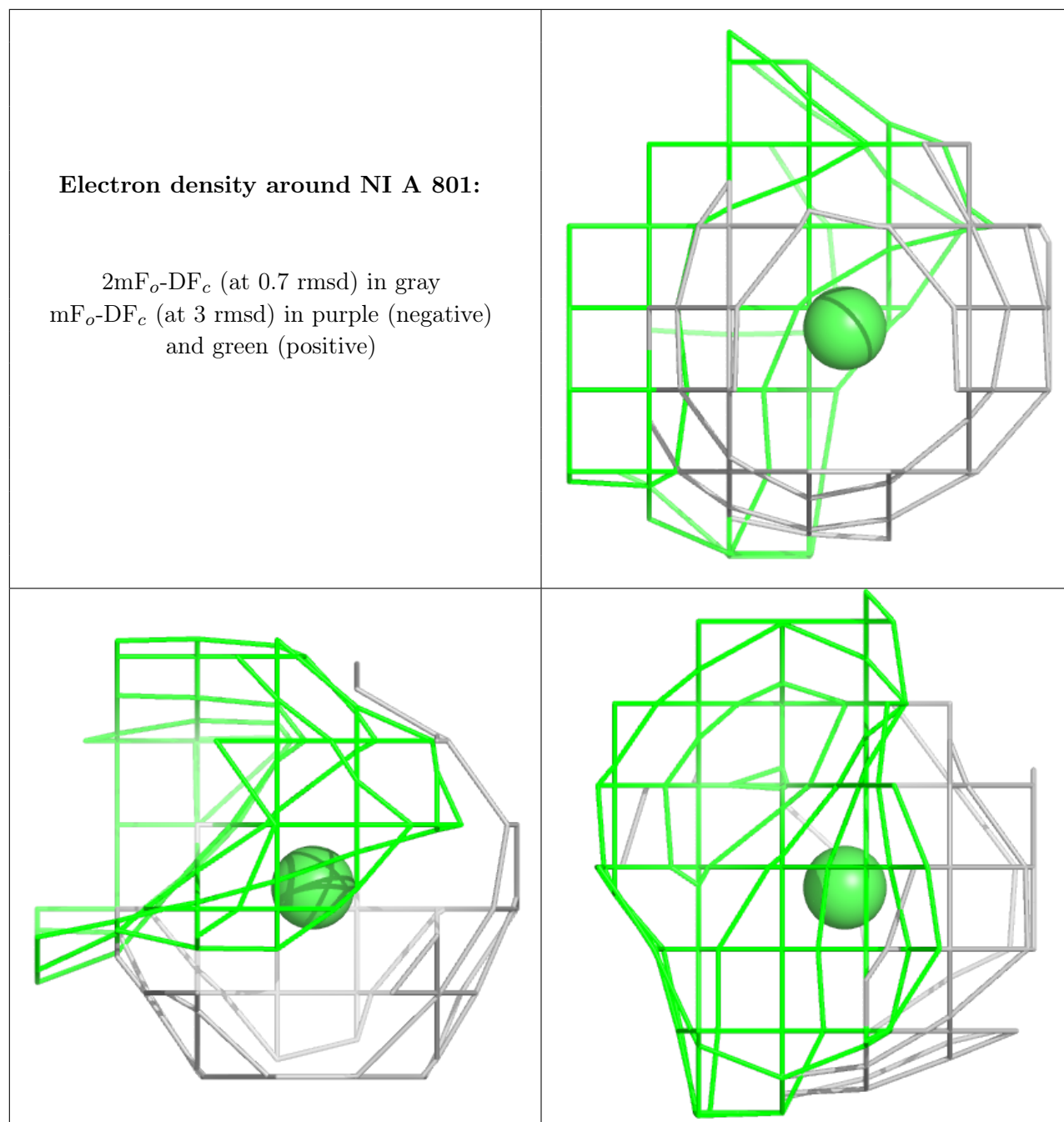
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

