



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2022 – 10:08 am BST

PDB ID : 7NYS
Title : monomeric acetyl-CoA synthase in closed conformation with carbon monoxide bound to the Ni proximal of cluster A
Authors : Kreibich, J.; Jeoung, J.H.; Dobbek, H.
Deposited on : 2021-03-23
Resolution : 2.00 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

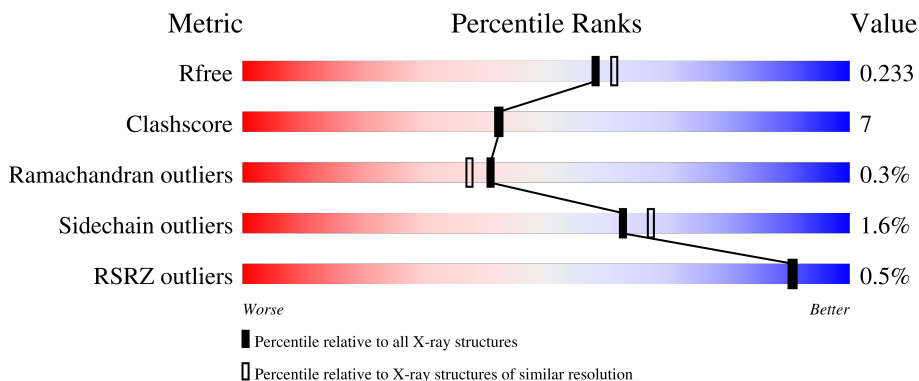
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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
6	UW8	B	804	-	-	X	-
7	MLI	B	810	-	-	X	X
8	PEG	B	807	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 24812 atoms, of which 11557 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.

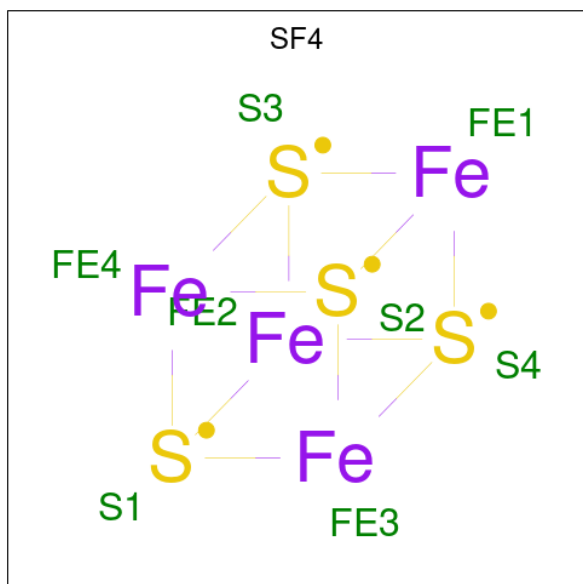
- Molecule 1 is a protein called CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	728	11550	3713	5762	969	1077	29	0	4	0
1	B	729	11524	3709	5744	967	1075	29	0	2	0

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 (three-letter code: SF4) (formula: Fe₄S₄).



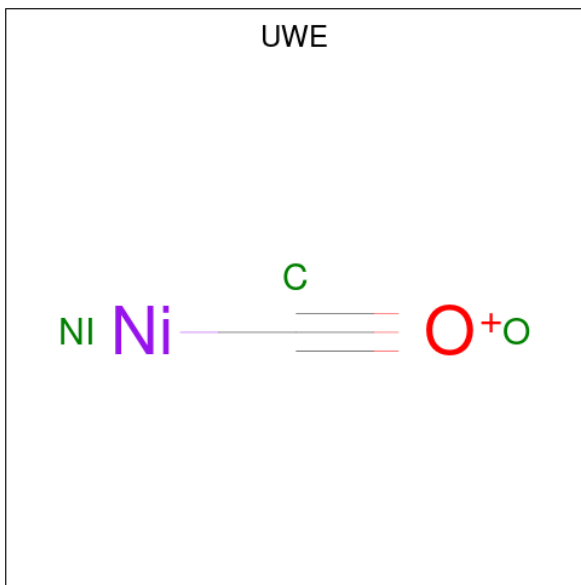
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0

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

- Molecule 3 is $\text{I}^{\text{3-}}$ -oxidanylidyne nickel (three-letter code: UWE) (formula: CNiO) (labeled as "Ligand of Interest" by depositor).



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

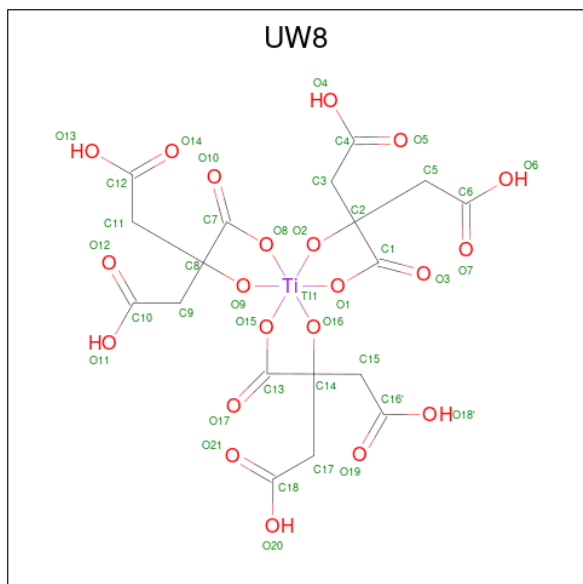
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

