



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:43 PM UTC

PDB ID : 7NZ5 / pdb_00007nz5
Title : monomeric acetyl-CoA synthase with Zn at the proximal position of cluster A
Authors : Kreibich, J.; Jeoung, J.H.; Dobbek, H.
Deposited on : 2021-03-23
Resolution : 1.90 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

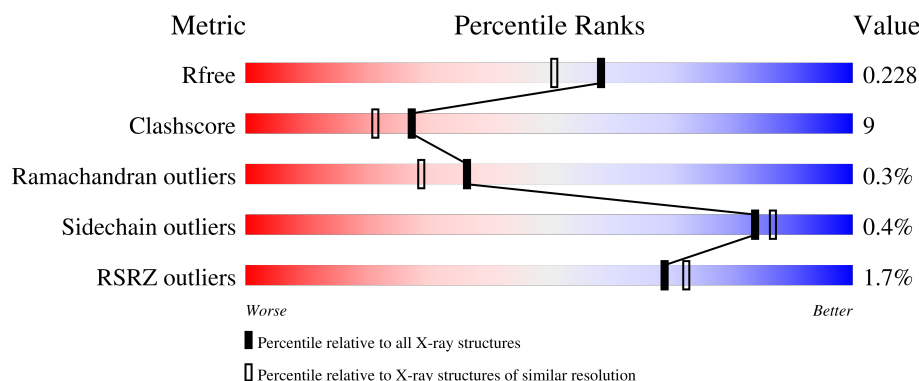
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	733	
1	B	733	

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
5	PEG	A	804	-	-	X	-
5	PEG	A	808	-	-	X	-
5	PEG	A	811	-	-	X	-
5	PEG	B	805	-	-	X	-
6	CIT	B	804	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 24865 atoms, of which 11616 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.

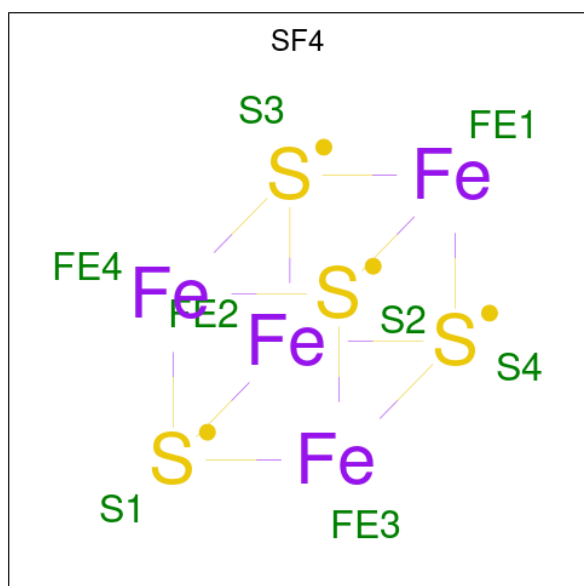
- Molecule 1 is a protein called CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	729	Total	C	H	N	O	S	0	2	0
			11537	3711	5754	967	1076	29			
1	B	729	Total	C	H	N	O	S	0	1	0
			11516	3705	5745	965	1072	29			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

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

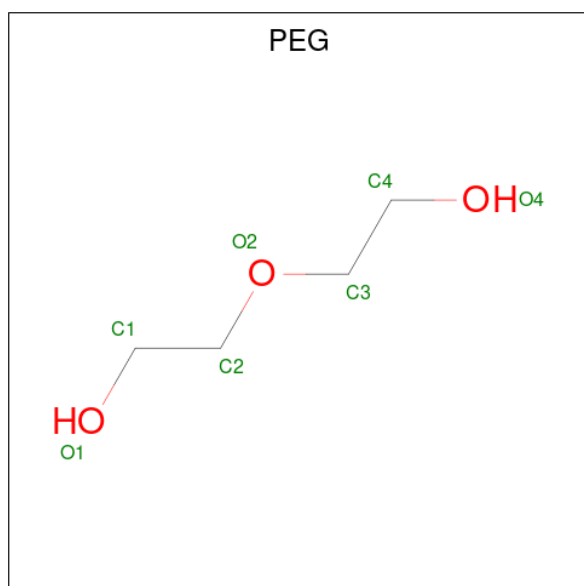
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	B	1	Total	Ni	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



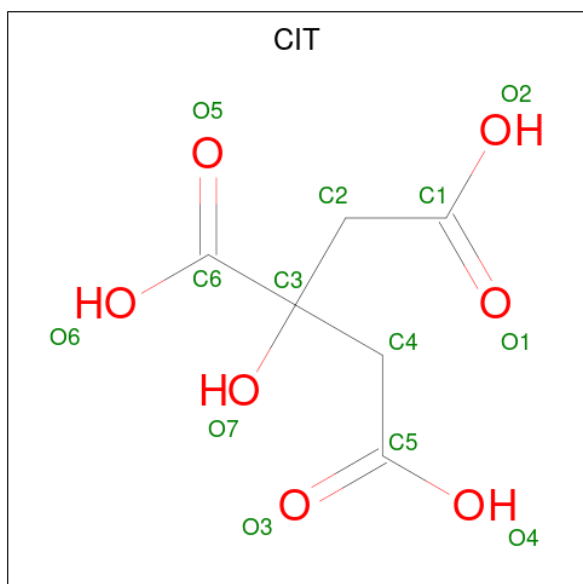
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		

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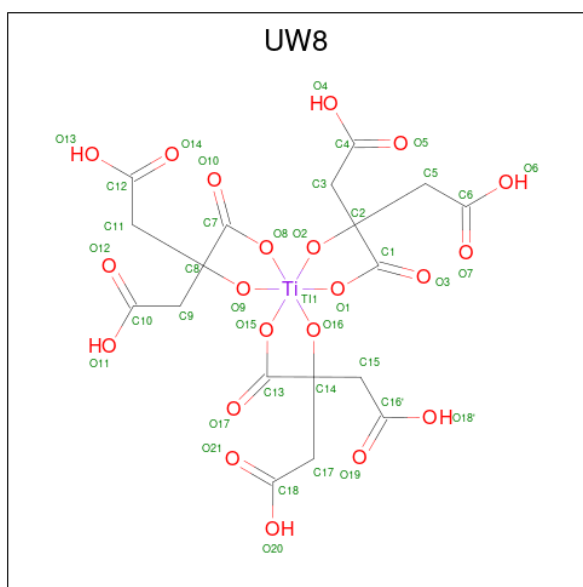
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



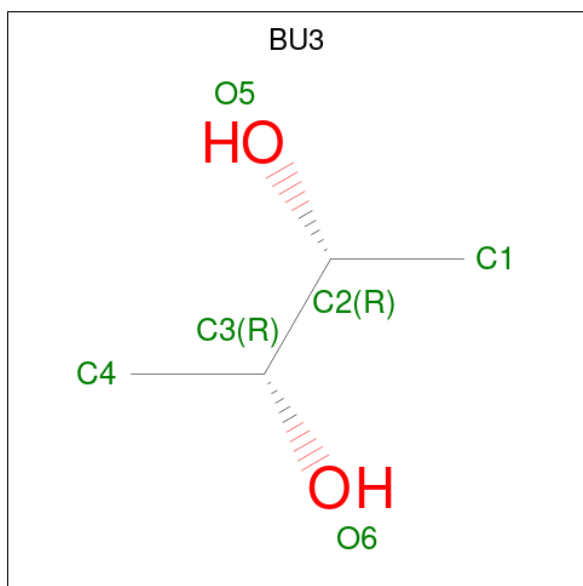
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			18	6	5	7		
6	A	1	Total	C	H	O	0	0
			18	6	5	7		
6	B	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 7 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 $\{5\}$.4 $\{5\}$]tridecan-3-yl]ethanoic acid (CCD ID: UW8) (formula: $C_{18}H_{18}O_{21}Ti$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	O	Ti	0	0
			49	17	12	19	1		

- Molecule 8 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			16	4	10	2		
8	A	1	Total	C	H	O	0	0
			16	4	10	2		