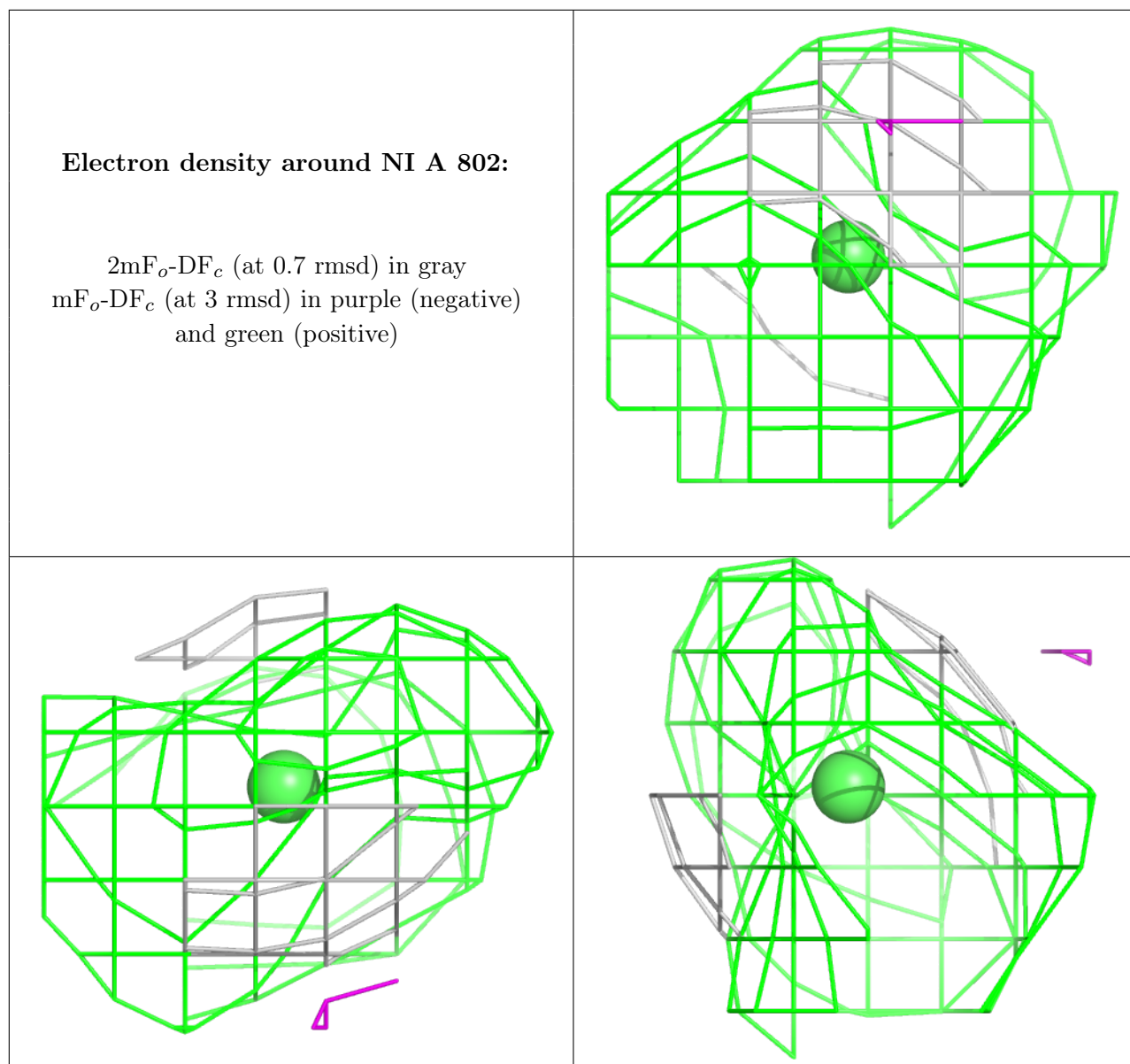


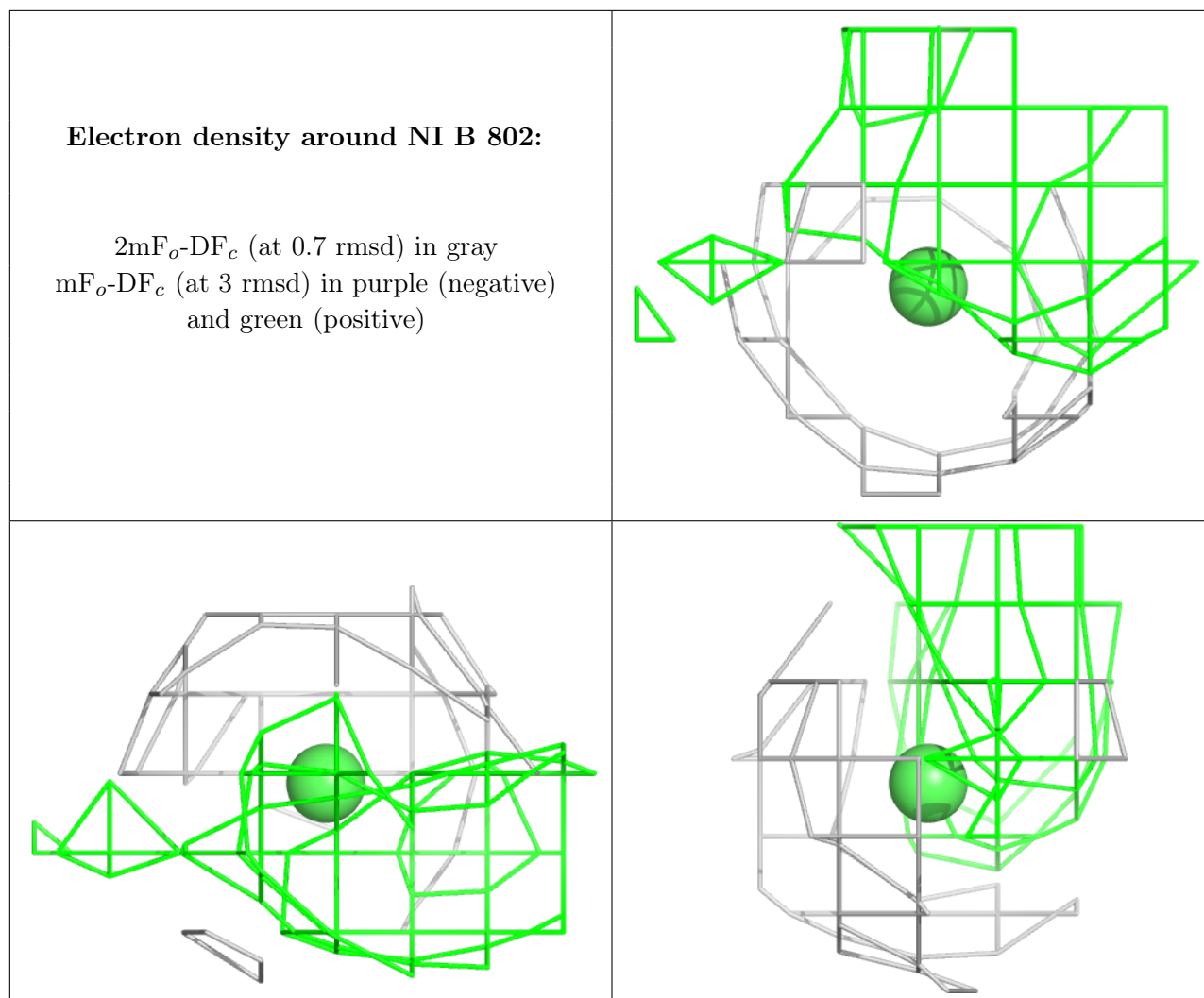
Electron density