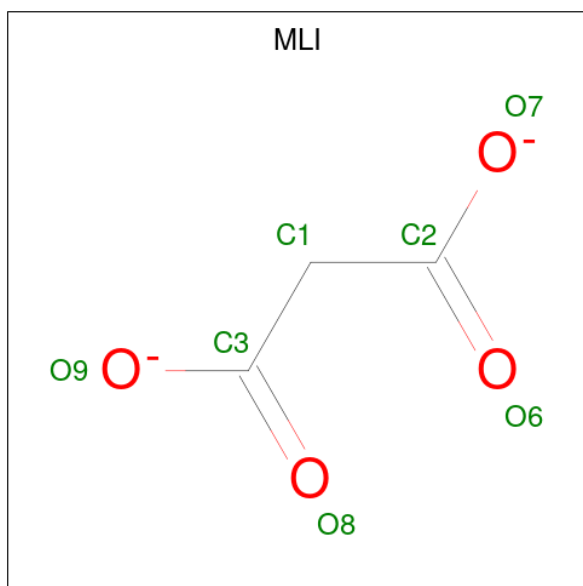
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	2	2	2	0	0

- Molecule 6 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 (three-letter code: UW8) (formula: C₁₈H₁₈O₂₁Ti).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	Ti		
6	B	1	51	18	11	21	1	0	0

- Molecule 7 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



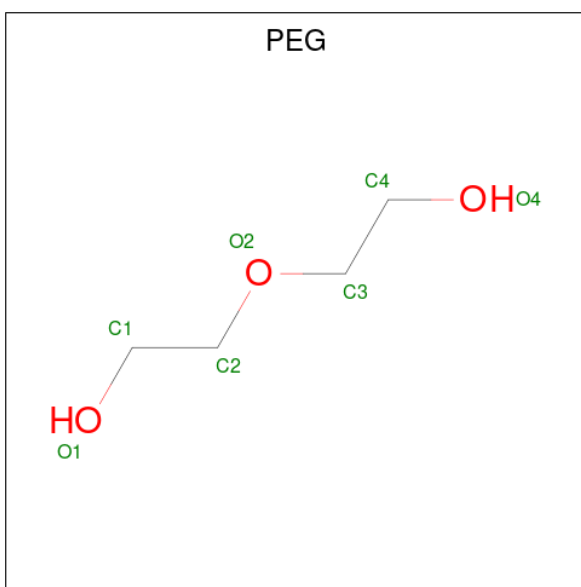
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	B	1	9	3	2	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			9	3	2	4		
7	B	1	Total	C	H	O	0	0
			9	3	2	4		
7	B	1	Total	C	H	O	0	0
			9	3	2	4		
7	B	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

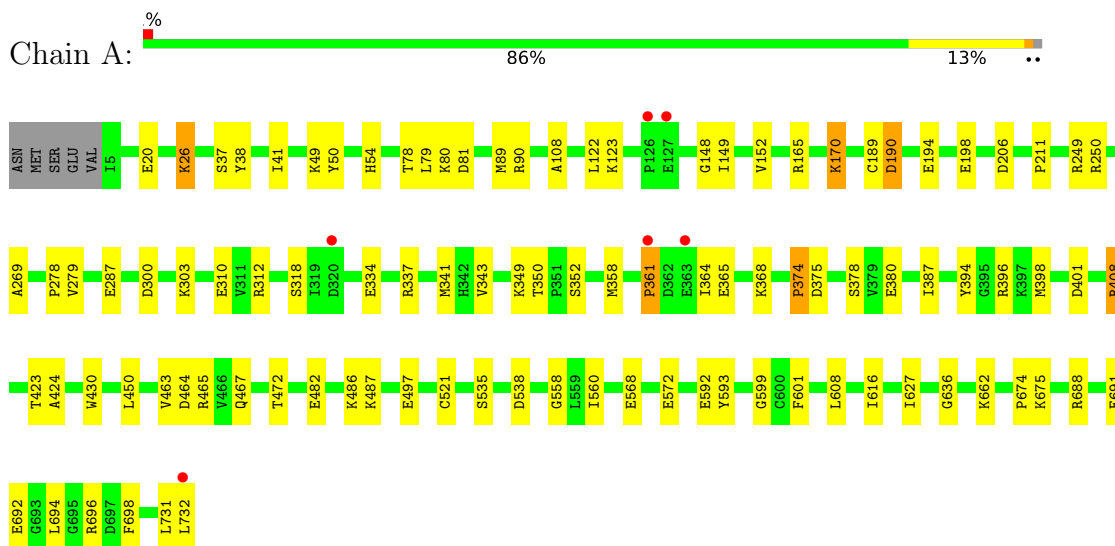
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	780	Total	O	0	0
			780	780		
9	B	785	Total	O	0	0
			785	785		