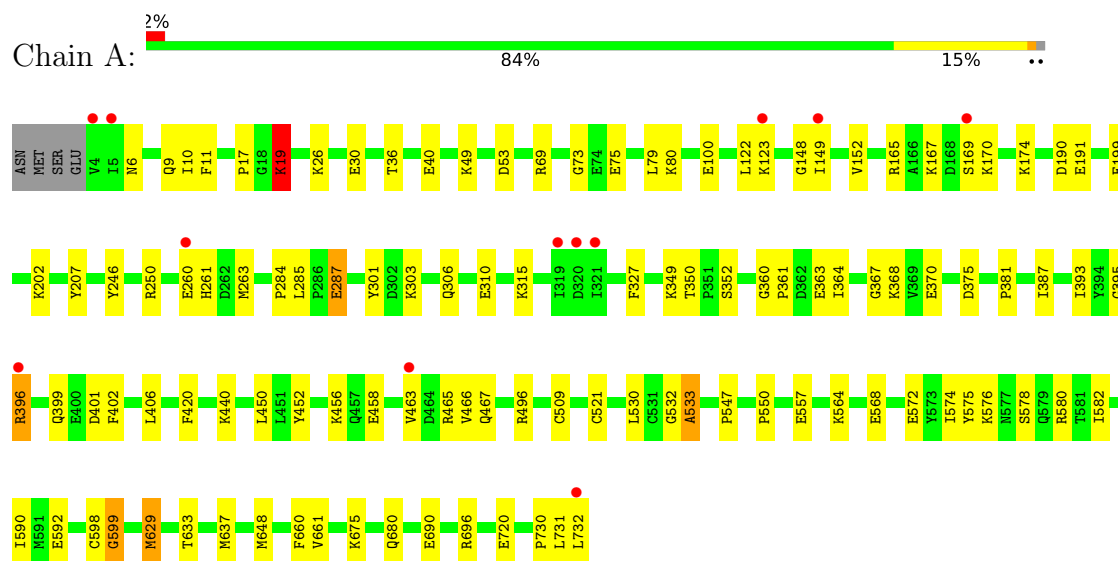
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	803	Total 803	O 803	0	0
9	B	735	Total 735	O 735	0	0

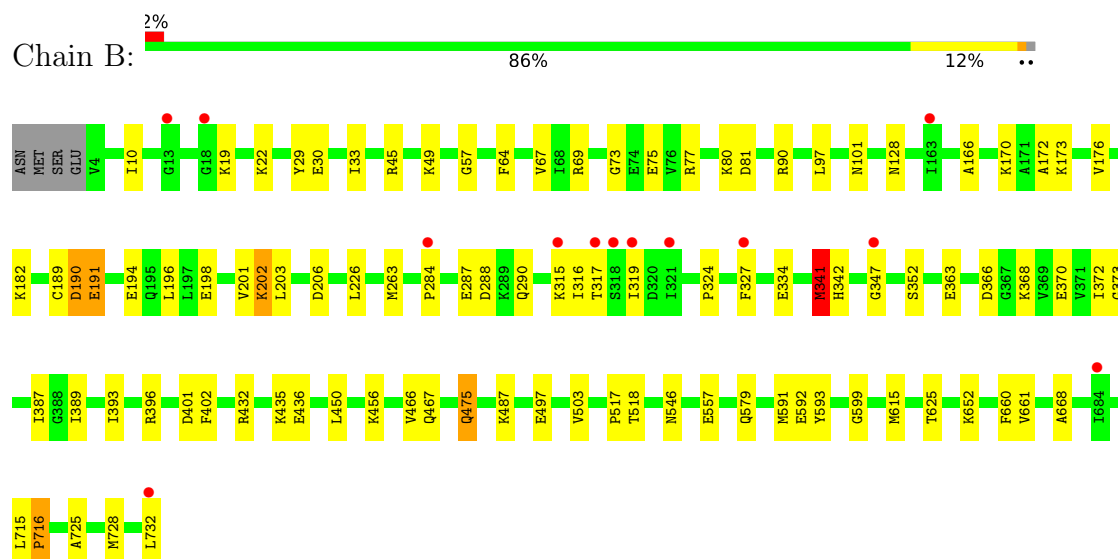
3 Residue-property plots [i](#)

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



- 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	69.25Å 98.81Å 238.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 1.90 46.19 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.0 (46.19-1.90) 88.0 (46.19-1.90)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.193 , 0.224 0.200 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24865	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: BU3, CIT, SF4, UW8, PEG, ZN, NI

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	0.64	12/5917 (0.2%)	0.72	13/8011 (0.2%)
1	B	0.52	11/5908 (0.2%)	0.64	5/7999 (0.1%)
All	All	0.58	23/11825 (0.2%)	0.68	18/16010 (0.1%)

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	1
1	B	0	2
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	PRO	N-CD	-15.52	1.26	1.47
1	B	716	PRO	N-CD	-15.12	1.26	1.47
1	B	128	ASN	C-N	14.55	1.50	1.33
1	A	19	LYS	CE-NZ	13.27	1.89	1.49
1	A	17	PRO	N-CD	11.89	1.64	1.47
1	A	350	THR	C-N	11.49	1.49	1.33
1	A	284	PRO	N-CD	-11.02	1.32	1.47
1	B	324	PRO	N-CD	-9.02	1.35	1.47
1	B	202	LYS	C-O	-7.48	1.15	1.24
1	A	629	MET	C-O	-7.15	1.15	1.23
1	A	260	GLU	C-O	-6.35	1.16	1.23
1	B	503	VAL	C-O	-6.23	1.17	1.24
1	B	191	GLU	CD-OE2	-6.23	1.13	1.25
1	A	285	LEU	C-O	-6.09	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	475	GLN	CB-CG	5.94	1.70	1.52
1	A	261	HIS	C-O	-5.94	1.16	1.23
1	B	201	VAL	C-O	-5.59	1.17	1.24
1	A	530	LEU	C-O	-5.56	1.17	1.24
1	A	533	ALA	C-O	-5.42	1.16	1.24
1	A	532	GLY	C-O	-5.34	1.16	1.24
1	B	203	LEU	C-O	-5.20	1.17	1.23
1	B	206	ASP	C-O	-5.14	1.17	1.24
1	B	284	PRO	N-CD	-5.02	1.40	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	LYS	CG-CD-CE	14.20	143.97	111.30
1	A	350	THR	O-C-N	-10.55	113.32	121.55
1	A	19	LYS	CD-CE-NZ	-8.89	83.47	111.90
1	B	128	ASN	CA-C-N	7.05	127.22	120.31
1	B	128	ASN	C-N-CA	7.05	127.22	120.31
1	A	350	THR	CA-C-N	6.42	126.39	119.78
1	A	350	THR	C-N-CA	6.42	126.39	119.78
1	A	599	GLY	CA-C-N	6.27	132.88	122.54
1	A	599	GLY	C-N-CA	6.27	132.88	122.54
1	A	396	ARG	N-CA-C	-6.01	104.73	111.28
1	A	19	LYS	O-C-N	-5.93	114.61	122.20
1	A	509	CYS	N-CA-CB	5.37	119.53	110.77
1	B	503	VAL	N-CA-CB	-5.33	101.34	111.21
1	B	128	ASN	O-C-N	-5.27	116.96	121.23
1	B	341	MET	CG-SD-CE	-5.25	89.35	100.90
1	A	395	GLY	CA-C-N	5.08	127.09	120.28
1	A	395	GLY	C-N-CA	5.08	127.09	120.28
1	A	287	GLU	CB-CG-CD	5.06	121.21	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	LYS	Mainchain
1	B	475	GLN	Sidechain,Mainchain

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	5783	5754	5752	100	32
1	B	5771	5745	5748	92	3
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	42	60	59	20	0
5	B	7	10	10	4	0
6	A	26	10	10	5	0
6	B	13	5	5	2	0
7	A	37	12	0	8	0
8	A	12	20	20	2	0
9	A	803	0	0	36	4
9	B	735	0	0	38	6
All	All	13249	11616	11604	212	38

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 9.