around UW8 B 806:

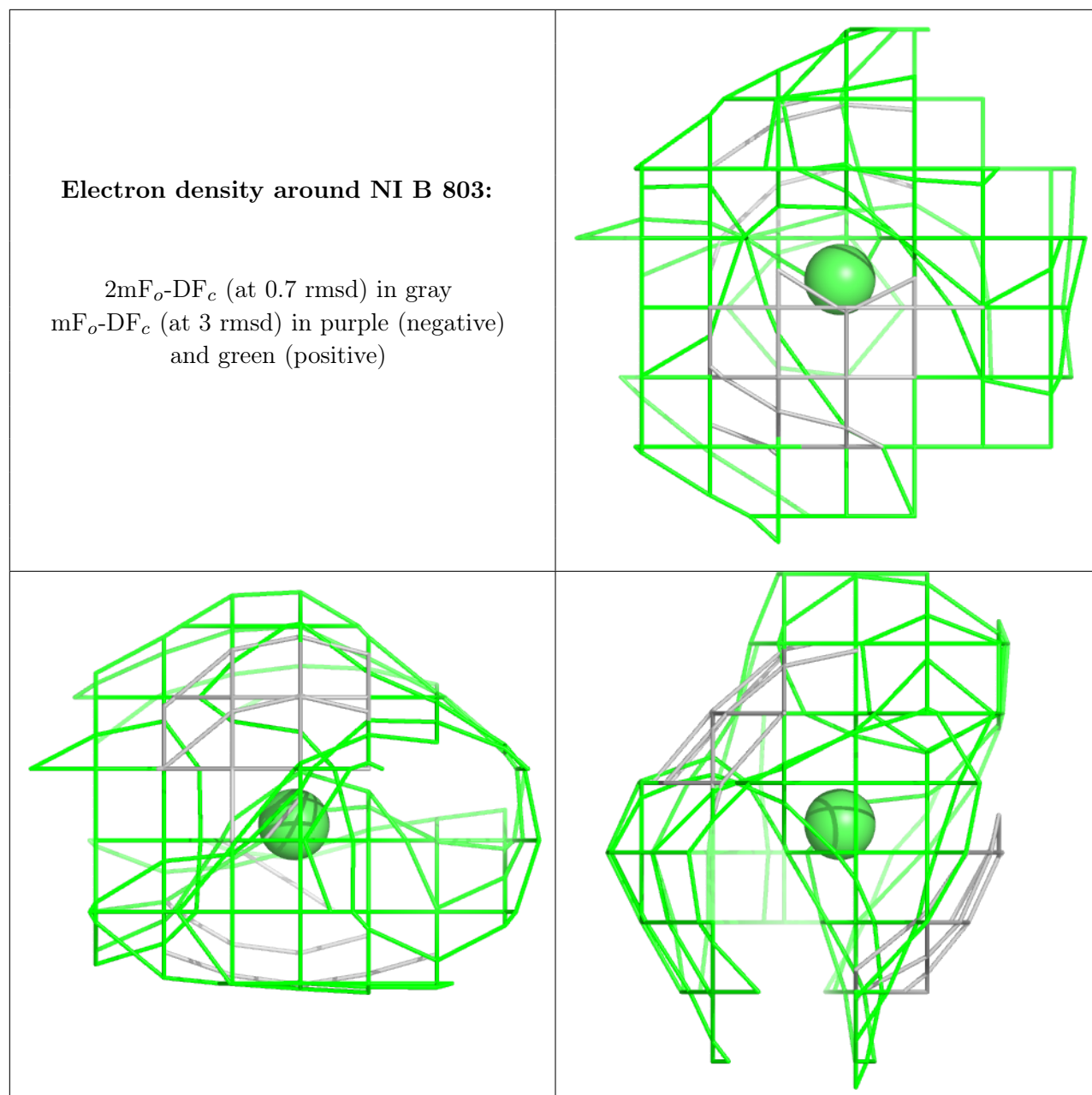
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)











6.5 Other polymers [i](#)

There are no such residues in this entry.