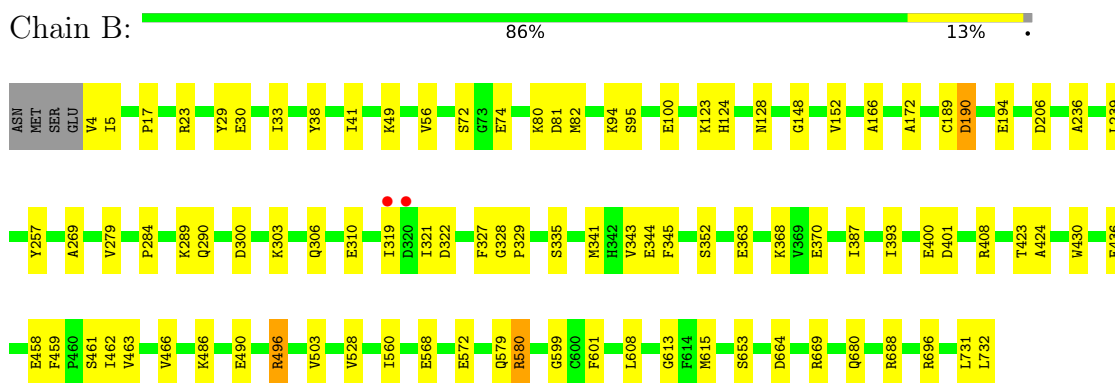
3 Residue-property plots [i](#)

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	70.28Å 99.20Å 238.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.00 48.56 – 1.89	Depositor EDS
% Data completeness (in resolution range)	84.5 (48.56-2.00) 74.0 (48.56-1.89)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.184 , 0.221 0.196 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24812	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: UWE, PEG, NI, SF4, MLI, UW8, CL

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	0.50	3/5922 (0.1%)	0.58	3/8016 (0.0%)
1	B	0.46	5/5914 (0.1%)	0.56	0/8007
All	All	0.48	8/11836 (0.1%)	0.57	3/16023 (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	1
1	B	0	2
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	PRO	N-CD	-12.69	1.30	1.47
1	A	361	PRO	N-CD	-11.90	1.31	1.47
1	A	374	PRO	N-CD	-11.13	1.32	1.47
1	B	329	PRO	N-CD	-9.30	1.34	1.47
1	A	350	THR	C-N	8.56	1.50	1.34
1	B	328	GLY	C-N	7.71	1.48	1.34
1	B	328	GLY	C-O	-5.49	1.14	1.23
1	B	81	ASP	C-O	5.19	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	ASP	CB-CG-OD2	-7.85	111.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	521	CYS	CA-CB-SG	5.01	123.02	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401[B]	ASP	Mainchain
1	B	335[A]	SER	Mainchain
1	B	335[B]	SER	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	5788	5762	5758	73	1
1	B	5780	5744	5751	86	1
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
6	B	40	11	0	10	1
7	B	35	10	10	3	0
8	B	21	30	30	0	0
9	A	780	0	0	28	2
9	B	785	0	0	30	4
All	All	13255	11557	11549	161	5