All (212) 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:19:LYS:CE	1:A:19:LYS:NZ	1.89	1.36
1:B:327:PHE:CE2	1:B:450:LEU:HD11	1.71	1.24
1:A:30:GLU:HG2	1:A:263:MET:CE	1.69	1.22
1:B:30:GLU:OE1	1:B:263:MET:HE1	1.41	1.19
1:A:149:ILE:HG22	9:A:1002:HOH:O	1.42	1.17
1:A:30:GLU:OE2	9:A:902:HOH:O	1.62	1.17
1:A:568:GLU:OE2	9:A:903:HOH:O	1.62	1.15
1:A:732:LEU:O	9:A:904:HOH:O	1.62	1.14
6:A:805:CIT:H42	9:A:1075:HOH:O	1.53	1.08
1:A:174:LYS:HZ3	5:A:811:PEG:H32	1.03	1.08
1:A:174:LYS:HZ3	5:A:811:PEG:C3	1.70	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LYS:NZ	5:A:811:PEG:C3	2.23	1.02
1:A:30:GLU:CG	1:A:263:MET:HE3	1.90	1.01
1:A:174:LYS:NZ	5:A:811:PEG:H32	1.76	0.99
1:A:287:GLU:HG3	9:A:1152:HOH:O	1.63	0.98
7:A:810:UW8:O3	9:A:905:HOH:O	1.83	0.95
1:A:675:LYS:NZ	9:A:906:HOH:O	2.00	0.94
1:A:30:GLU:HG2	1:A:263:MET:HE3	0.94	0.93
1:B:194:GLU:OE2	1:B:194:GLU:N	2.02	0.92
1:B:191:GLU:OE1	9:B:902:HOH:O	1.85	0.92
1:A:19:LYS:NZ	1:A:19:LYS:HD2	1.87	0.89
1:A:629:MET:HE1	1:A:637:MET:SD	2.13	0.89
1:A:49:LYS:NZ	7:A:810:UW8:O15	2.05	0.89
1:A:19:LYS:NZ	1:A:19:LYS:CD	2.36	0.88
1:B:327:PHE:CE2	1:B:450:LEU:CD1	2.57	0.88
1:B:327:PHE:HE2	1:B:450:LEU:HD11	1.37	0.88
1:A:360:GLY:N	1:A:363:GLU:OE1	2.08	0.87
5:B:805:PEG:C3	9:B:1069:HOH:O	2.25	0.84
1:A:174:LYS:NZ	5:A:811:PEG:H31	1.90	0.84
1:B:557:GLU:OE1	9:B:904:HOH:O	1.98	0.82
1:A:36:THR:O	1:A:40[B]:GLU:HG3	1.79	0.82
5:A:804:PEG:H42	9:A:909:HOH:O	1.79	0.82
1:B:373:GLY:O	9:B:903:HOH:O	1.97	0.82
1:A:169:SER:OG	1:A:199:GLU:OE2	1.98	0.81
1:B:732:LEU:HA	9:B:1053:HOH:O	1.81	0.81
5:A:804:PEG:C4	9:A:909:HOH:O	2.27	0.80
1:B:22:LYS:HD2	1:B:97:LEU:HD12	1.63	0.80
1:B:592:GLU:OE1	9:B:906:HOH:O	1.99	0.80
1:B:363:GLU:OE2	9:B:905:HOH:O	1.99	0.79
1:B:732:LEU:HB2	9:B:1053:HOH:O	1.83	0.79
1:B:732:LEU:CA	9:B:1053:HOH:O	2.29	0.78
1:B:30:GLU:CD	1:B:263:MET:HE1	2.08	0.78
5:B:805:PEG:O1	9:B:907:HOH:O	2.01	0.77
1:B:288:ASP:OD2	9:B:908:HOH:O	2.02	0.77
1:A:30:GLU:OE2	9:A:907:HOH:O	2.02	0.77
5:B:805:PEG:H31	9:B:1069:HOH:O	1.85	0.76
1:B:436:GLU:HG3	9:B:1253:HOH:O	1.83	0.76
1:B:347:GLY:O	9:B:909:HOH:O	2.04	0.75
1:A:533:ALA:HA	5:A:808:PEG:H31	1.68	0.74
1:B:334:GLU:OE1	9:B:910:HOH:O	2.05	0.74
1:B:370:GLU:OE1	1:B:372:ILE:HD11	1.88	0.74
1:A:368:LYS:HD3	1:A:467:GLN:NE2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:LYS:HE2	9:B:928:HOH:O	1.88	0.72
1:B:170:LYS:O	9:B:912:HOH:O	2.08	0.71
1:A:368:LYS:HD3	1:A:467:GLN:HE21	1.56	0.71
1:A:174:LYS:HZ1	5:A:811:PEG:H31	1.53	0.71
1:B:334:GLU:OE2	9:B:913:HOH:O	2.08	0.70
5:A:804:PEG:O4	9:A:909:HOH:O	2.09	0.70
1:A:26:LYS:HG2	9:B:1404:HOH:O	1.91	0.70
1:A:303:LYS:HD2	9:A:951:HOH:O	1.92	0.70
1:A:557:GLU:OE1	9:A:910:HOH:O	2.09	0.69
1:A:327:PHE:CE2	1:A:450:LEU:HD11	2.27	0.69
1:A:202:LYS:HD3	1:A:207:TYR:CE1	2.28	0.68
1:A:375:ASP:OD2	9:A:911:HOH:O	2.11	0.68
1:A:533:ALA:HB2	5:A:808:PEG:H41	1.76	0.68
1:B:57:GLY:O	9:B:914:HOH:O	2.11	0.67
6:B:804:CIT:O2	6:B:804:CIT:O7	2.10	0.67
1:A:174:LYS:HZ1	5:A:811:PEG:C3	2.06	0.67
1:A:40[B]:GLU:OE2	9:A:912:HOH:O	2.12	0.66
1:B:202:LYS:HE2	9:B:1203:HOH:O	1.95	0.66
1:A:75:GLU:OE1	9:A:913:HOH:O	2.13	0.66
1:B:29:TYR:CE1	1:B:33:ILE:HD11	2.30	0.66
1:A:303:LYS:HA	1:A:303:LYS:HE3	1.78	0.65
1:B:327:PHE:CD2	1:B:450:LEU:HD11	2.31	0.65
1:A:629:MET:HE3	1:A:633:THR:HG22	1.79	0.64
1:A:452:TYR:CZ	1:A:456:LYS:HD2	2.32	0.64
5:A:804:PEG:H11	5:A:804:PEG:H41	1.80	0.64
1:A:533:ALA:HA	5:A:808:PEG:C3	2.27	0.64
1:B:101:ASN:OD1	9:B:915:HOH:O	2.14	0.64
1:B:19:LYS:HE3	1:B:19:LYS:HA	1.78	0.64
1:A:361:PRO:O	1:A:465:ARG:NH1	2.31	0.63
1:A:572:GLU:OE2	6:A:805:CIT:O5	2.17	0.63
5:B:805:PEG:H32	9:B:1069:HOH:O	1.95	0.63
1:A:590:ILE:HG22	1:A:648:MET:HE2	1.82	0.62
1:B:19:LYS:HA	1:B:19:LYS:CE	2.30	0.62
1:A:100:GLU:HG3	9:A:1418:HOH:O	2.00	0.61
1:B:194:GLU:H	1:B:194:GLU:CD	2.03	0.61
1:A:49:LYS:NZ	7:A:810:UW8:O1	2.35	0.60
1:A:440:LYS:NZ	8:A:812:BU3:H42	2.18	0.59
1:B:368:LYS:HD2	1:B:467:GLN:NE2	2.16	0.59
1:A:19:LYS:HD2	1:A:19:LYS:HZ2	1.65	0.58
1:A:458:GLU:OE2	9:A:915:HOH:O	2.17	0.58
1:A:263:MET:HE1	1:B:90:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ALA:HB2	5:A:808:PEG:C4	2.33	0.57
1:B:341:MET:HG3	1:B:432:ARG:CZ	2.34	0.57
1:A:53:ASP:OD1	1:A:80:LYS:HE3	2.04	0.57
1:B:10:ILE:HG23	9:B:1393:HOH:O	2.03	0.57
1:A:170:LYS:HA	1:A:170:LYS:HE2	1.86	0.57
1:A:720:GLU:OE2	9:A:916:HOH:O	2.17	0.57
1:B:327:PHE:O	9:B:916:HOH:O	2.17	0.57
1:B:393:ILE:HD13	1:B:466:VAL:HG22	1.87	0.57
1:A:30:GLU:CG	1:A:263:MET:CE	2.62	0.57
1:B:287:GLU:HA	1:B:290:GLN:HE21	1.70	0.57
1:B:725:ALA:HA	1:B:728:MET:HE3	1.86	0.56
1:A:303:LYS:HE3	1:A:303:LYS:CA	2.35	0.56
1:B:327:PHE:CD2	1:B:450:LEU:CD1	2.87	0.56
1:B:615:MET:HE1	1:B:625:THR:CB	2.36	0.56
1:A:440:LYS:HZ3	8:A:812:BU3:H42	1.71	0.56
5:A:804:PEG:O1	9:A:917:HOH:O	2.18	0.56
1:A:10:ILE:HD11	1:A:11:PHE:CZ	2.41	0.56
1:B:546:ASN:ND2	9:B:931:HOH:O	2.37	0.56
1:B:30:GLU:CD	1:B:263:MET:CE	2.79	0.55
7:A:810:UW8:C16'	1:B:49:LYS:HD2	2.35	0.55
1:B:22:LYS:HD2	1:B:97:LEU:CD1	2.36	0.55
1:B:389:ILE:HD12	9:B:1112:HOH:O	2.07	0.54
1:A:352:SER:HA	1:A:387:ILE:O	2.08	0.54
1:B:80:LYS:HG2	1:B:81:ASP:N	2.23	0.54
1:B:202:LYS:HD2	1:B:202:LYS:N	2.22	0.54
5:A:804:PEG:H41	5:A:804:PEG:C1	2.38	0.54
1:A:590:ILE:HG22	1:A:648:MET:CE	2.38	0.53
1:B:668:ALA:HB1	1:B:728:MET:HE1	1.90	0.52
1:A:165:ARG:HD2	1:A:191:GLU:OE1	2.10	0.52
1:B:487:LYS:NZ	9:B:933:HOH:O	2.39	0.52
1:A:303:LYS:CE	9:A:951:HOH:O	2.58	0.51
1:B:518:THR:HG22	1:B:579:GLN:NE2	2.25	0.51
1:A:730:PRO:HB2	1:A:732:LEU:HD23	1.93	0.51
1:B:652:LYS:HE3	9:B:1118:HOH:O	2.11	0.51
1:A:6:ASN:O	1:A:9:GLN:HG2	2.11	0.50
1:A:401[B]:ASP:OD2	9:A:918:HOH:O	2.19	0.50
1:A:731:LEU:O	1:A:732:LEU:C	2.54	0.50
1:B:327:PHE:CD1	1:B:327:PHE:C	2.89	0.50
6:A:805:CIT:H22	9:A:1075:HOH:O	2.11	0.49
1:B:352:SER:HA	1:B:387:ILE:O	2.12	0.49
1:B:30:GLU:HG2	1:B:263:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLN:HG3	1:A:310:GLU:OE2	2.13	0.49
1:B:518:THR:HA	1:B:579:GLN:HE22	1.78	0.49
1:A:463:VAL:CG1	1:A:466:VAL:CG2	2.90	0.49
1:B:396:ARG:NE	9:B:948:HOH:O	2.46	0.49
1:A:399:GLN:HB2	1:A:401[B]:ASP:OD1	2.12	0.48
1:B:518:THR:HG22	1:B:579:GLN:HE21	1.78	0.48
1:B:715:LEU:N	1:B:716:PRO:HD2	2.28	0.48
6:A:805:CIT:O4	6:A:805:CIT:O7	2.31	0.48
1:A:401[B]:ASP:OD1	1:A:402:PHE:N	2.46	0.48
1:A:452:TYR:CE2	1:A:456:LYS:HE2	2.49	0.48
1:B:317:THR:HG23	1:B:317:THR:O	2.13	0.48
1:A:420:PHE:O	9:A:919:HOH:O	2.20	0.47
1:A:496:ARG:HD3	9:A:1498:HOH:O	2.13	0.47
1:A:680:GLN:NE2	9:A:947:HOH:O	2.44	0.47
1:B:77:ARG:NH1	9:B:919:HOH:O	2.23	0.47
1:B:173:LYS:NZ	9:B:952:HOH:O	2.47	0.47
1:A:246:TYR:CE2	1:A:250:ARG:HD2	2.50	0.47
5:A:807:PEG:H22	9:A:969:HOH:O	2.15	0.47
1:A:564:LYS:NZ	1:A:592:GLU:OE2	2.47	0.46
1:B:69:ARG:O	1:B:73:GLY:HA2	2.14	0.46
1:A:30:GLU:HG2	1:A:263:MET:SD	2.55	0.46
1:A:572:GLU:O	1:A:576:LYS:HG3	2.16	0.46
1:A:550:PRO:HD2	9:A:1390:HOH:O	2.14	0.46
1:B:315:LYS:HG2	9:B:1132:HOH:O	2.16	0.45
1:A:367:GLY:HA2	1:A:452:TYR:CE2	2.52	0.45
1:A:690:GLU:OE1	1:A:696:ARG:HD2	2.17	0.45
5:A:804:PEG:C4	5:A:804:PEG:H11	2.41	0.45
1:A:315:LYS:HA	1:A:315:LYS:CE	2.46	0.45
7:A:810:UW8:C15	1:B:49:LYS:HD2	2.46	0.45
1:B:341:MET:C	1:B:341:MET:HE2	2.42	0.45
1:A:364:ILE:HG13	1:A:467:GLN:HB2	1.99	0.45
1:B:182:LYS:HB3	1:B:316:ILE:CD1	2.46	0.45
1:A:79:LEU:HD21	1:A:122:LEU:HD11	1.98	0.45
1:A:69:ARG:O	1:A:73:GLY:HA2	2.17	0.45
1:B:591:MET:HE3	9:B:981:HOH:O	2.17	0.45
1:B:366:ASP:OD1	1:B:456:LYS:NZ	2.43	0.44
7:A:810:UW8:O18'	1:B:49:LYS:HD2	2.18	0.44
1:B:668:ALA:CB	1:B:728:MET:HE1	2.47	0.44
1:B:67:VAL:HG22	1:B:226:LEU:HD12	2.00	0.44
5:A:807:PEG:C2	9:A:969:HOH:O	2.65	0.44
7:A:810:UW8:O18'	1:B:49:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PHE:C	1:A:327:PHE:CD1	2.96	0.43
1:B:191:GLU:HB3	9:B:1310:HOH:O	2.18	0.43
1:A:575:TYR:HA	1:A:582:ILE:O	2.18	0.43
6:B:804:CIT:H42	9:B:927:HOH:O	2.18	0.43
6:A:805:CIT:H42	9:A:999:HOH:O	2.17	0.43
7:A:810:UW8:O7	7:A:810:UW8:C1	2.64	0.43
1:B:615:MET:HE1	1:B:625:THR:OG1	2.19	0.43
1:A:547:PRO:HG3	9:A:1387:HOH:O	2.18	0.42
1:B:80:LYS:HD3	9:B:1073:HOH:O	2.19	0.42
1:A:660:PHE:O	1:A:661:VAL:C	2.61	0.42
1:B:189:CYS:O	1:B:190:ASP:HB2	2.19	0.42
1:A:574:ILE:O	1:A:578:SER:HB3	2.19	0.42
1:B:176:VAL:HG21	1:B:196:LEU:HD21	2.01	0.42
1:B:341:MET:HE2	1:B:341:MET:HB3	1.71	0.42
1:A:315:LYS:HA	1:A:315:LYS:HE2	2.01	0.42
1:A:149:ILE:CG2	9:A:1002:HOH:O	2.25	0.41
1:A:368:LYS:NZ	1:A:370:GLU:CD	2.78	0.41
1:B:401[B]:ASP:OD1	1:B:402:PHE:N	2.53	0.41
1:B:45:ARG:NE	9:B:917:HOH:O	2.19	0.41
1:B:182:LYS:HB3	1:B:316:ILE:HD13	2.02	0.41
1:B:660:PHE:O	1:B:661:VAL:C	2.62	0.41
1:A:393:ILE:CD1	1:A:406:LEU:HD23	2.51	0.41
1:A:401[B]:ASP:HB3	9:A:1300:HOH:O	2.19	0.41
1:B:166:ALA:HB3	1:B:172:ALA:HB2	2.01	0.41
1:B:194:GLU:O	1:B:198:GLU:HG3	2.21	0.41
1:B:342:HIS:HB2	1:B:435:LYS:HA	2.02	0.41
1:B:715:LEU:N	1:B:716:PRO:CD	2.83	0.41
1:B:170:LYS:N	1:B:170:LYS:HD3	2.34	0.41
1:A:167:LYS:HG3	1:A:301:TYR:CE1	2.55	0.41
1:B:592:GLU:HG2	1:B:593:TYR:CD2	2.56	0.41
1:A:401[A]:ASP:CG	9:A:1300:HOH:O	2.63	0.41
1:A:452:TYR:CE1	1:A:456:LYS:HD2	2.56	0.41
1:A:287:GLU:CG	9:A:1152:HOH:O	2.41	0.41
1:B:517:PRO:C	1:B:579:GLN:HE22	2.29	0.41
1:A:148:GLY:O	1:A:152:VAL:HG13	2.21	0.40
1:B:64:PHE:CZ	1:B:75:GLU:HG3	2.57	0.40
1:B:319:ILE:O	1:B:319:ILE:HG13	2.21	0.40