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 (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ILE:HD11	1:B:327:PHE:CZ	1.25	1.64
1:B:319:ILE:HD11	1:B:327:PHE:CE2	1.53	1.43
1:B:319:ILE:CD1	1:B:327:PHE:CZ	2.14	1.29
1:A:675:LYS:HE2	9:A:1271:HOH:O	1.19	1.27
1:A:568:GLU:HG2	9:A:1504:HOH:O	1.33	1.26
1:B:368:LYS:HE3	9:B:905:HOH:O	1.35	1.26
1:A:149:ILE:CG2	9:A:1565:HOH:O	1.84	1.22
1:A:287:GLU:OE1	9:A:903:HOH:O	1.54	1.19
1:A:149:ILE:HG21	9:A:1565:HOH:O	1.42	1.15
1:A:487:LYS:HE3	9:A:1302:HOH:O	1.48	1.14
1:B:572:GLU:OE1	9:B:902:HOH:O	1.65	1.14
1:B:100:GLU:OE1	9:B:903:HOH:O	1.73	1.07
1:B:688:ARG:HD2	9:B:933:HOH:O	1.55	1.03
1:B:319:ILE:CD1	1:B:327:PHE:CE2	2.40	1.03
1:A:198:GLU:OE2	9:A:904:HOH:O	1.80	0.99
1:B:319:ILE:HD11	1:B:327:PHE:HZ	1.17	0.97
1:B:290:GLN:HG2	9:B:1460:HOH:O	1.67	0.95
1:A:375:ASP:O	1:A:378:SER:OG	1.84	0.95
1:A:732:LEU:HD12	9:A:1121:HOH:O	1.68	0.93
1:B:319:ILE:CD1	1:B:327:PHE:HZ	1.70	0.91
1:A:20:GLU:O	9:A:905:HOH:O	1.90	0.89
1:A:310:GLU:HB3	9:A:1482:HOH:O	1.72	0.87
1:B:49:LYS:NZ	6:B:804:UW8:O16	2.07	0.85
1:B:319:ILE:CG1	1:B:327:PHE:HZ	1.89	0.85
1:A:572:GLU:HG2	9:A:1491:HOH:O	1.75	0.85
1:B:688:ARG:CD	9:B:933:HOH:O	2.17	0.85
1:A:49:LYS:NZ	6:B:804:UW8:O15	2.09	0.85
1:B:128:ASN:ND2	9:B:908:HOH:O	2.09	0.84
1:A:361:PRO:O	9:A:901:HOH:O	1.95	0.82
1:A:408:ARG:HD3	9:A:921:HOH:O	1.81	0.81
1:B:236:ALA:HB3	1:B:239:LEU:CD1	2.09	0.81
1:B:363:GLU:OE2	9:B:904:HOH:O	1.98	0.80
1:A:636:GLY:O	9:A:906:HOH:O	2.00	0.79
1:A:334:GLU:OE1	9:A:907:HOH:O	2.03	0.77
1:B:528:VAL:HG11	1:B:653:SER:OG	1.85	0.76
1:B:732:LEU:HA	9:B:1354:HOH:O	1.87	0.75
1:B:370:GLU:OE1	9:B:905:HOH:O	2.04	0.74
6:B:804:UW8:O3	9:B:906:HOH:O	2.06	0.74
1:A:688:ARG:NH2	1:A:692:GLU:OE1	2.22	0.73
1:A:688:ARG:HD2	9:A:1229:HOH:O	1.90	0.71
1:B:580:ARG:NH2	9:B:920:HOH:O	2.23	0.71
1:A:337:ARG:NH1	9:A:909:HOH:O	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLU:OE1	9:B:909:HOH:O	2.10	0.70
1:B:124:HIS:O	9:B:907:HOH:O	2.09	0.69
1:B:236:ALA:HB3	1:B:239:LEU:HD11	1.73	0.69
1:B:436:GLU:OE1	7:B:810:MLI:O7	2.11	0.69
1:A:662:LYS:NZ	9:A:914:HOH:O	2.25	0.68
1:A:165:ARG:NH1	9:A:915:HOH:O	2.27	0.68
1:A:26:LYS:HE2	1:B:95:SER:HB3	1.76	0.68
1:B:393:ILE:HD13	1:B:466:VAL:HG22	1.76	0.67
1:B:300:ASP:OD2	1:B:303:LYS:HE3	1.96	0.65
1:B:319:ILE:CG1	1:B:327:PHE:CZ	2.73	0.65
1:A:206:ASP:OD1	9:A:908:HOH:O	2.14	0.64
1:B:284:PRO:O	9:B:910:HOH:O	2.14	0.64
1:B:732:LEU:HD13	9:B:1629:HOH:O	1.98	0.64
1:A:54:HIS:HE1	9:A:1026:HOH:O	1.81	0.63
1:A:368:LYS:HE3	1:A:467:GLN:NE2	2.14	0.62
1:A:49:LYS:NZ	6:B:804:UW8:O1	2.32	0.62
1:A:250:ARG:HG2	9:A:1167:HOH:O	2.01	0.61
1:A:89:MET:HE2	1:A:108:ALA:HA	1.81	0.61
1:B:400:GLU:OE2	9:B:911:HOH:O	2.16	0.60
1:B:236:ALA:HB3	1:B:239:LEU:HD12	1.81	0.59
6:B:804:UW8:O6	9:B:912:HOH:O	2.17	0.59
1:B:731:LEU:O	1:B:732:LEU:CB	2.47	0.58
1:A:731:LEU:O	1:A:732:LEU:HG	2.04	0.57
1:A:568:GLU:CG	9:A:1504:HOH:O	2.14	0.57
1:A:368:LYS:HE3	1:A:467:GLN:HE22	1.70	0.57
1:B:319:ILE:HG13	1:B:327:PHE:HZ	1.68	0.56
1:A:463:VAL:O	1:A:463:VAL:HG23	2.06	0.56
1:B:72:SER:OG	1:B:74:GLU:OE1	2.17	0.56
1:A:535[A]:SER:OG	1:A:538:ASP:OD2	2.23	0.55
1:B:579:GLN:HA	1:B:580:ARG:HH21	1.72	0.55
1:B:5:ILE:O	9:B:913:HOH:O	2.18	0.55
1:A:123:LYS:NZ	6:B:804:UW8:O3	2.40	0.55
1:B:688:ARG:NE	9:B:933:HOH:O	2.35	0.54
1:B:123:LYS:NZ	6:B:804:UW8:C9	2.72	0.53
1:B:408:ARG:HD2	9:B:1477:HOH:O	2.08	0.53
1:B:29:TYR:CE1	1:B:33:ILE:HD11	2.44	0.53
1:B:94:LYS:NZ	9:B:944:HOH:O	2.42	0.52
1:A:560:ILE:HD11	1:A:568:GLU:HG3	1.92	0.52
1:A:608:LEU:HD21	1:A:627:ILE:HB	1.92	0.52
1:B:613:GLY:HA2	1:B:669:ARG:HG2	1.92	0.52
1:A:572:GLU:CG	9:A:1491:HOH:O	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ILE:CD1	1:B:466:VAL:HG22	2.40	0.52
1:A:78:THR:OG1	1:A:80:LYS:HG2	2.11	0.51
1:B:560:ILE:HD11	1:B:568:GLU:HG3	1.92	0.51
1:A:380:GLU:HG3	9:A:1607:HOH:O	2.11	0.51
1:B:463:VAL:HG23	1:B:463:VAL:O	2.11	0.50
1:B:123:LYS:HZ2	6:B:804:UW8:C9	2.24	0.50
1:A:394:TYR:HB3	1:A:465:ARG:HG3	1.93	0.50
1:A:423:THR:HG22	1:A:430:TRP:HB3	1.94	0.49
1:B:321:ILE:HG13	1:B:321:ILE:O	2.12	0.49
6:B:804:UW8:O18'	6:B:804:UW8:C13	2.60	0.49
1:A:80:LYS:HG3	1:A:81:ASP:N	2.28	0.49
1:B:664:ASP:O	1:B:669:ARG:NE	2.43	0.49
1:B:306:GLN:O	1:B:310:GLU:HG3	2.13	0.48
1:B:319:ILE:CD1	1:B:327:PHE:HE2	2.19	0.48
1:A:79:LEU:HD21	1:A:122:LEU:HD11	1.95	0.48
1:A:535[B]:SER:HB2	1:A:538:ASP:OD2	2.12	0.48
1:B:401[B]:ASP:OD2	9:B:914:HOH:O	2.19	0.48
1:B:528:VAL:CG1	1:B:653:SER:OG	2.59	0.48
1:B:269:ALA:HB1	1:B:279:VAL:HG21	1.95	0.47
1:B:461:SER:OG	1:B:462:ILE:HG23	2.14	0.47
1:B:731:LEU:O	1:B:732:LEU:HB3	2.13	0.47
1:B:29:TYR:CZ	1:B:33:ILE:HD11	2.49	0.47
1:B:459:PHE:O	1:B:463:VAL:HG22	2.15	0.47
1:B:490:GLU:OE2	9:B:911:HOH:O	2.20	0.46
1:A:592:GLU:HG2	1:A:593:TYR:CD2	2.50	0.46
1:B:423:THR:HG22	1:B:430:TRP:HB3	1.98	0.46
1:B:352:SER:HA	1:B:387:ILE:O	2.15	0.46
1:B:56:VAL:HG21	1:B:82:MET:HE1	1.97	0.46
1:B:486:LYS:O	1:B:490:GLU:HG2	2.15	0.46
1:A:364:ILE:HG23	1:A:465:ARG:HD2	1.98	0.46
1:A:463:VAL:O	1:A:463:VAL:CG2	2.64	0.46
1:B:166:ALA:HB3	1:B:172:ALA:HB2	1.97	0.46
1:B:669:ARG:CD	1:B:731:LEU:HD11	2.45	0.46
1:B:148:GLY:O	1:B:152:VAL:HG13	2.16	0.46
1:B:4:VAL:HG12	1:B:4:VAL:O	2.16	0.45
1:B:319:ILE:HD12	1:B:321:ILE:HD11	1.97	0.45
1:A:194:GLU:O	1:A:198:GLU:HG3	2.16	0.45
1:B:319:ILE:HD12	1:B:321:ILE:CD1	2.46	0.45
1:A:170:LYS:HB2	1:A:170:LYS:HE2	1.77	0.45
1:A:341:MET:SD	1:A:343:VAL:N	2.90	0.44
1:B:732:LEU:CD1	9:B:1629:HOH:O	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:LYS:HG2	9:A:1439:HOH:O	2.16	0.44
1:B:341:MET:SD	1:B:343:VAL:N	2.90	0.44
1:B:206:ASP:OD1	9:B:916:HOH:O	2.21	0.44
1:A:374:PRO:HD2	1:A:472:THR:OG1	2.18	0.44
1:A:249:ARG:HD3	9:A:1580:HOH:O	2.17	0.44
1:A:26:LYS:NZ	9:A:957:HOH:O	2.50	0.44
7:B:810:MLI:O8	9:B:915:HOH:O	2.21	0.43
1:B:458:GLU:OE2	9:B:917:HOH:O	2.21	0.43
1:B:608:LEU:HD11	1:B:615:MET:HB3	2.00	0.43
1:B:423:THR:O	1:B:424:ALA:HB3	2.19	0.43
1:A:423:THR:O	1:A:424:ALA:HB3	2.18	0.43
1:A:616:ILE:O	1:A:674:PRO:HD3	2.19	0.43
1:B:23:ARG:HD2	1:B:289:LYS:HD2	2.00	0.42
1:A:450:LEU:C	1:A:450:LEU:HD23	2.40	0.42
1:A:38:TYR:CD1	1:B:41:ILE:HB	2.55	0.42
1:A:269:ALA:HB1	1:A:279:VAL:HG21	2.02	0.42
1:A:278:PRO:HD2	1:A:312:ARG:HD3	2.02	0.42
1:A:688:ARG:NH1	1:A:691:GLU:OE1	2.53	0.42
1:B:732:LEU:HB3	7:B:811:MLI:O9	2.19	0.42
1:A:358:MET:HE3	1:A:398:MET:HB3	2.01	0.42
1:A:300:ASP:HB3	1:A:303:LYS:HD2	2.01	0.42
1:A:694:LEU:HD22	1:A:698:PHE:CD1	2.55	0.42
1:A:352:SER:HA	1:A:387:ILE:O	2.20	0.42
1:B:579:GLN:HA	1:B:580:ARG:NH2	2.34	0.42
1:B:194:GLU:HG3	9:B:1279:HOH:O	2.20	0.42
6:B:804:UW8:C6	9:B:912:HOH:O	2.64	0.41
1:A:41:ILE:HD13	1:B:38:TYR:HB3	2.01	0.41
1:A:148:GLY:O	1:A:152:VAL:HG13	2.20	0.41
1:A:482:GLU:O	1:A:486:LYS:HG3	2.20	0.41
1:B:189:CYS:O	1:B:190:ASP:HB2	2.21	0.41
1:B:322:ASP:O	1:B:322:ASP:CG	2.58	0.41
1:B:463:VAL:O	1:B:463:VAL:CG2	2.68	0.41
1:A:37:SER:OG	1:A:90:ARG:NH2	2.54	0.41
1:A:49:LYS:HE2	1:A:50:TYR:CZ	2.56	0.41
1:A:558:GLY:HA3	1:A:568:GLU:HB2	2.02	0.41
1:A:189:CYS:O	1:A:190:ASP:HB2	2.21	0.40
1:B:343:VAL:HG22	1:B:344:GLU:N	2.36	0.40