All (38) 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)
1:A:396:ARG:CZ	1:A:580:ARG:NH2[4_545]	0.61	1.59
1:A:396:ARG:NH2	1:A:580:ARG:NH1[4_545]	0.84	1.36
1:A:396:ARG:NH2	1:A:580:ARG:CZ[4_545]	0.94	1.26
1:A:396:ARG:CZ	1:A:580:ARG:CZ[4_545]	0.96	1.24
1:A:396:ARG:HH22	1:A:580:ARG:NH1[4_545]	0.45	1.15
1:A:396:ARG:HH12	1:A:580:ARG:NE[4_545]	0.52	1.08
1:A:396:ARG:NH1	1:A:580:ARG:NE[4_545]	1.14	1.06
1:A:396:ARG:HH12	1:A:580:ARG:HE[4_545]	0.55	1.05
1:A:496:ARG:NH2	1:B:497:GLU:OE1[2_454]	1.18	1.02
1:A:396:ARG:NE	1:A:580:ARG:NH2[4_545]	1.25	0.95
1:A:396:ARG:HH21	1:A:580:ARG:HH12[4_545]	0.72	0.88
1:A:396:ARG:NH1	1:A:580:ARG:CZ[4_545]	1.40	0.80
1:A:396:ARG:NH1	1:A:580:ARG:HE[4_545]	0.88	0.72
1:A:496:ARG:HH21	1:B:497:GLU:OE1[2_454]	0.88	0.72
1:A:396:ARG:NH2	1:A:580:ARG:NH2[4_545]	1.51	0.69
1:A:396:ARG:HH22	1:A:580:ARG:HH11[4_545]	1.01	0.59
1:A:396:ARG:NH1	1:A:580:ARG:NH2[4_545]	1.61	0.59
1:A:396:ARG:NH2	1:A:580:ARG:HH12[4_545]	1.05	0.55
1:A:396:ARG:HH22	1:A:580:ARG:CZ[4_545]	1.08	0.52
9:A:1468:HOH:O	9:B:1392:HOH:O[2_454]	1.72	0.48
1:A:396:ARG:CZ	1:A:580:ARG:HH21[4_545]	1.18	0.42
1:A:396:ARG:HH11	1:A:580:ARG:HE[4_545]	1.21	0.39
1:A:396:ARG:HH22	1:A:580:ARG:HH12[4_545]	1.21	0.39
1:A:496:ARG:HH22	1:B:497:GLU:OE1[2_454]	1.22	0.38
1:A:396:ARG:NE	1:A:580:ARG:HH22[4_545]	1.26	0.34
1:A:396:ARG:HH21	1:A:580:ARG:NH1[4_545]	1.27	0.33
1:A:396:ARG:HE	1:A:580:ARG:HH22[4_545]	1.28	0.32
1:A:396:ARG:CZ	1:A:580:ARG:HH22[4_545]	1.31	0.29
1:A:396:ARG:CZ	1:A:580:ARG:NE[4_545]	1.91	0.29
1:A:396:ARG:NE	1:A:580:ARG:HH21[4_545]	1.35	0.25
9:A:1581:HOH:O	9:B:1515:HOH:O[2_454]	1.95	0.25
9:B:1347:HOH:O	9:B:1387:HOH:O[3_455]	1.97	0.23
9:B:1415:HOH:O	9:B:1520:HOH:O[1_655]	1.98	0.22
1:A:396:ARG:CZ	1:A:580:ARG:NH1[4_545]	2.03	0.17
1:A:396:ARG:NH1	1:A:580:ARG:HH21[4_545]	1.45	0.15
9:A:1626:HOH:O	9:B:1486:HOH:O[3_555]	2.05	0.15
1:A:396:ARG:HH12	1:A:580:ARG:CZ[4_545]	1.50	0.10
9:A:1598:HOH:O	9:B:1499:HOH:O[3_555]	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	729/733 (100%)	716 (98%)	11 (2%)	2 (0%)	36	29
1	B	728/733 (99%)	711 (98%)	15 (2%)	2 (0%)	36	29
All	All	1457/1466 (99%)	1427 (98%)	26 (2%)	4 (0%)	36	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ASP
1	B	190	ASP
1	B	599	GLY
1	A	599	GLY