All (5) 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:B:804:UW8:H11B	9:B:1679:HOH:O[3_455]	1.35	0.25
1:A:497:GLU:OE1	1:B:496:ARG:HH21[2_454]	1.40	0.20
9:A:1134:HOH:O	9:B:1486:HOH:O[3_455]	2.12	0.08
9:A:1600:HOH:O	9:B:1271:HOH:O[3_555]	2.12	0.08
9:B:1380:HOH:O	9:B:1517:HOH:O[3_455]	2.13	0.07

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	730/733 (100%)	715 (98%)	13 (2%)	2 (0%)	41	37
1	B	729/733 (100%)	712 (98%)	15 (2%)	2 (0%)	41	37
All	All	1459/1466 (100%)	1427 (98%)	28 (2%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

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

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	614/615 (100%)	604 (98%)	10 (2%)	62	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	613/615 (100%)	604 (98%)	9 (2%)	65	69
All	All	1227/1230 (100%)	1208 (98%)	19 (2%)	62	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	170	LYS
1	A	211	PRO
1	A	318	SER
1	A	349	LYS
1	A	365	GLU
1	A	396	ARG
1	A	408	ARG
1	A	601	PHE
1	A	696	ARG
1	B	80	LYS
1	B	257	TYR
1	B	345	PHE
1	B	496	ARG
1	B	503	VAL
1	B	580	ARG
1	B	601	PHE
1	B	680	GLN
1	B	696	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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
8	PEG	B	808	-	6,6,6	0.49	0	5,5,5	0.24	0
7	MLI	B	806	-	0,6,6	-	-	0,7,7	-	-
3	UWE	B	802	1	1,2,2	2.62	1 (100%)	-	-	-
3	UWE	A	802	1	1,2,2	2.09	1 (100%)	-	-	-
7	MLI	B	805	-	0,6,6	-	-	0,7,7	-	-
2	SF4	B	801	1	0,12,12	-	-	-	-	-
8	PEG	B	812	-	6,6,6	0.53	0	5,5,5	0.43	0
7	MLI	B	809	-	0,6,6	-	-	0,7,7	-	-
7	MLI	B	810	-	0,6,6	-	-	0,7,7	-	-
6	UW8	B	804	-	24,42,42	5.62	9 (37%)	33,72,72	2.16	11 (33%)
8	PEG	B	807	-	6,6,6	0.48	0	5,5,5	0.22	0
2	SF4	A	801	1	0,12,12	-	-	-	-	-
7	MLI	B	811	-	0,6,6	-	-	0,7,7	-	-

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
8	PEG	B	808	-	-	0/4/4/4	-
7	MLI	B	806	-	-	0/0/4/4	-
7	MLI	B	805	-	-	0/0/4/4	-
2	SF4	B	801	1	-	-	0/6/5/5
8	PEG	B	812	-	-	2/4/4/4	-
7	MLI	B	809	-	-	0/0/4/4	-
7	MLI	B	810	-	-	0/0/4/4	-
6	UW8	B	804	-	-	6/18/93/93	0/3/3/3
8	PEG	B	807	-	-	1/4/4/4	-
2	SF4	A	801	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MLI	B	811	-	-	0/0/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	804	UW8	O1-C1	15.51	1.45	1.28
6	B	804	UW8	O15-C13	15.26	1.44	1.28
6	B	804	UW8	O8-C7	14.82	1.44	1.28
6	B	804	UW8	O16-C14	3.92	1.45	1.41
6	B	804	UW8	O9-C8	2.91	1.44	1.41
3	B	802	UWE	O-C	-2.62	1.06	1.15
6	B	804	UW8	O2-C2	2.61	1.43	1.41
6	B	804	UW8	C2-C1	-2.48	1.49	1.54
6	B	804	UW8	C8-C7	-2.17	1.50	1.54
3	A	802	UWE	O-C	2.09	1.22	1.15
6	B	804	UW8	C14-C13	-2.00	1.50	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	804	UW8	C8-C9-C10	-6.93	105.13	115.47
6	B	804	UW8	C2-C3-C4	-5.44	107.36	115.47
6	B	804	UW8	O2-C2-C1	-4.22	104.84	107.28
6	B	804	UW8	C8-C11-C12	-2.83	111.25	115.47
6	B	804	UW8	C14-C17-C18	-2.82	111.27	115.47
6	B	804	UW8	O8-C7-O10	-2.42	121.97	124.30
6	B	804	UW8	O16-C14-C15	2.40	113.28	110.07
6	B	804	UW8	C2-C5-C6	-2.39	111.90	115.47
6	B	804	UW8	O1-C1-O3	-2.22	122.16	124.30
6	B	804	UW8	O9-C8-C7	-2.04	106.10	107.28
6	B	804	UW8	O15-C13-O17	-2.03	122.34	124.30

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	804	UW8	O2-C2-C5-C6
6	B	804	UW8	C1-C2-C5-C6
6	B	804	UW8	O16-C14-C15-C16'
6	B	804	UW8	C3-C2-C5-C6
6	B	804	UW8	C17-C14-C15-C16'

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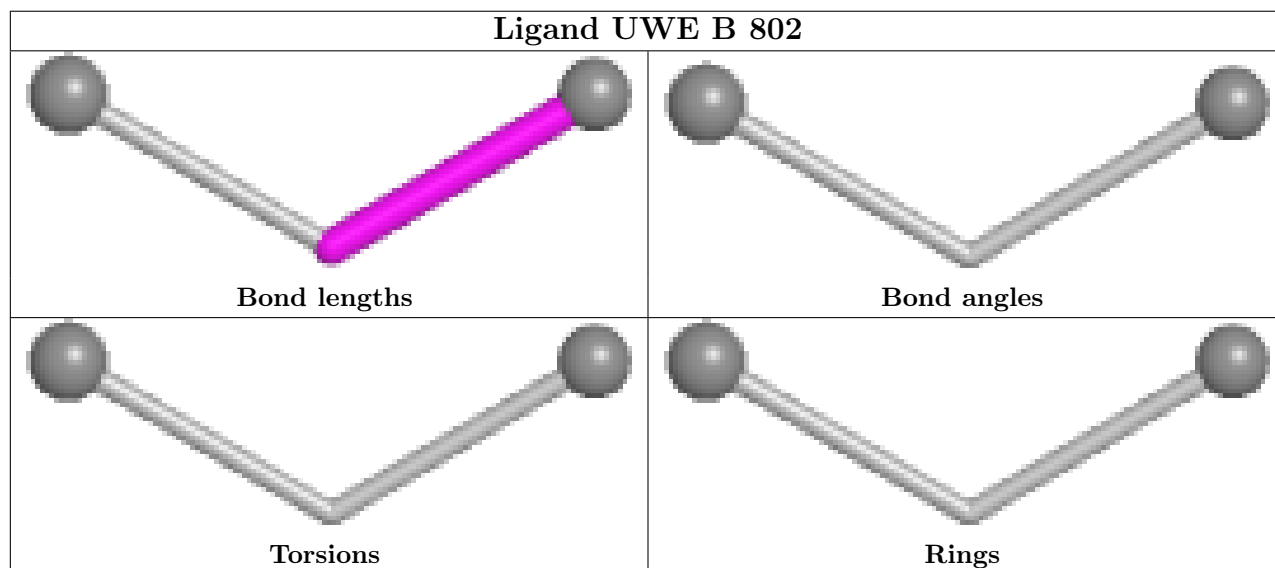
Mol	Chain	Res	Type	Atoms
6	B	804	UW8	C13-C14-C15-C16'
8	B	807	PEG	O2-C3-C4-O4
8	B	812	PEG	O2-C3-C4-O4
8	B	812	PEG	C1-C2-O2-C3