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	613/615 (100%)	609 (99%)	4 (1%)	76	78
1	B	612/615 (100%)	611 (100%)	1 (0%)	87	90
All	All	1225/1230 (100%)	1220 (100%)	5 (0%)	84	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	349	LYS

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Mol	Chain	Res	Type
1	A	521	CYS
1	A	598	CYS
1	B	341	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	467	GLN
1	A	577	ASN
1	A	579	GLN
1	B	306	GLN
1	B	579	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 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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
7	UW8	A	810	-	37,39,42	5.93	15 (40%)	44,68,72	7.55	21 (47%)
5	PEG	A	807	-	6,6,6	0.49	0	5,5,5	0.28	0
8	BU3	A	812	-	4,5,5	0.72	0	6,6,6	1.56	1 (16%)
5	PEG	A	808	-	6,6,6	0.52	0	5,5,5	0.40	0
6	CIT	A	813	-	12,12,12	1.83	3 (25%)	17,17,17	1.27	2 (11%)
2	SF4	A	801	1	0,12,12	-	-	-	-	-
5	PEG	A	811	-	6,6,6	0.16	0	5,5,5	0.16	0
5	PEG	A	804	-	6,6,6	0.55	0	5,5,5	0.36	0
2	SF4	B	801	1	0,12,12	-	-	-	-	-
5	PEG	A	809	-	6,6,6	0.50	0	5,5,5	0.24	0
6	CIT	A	805	-	12,12,12	1.04	1 (8%)	17,17,17	1.38	3 (17%)
5	PEG	A	806	-	6,6,6	0.51	0	5,5,5	0.24	0
8	BU3	A	814	-	4,5,5	0.49	0	6,6,6	0.67	0
6	CIT	B	804	-	12,12,12	1.17	1 (8%)	17,17,17	1.44	3 (17%)
5	PEG	B	805	-	6,6,6	0.52	0	5,5,5	0.23	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
7	UW8	A	810	-	-	9/25/88/93	0/3/3/3
5	PEG	A	807	-	-	1/4/4/4	-
8	BU3	A	812	-	-	4/4/4/4	-
5	PEG	A	808	-	-	3/4/4/4	-
6	CIT	A	813	-	-	9/16/16/16	-
2	SF4	A	801	1	-	-	0/6/5/5
5	PEG	A	811	-	-	4/4/4/4	-
5	PEG	A	804	-	-	1/4/4/4	-
5	PEG	A	809	-	-	3/4/4/4	-
6	CIT	A	805	-	-	10/16/16/16	-
2	SF4	B	801	1	-	-	0/6/5/5
5	PEG	A	806	-	-	3/4/4/4	-
8	BU3	A	814	-	-	0/4/4/4	-
6	CIT	B	804	-	-	14/16/16/16	-
5	PEG	B	805	-	-	2/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	810	UW8	C2-C1	-16.15	1.28	1.54
7	A	810	UW8	O1-C1	15.75	1.46	1.28
7	A	810	UW8	O15-C13	15.51	1.46	1.28
7	A	810	UW8	O3-C1	13.00	1.49	1.20
7	A	810	UW8	O8-C7	11.63	1.41	1.28
7	A	810	UW8	O16-C14	7.44	1.48	1.41
7	A	810	UW8	C3-C2	-7.31	1.42	1.53
7	A	810	UW8	O2-C2	-5.07	1.36	1.41
7	A	810	UW8	O18'-C16'	4.89	1.47	1.30
7	A	810	UW8	O9-C8	4.03	1.45	1.41
6	A	813	CIT	O6-C6	-3.99	1.16	1.30
7	A	810	UW8	O1-TI1	-3.72	1.89	2.04
7	A	810	UW8	O19-C16'	3.54	1.33	1.22
7	A	810	UW8	O9-TI1	-2.96	1.79	1.88
6	A	813	CIT	O4-C5	-2.86	1.21	1.30
7	A	810	UW8	C14-C13	-2.78	1.49	1.54
6	A	813	CIT	O2-C1	-2.75	1.21	1.30
7	A	810	UW8	C5-C2	-2.68	1.49	1.53
6	B	804	CIT	O4-C5	-2.42	1.22	1.30
6	A	805	CIT	O2-C1	-2.33	1.23	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	810	UW8	O2-C2-C1	-38.39	85.72	107.28
7	A	810	UW8	O1-C1-O3	-21.56	104.15	124.30
7	A	810	UW8	O1-C1-C2	15.50	129.43	113.94
7	A	810	UW8	O16-C14-C13	-7.77	102.92	107.28
7	A	810	UW8	C2-C5-C6	5.88	127.05	113.42
7	A	810	UW8	O16-C14-C15	5.72	117.59	110.07
7	A	810	UW8	O8-C7-O10	-4.82	119.79	124.30
7	A	810	UW8	C5-C2-C3	4.81	122.13	109.74
7	A	810	UW8	C17-C14-C15	-3.88	99.74	109.74
7	A	810	UW8	O16-C14-C17	3.88	115.17	110.07
7	A	810	UW8	C8-C11-C12	-3.76	104.77	113.40
7	A	810	UW8	O9-C8-C11	3.71	114.95	110.07
6	A	805	CIT	O5-C6-C3	-3.40	115.51	122.09
7	A	810	UW8	O4-C4-C3	3.25	124.63	114.35
6	B	804	CIT	O3-C5-C4	-2.99	114.49	122.95
7	A	810	UW8	O14-C12-C11	-2.95	114.61	122.95
7	A	810	UW8	O18'-C16'-O19	-2.94	115.77	123.33
6	B	804	CIT	O5-C6-C3	-2.87	116.52	122.09
7	A	810	UW8	C14-C15-C16'	2.81	119.93	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	812	BU3	O6-C3-C4	2.73	117.84	109.68
7	A	810	UW8	O13-C12-C11	2.65	122.75	114.35
7	A	810	UW8	O15-C13-C14	-2.54	111.41	113.94
6	A	813	CIT	C4-C3-C6	-2.53	104.44	110.03
6	A	805	CIT	O6-C6-C3	2.45	117.83	113.14
7	A	810	UW8	O2-C2-C3	2.38	113.20	110.07
6	B	804	CIT	O6-C6-C3	2.27	117.49	113.14
7	A	810	UW8	O5-C4-C3	-2.15	116.86	122.95
7	A	810	UW8	O9-C8-C7	-2.12	106.09	107.28
6	A	813	CIT	O7-C3-C6	2.05	111.87	108.96
6	A	805	CIT	O7-C3-C6	2.04	111.85	108.96

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	805	CIT	C1-C2-C3-O7
6	A	805	CIT	C1-C2-C3-C4
6	A	805	CIT	C1-C2-C3-C6
6	A	813	CIT	C1-C2-C3-O7
6	A	813	CIT	C1-C2-C3-C4
6	A	813	CIT	C1-C2-C3-C6
6	A	813	CIT	C2-C3-C6-O5
6	A	813	CIT	C2-C3-C6-O6
6	A	813	CIT	O7-C3-C6-O5
6	A	813	CIT	O7-C3-C6-O6
6	B	804	CIT	C2-C3-C4-C5
7	A	810	UW8	O2-C2-C3-C4
7	A	810	UW8	C1-C2-C3-C4
7	A	810	UW8	C5-C2-C3-C4
7	A	810	UW8	O2-C2-C5-C6
7	A	810	UW8	C1-C2-C5-C6
7	A	810	UW8	C3-C2-C5-C6
8	A	812	BU3	O5-C2-C3-O6
8	A	812	BU3	C1-C2-C3-O6
8	A	812	BU3	O5-C2-C3-C4
6	B	804	CIT	C6-C3-C4-C5
5	A	806	PEG	O2-C3-C4-O4
5	A	809	PEG	O1-C1-C2-O2
5	A	809	PEG	O2-C3-C4-O4
5	A	806	PEG	O1-C1-C2-O2
5	A	807	PEG	O2-C3-C4-O4

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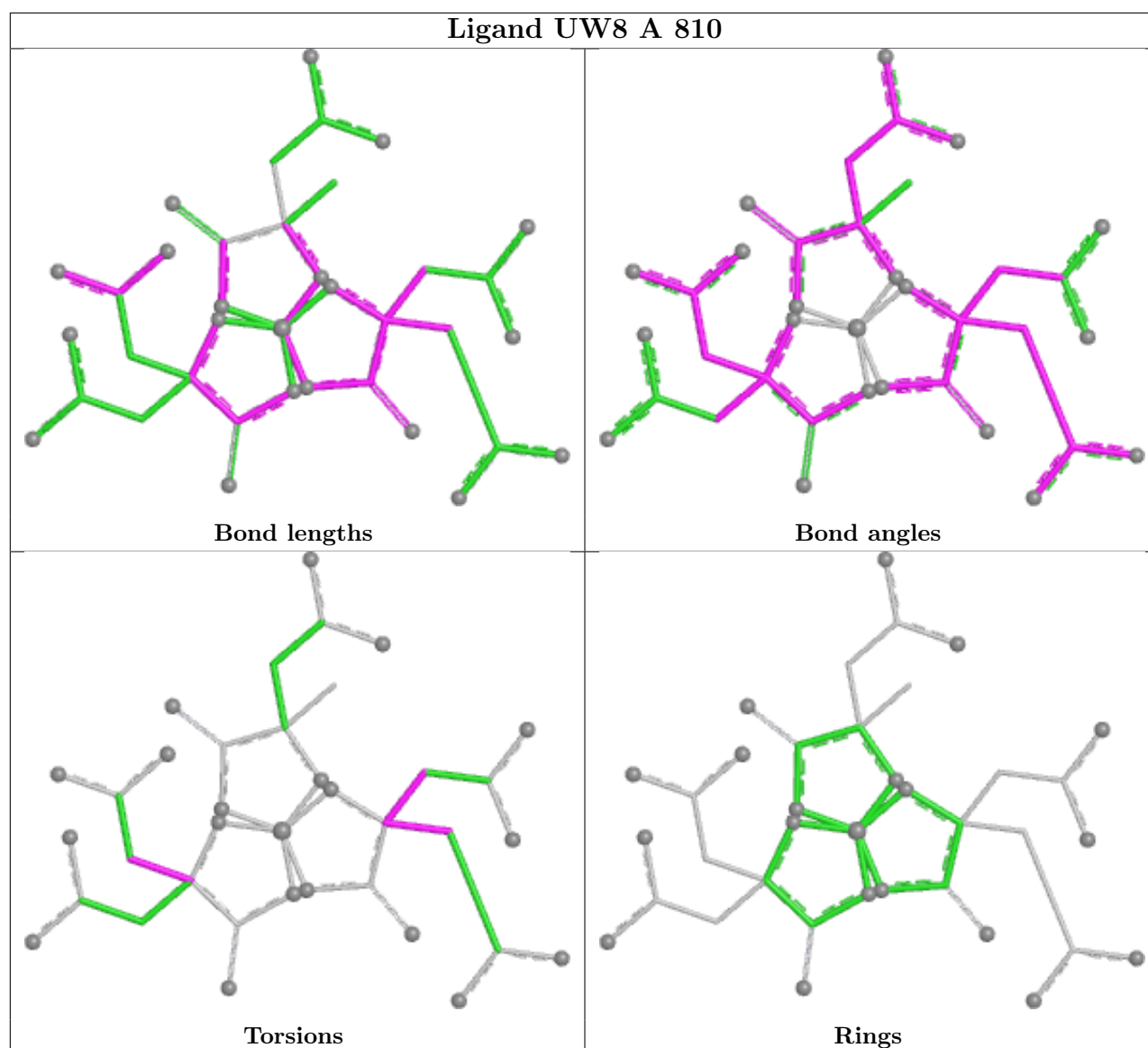
Mol	Chain	Res	Type	Atoms
5	A	808	PEG	O2-C3-C4-O4
6	A	805	CIT	C2-C3-C6-O6
5	B	805	PEG	O1-C1-C2-O2
6	B	804	CIT	C1-C2-C3-O7
6	B	804	CIT	C1-C2-C3-C6
6	B	804	CIT	O7-C3-C4-C5
6	A	813	CIT	C3-C4-C5-O3
6	A	813	CIT	C3-C4-C5-O4
6	B	804	CIT	O1-C1-C2-C3
6	B	804	CIT	O2-C1-C2-C3
6	B	804	CIT	O7-C3-C6-O5
6	B	804	CIT	C1-C2-C3-C4
5	A	811	PEG	C4-C3-O2-C2
5	A	806	PEG	C1-C2-O2-C3
5	A	809	PEG	C4-C3-O2-C2
5	A	808	PEG	O1-C1-C2-O2
5	A	811	PEG	O1-C1-C2-O2
6	A	805	CIT	C4-C3-C6-O6
6	B	804	CIT	C2-C3-C6-O5
7	A	810	UW8	C17-C14-C15-C16'
5	A	811	PEG	O2-C3-C4-O4
8	A	812	BU3	C1-C2-C3-C4
5	A	804	PEG	C1-C2-O2-C3
5	A	811	PEG	C1-C2-O2-C3
7	A	810	UW8	C13-C14-C15-C16'
6	A	805	CIT	C2-C3-C6-O5
6	B	804	CIT	C2-C3-C6-O6
6	B	804	CIT	C4-C3-C6-O5
6	B	804	CIT	C4-C3-C6-O6
7	A	810	UW8	O16-C14-C15-C16'
6	A	805	CIT	C2-C3-C4-C5
5	B	805	PEG	C4-C3-O2-C2
5	A	808	PEG	C1-C2-O2-C3
6	A	805	CIT	O7-C3-C6-O6
6	B	804	CIT	O7-C3-C6-O6
6	A	805	CIT	C4-C3-C6-O5
6	A	805	CIT	C3-C4-C5-O4

There are no ring outliers.

9 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	810	UW8	8	0
5	A	807	PEG	2	0
8	A	812	BU3	2	0
5	A	808	PEG	4	0
5	A	811	PEG	7	0
5	A	804	PEG	7	0
6	A	805	CIT	5	0
6	B	804	CIT	2	0
5	B	805	PEG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	729/733 (99%)	-0.02	12 (1%) 70 74	12, 24, 48, 70	2 (0%)
1	B	729/733 (99%)	0.03	13 (1%) 67 71	13, 25, 47, 83	1 (0%)
All	All	1458/1466 (99%)	0.01	25 (1%) 69 72	12, 25, 48, 83	3 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	PHE	4.7
1	A	732	LEU	3.7
1	A	4	VAL	3.2
1	B	321	ILE	3.0
1	B	284	PRO	2.7
1	B	732	LEU	2.7
1	A	321	ILE	2.7
1	A	396	ARG	2.7
1	A	123	LYS	2.6
1	B	347	GLY	2.5
1	B	684	ILE	2.5
1	A	149	ILE	2.5
1	B	319	ILE	2.5
1	B	318	SER	2.4
1	B	13	GLY	2.3
1	A	5	ILE	2.2
1	A	319	ILE	2.2
1	B	317	THR	2.2
1	A	260	GLU	2.2
1	A	320	ASP	2.2
1	B	18	GLY	2.2
1	B	163	ILE	2.1
1	A	463	VAL	2.1
1	B	315	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	169	SER	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.

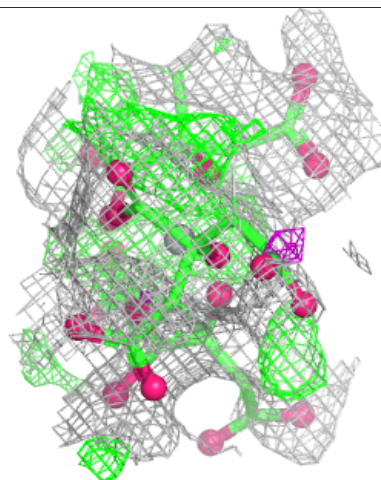
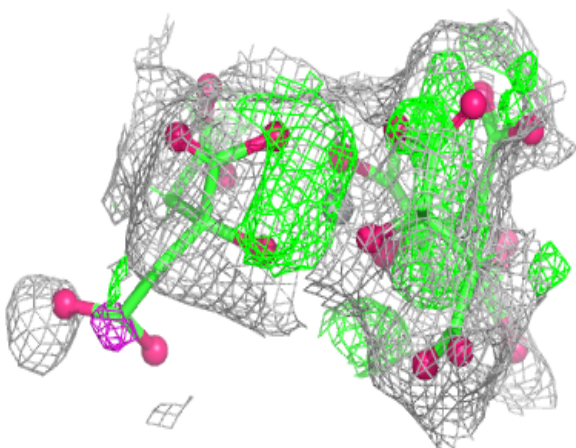
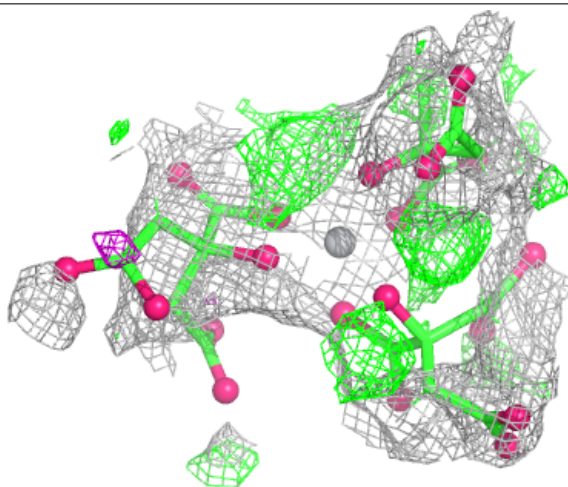
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CIT	B	804	13/13	0.51	0.16	58,73,83,88	0
7	UW8	A	810	37/40	0.65	0.18	65,81,100,105	0
5	PEG	A	811	7/7	0.66	0.15	42,51,61,61	0
6	CIT	A	805	13/13	0.67	0.14	49,60,78,78	0
8	BU3	A	814	6/6	0.69	0.17	35,47,58,63	0
6	CIT	A	813	13/13	0.70	0.14	33,43,52,58	0
5	PEG	A	807	7/7	0.72	0.15	41,59,71,71	0
5	PEG	A	809	7/7	0.72	0.16	37,52,63,63	0
5	PEG	A	806	7/7	0.75	0.14	42,50,61,61	0
8	BU3	A	812	6/6	0.76	0.14	37,46,56,56	0
5	PEG	A	804	7/7	0.77	0.13	33,40,44,50	0
5	PEG	A	808	7/7	0.78	0.11	35,44,55,57	0
5	PEG	B	805	7/7	0.80	0.13	28,46,58,58	0
3	ZN	A	802	1/1	0.97	0.04	9,9,9,9	1
3	ZN	B	802	1/1	0.98	0.06	6,6,6,6	1
2	SF4	B	801	8/8	0.99	0.03	12,12,14,16	0
4	NI	A	803	1/1	0.99	0.04	15,15,15,15	0
2	SF4	A	801	8/8	0.99	0.03	14,15,15,16	0
4	NI	B	803	1/1	1.00	0.04	12,12,12,12	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

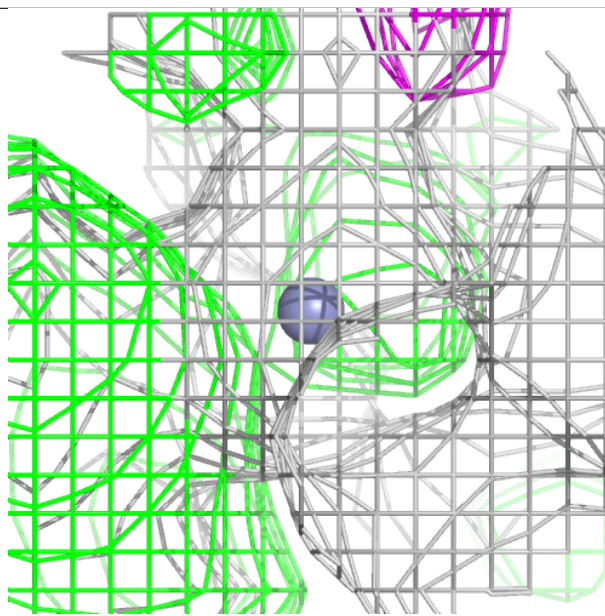
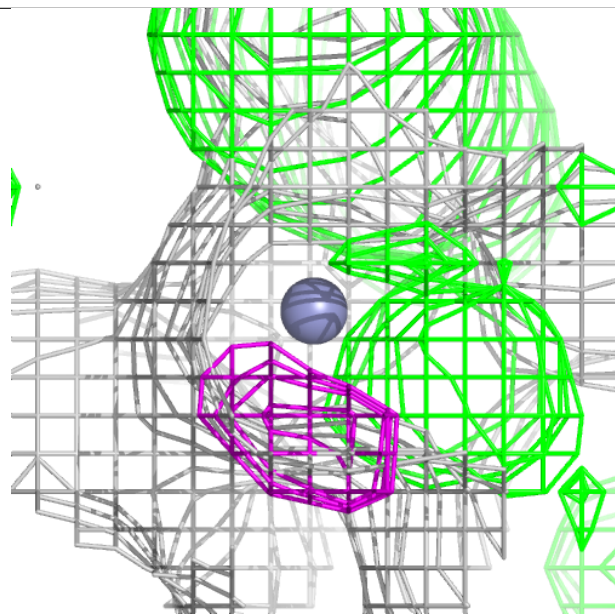
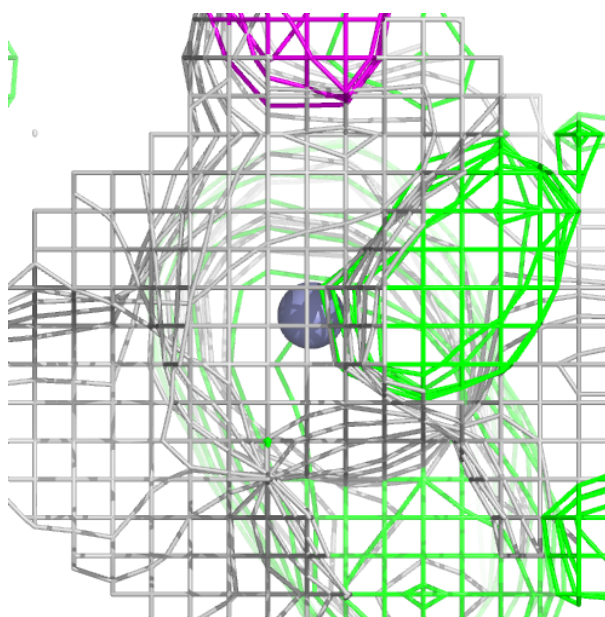
Electron density around UW8 A 810:

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



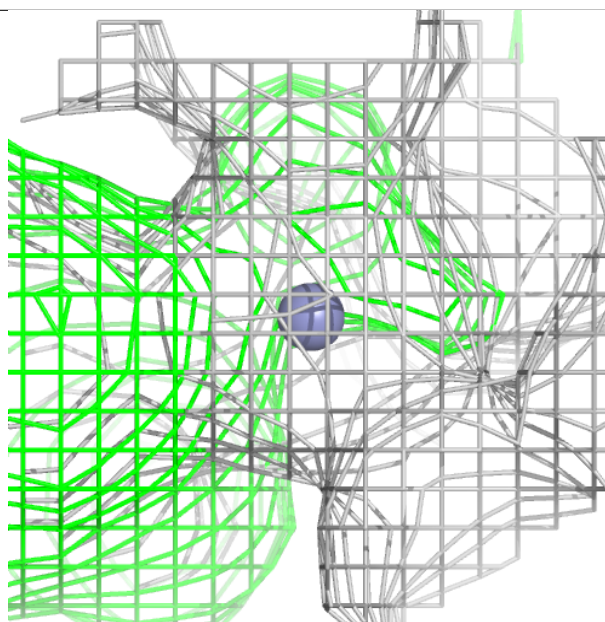
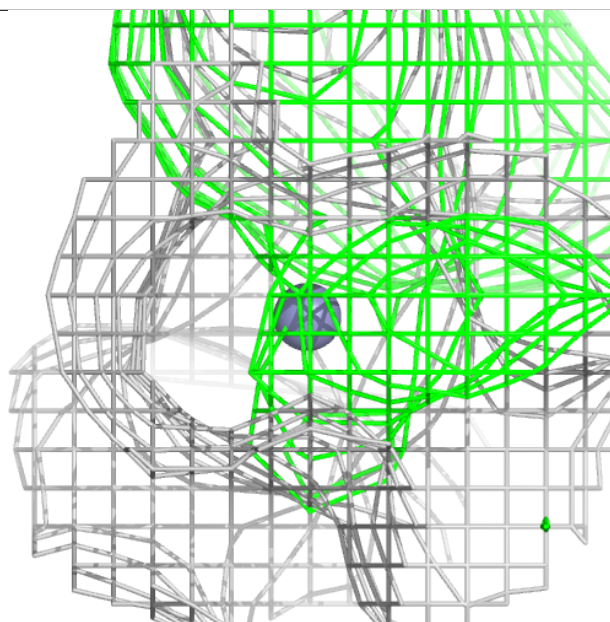
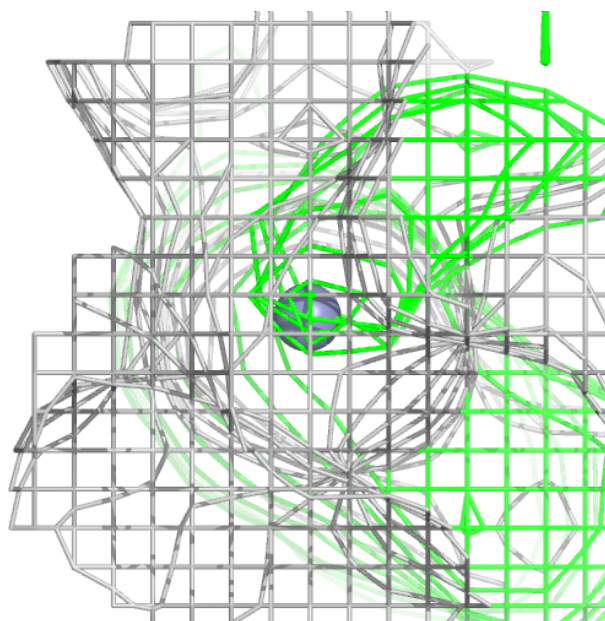
Electron density around ZN A 802:

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



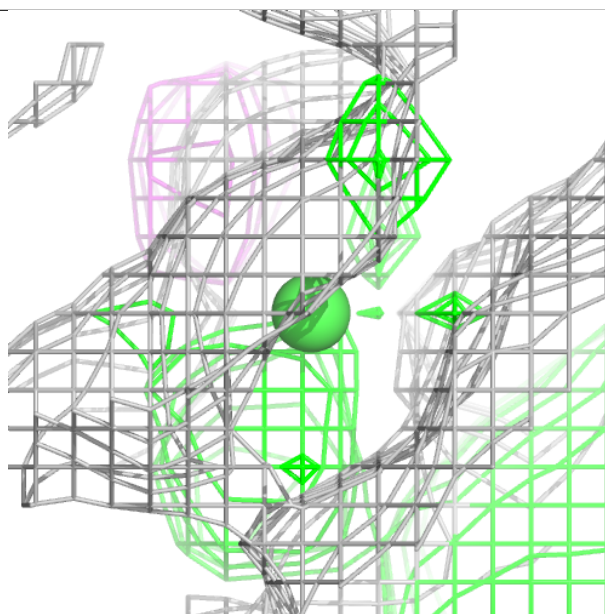
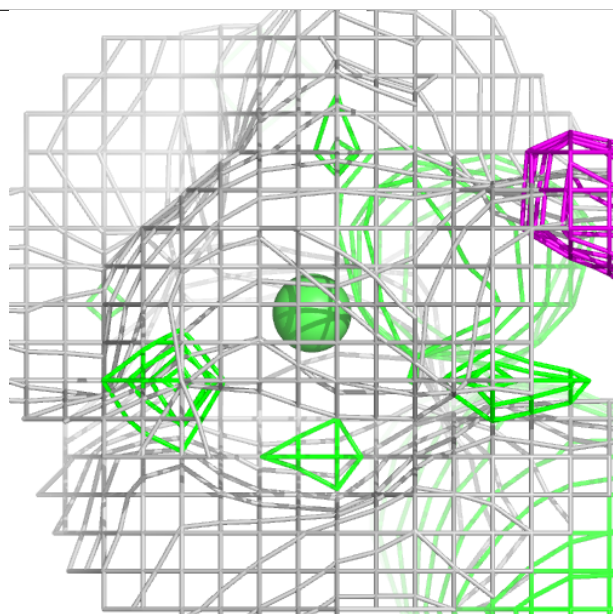
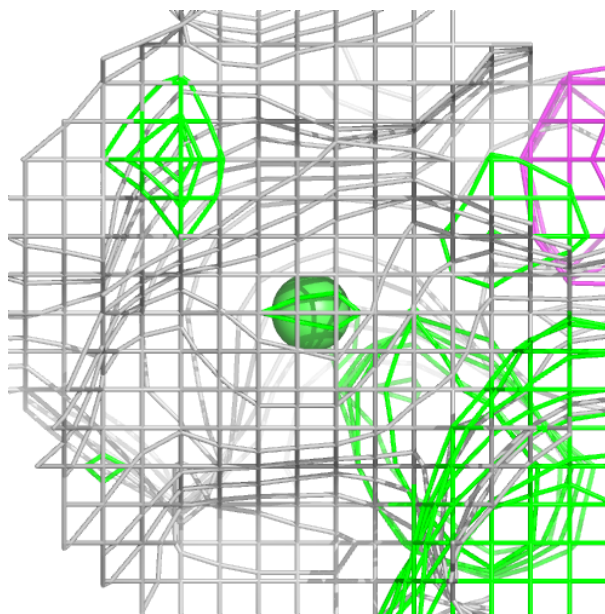
Electron density around ZN B 802:

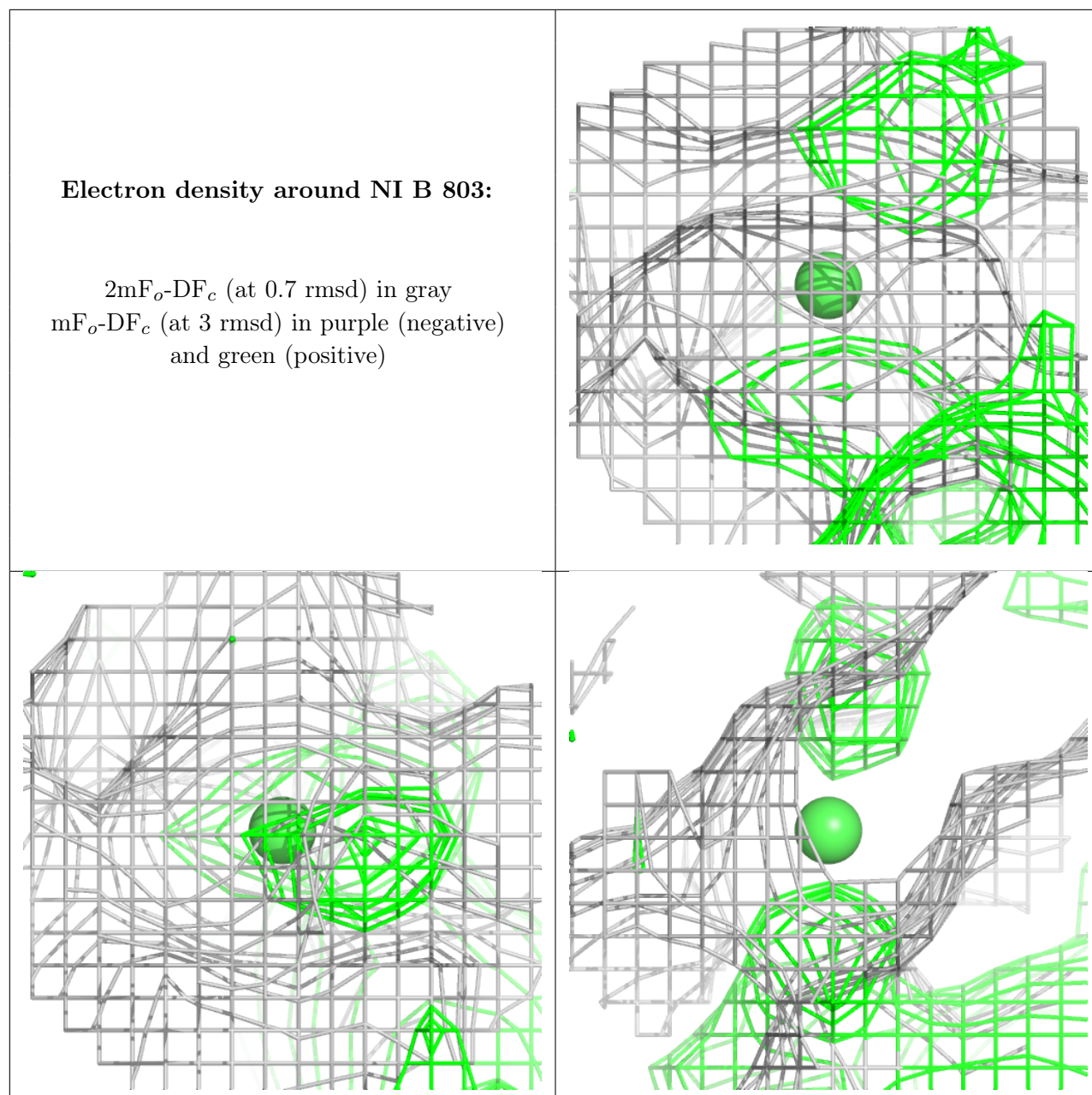
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI A 803:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.