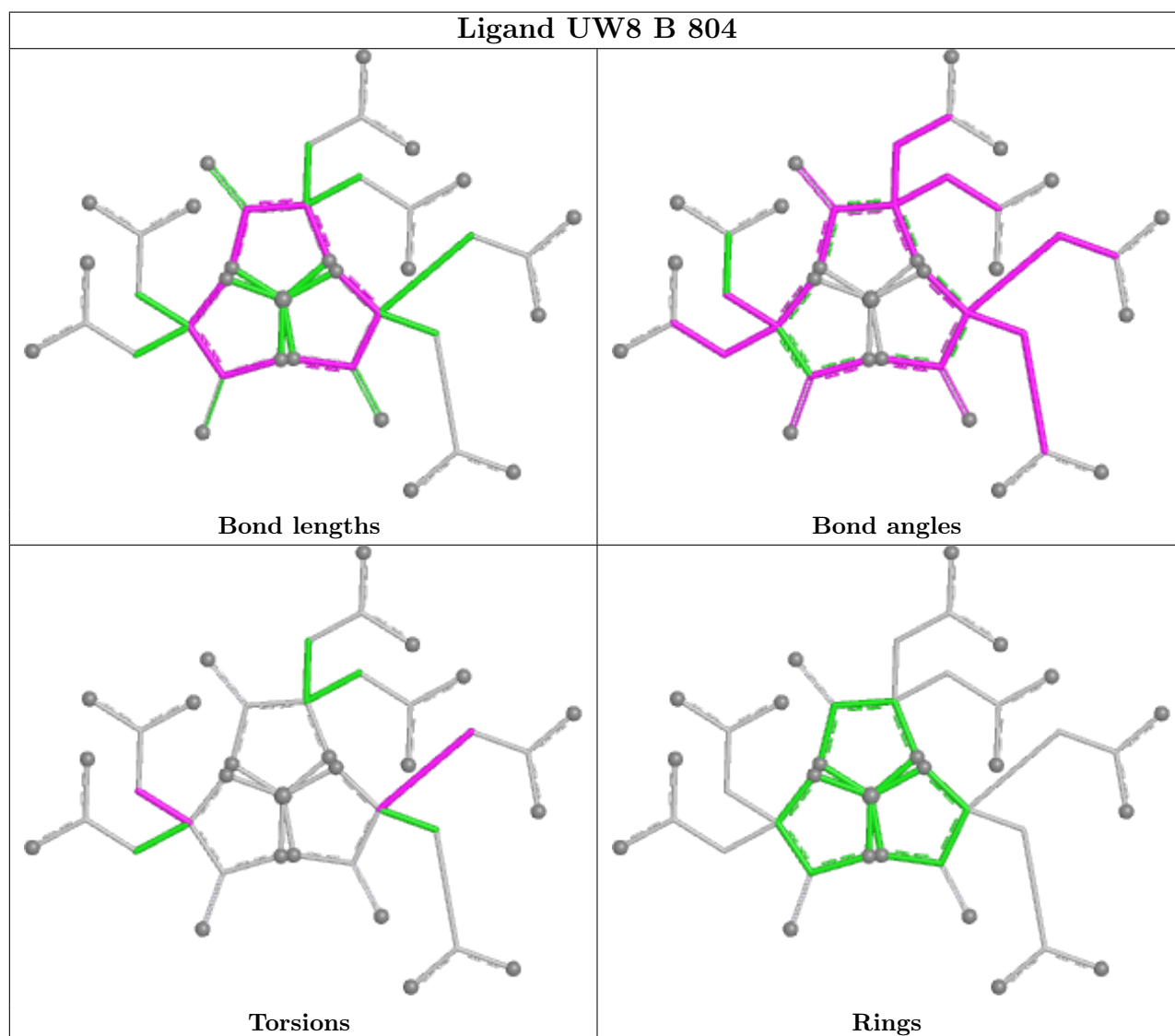
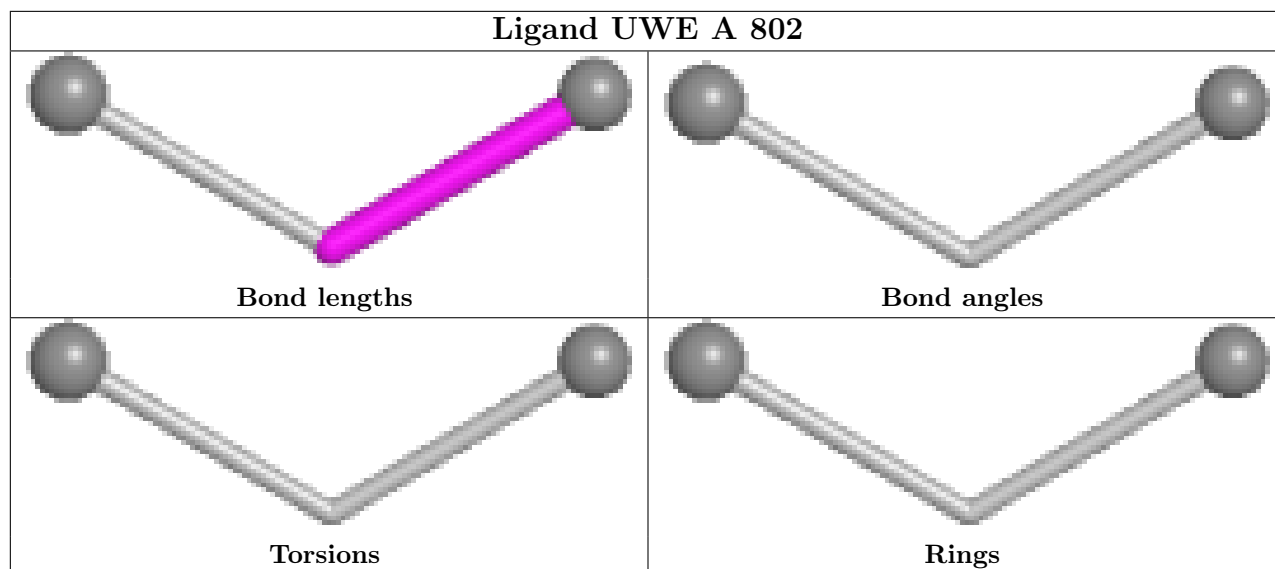
There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	810	MLI	2	0
6	B	804	UW8	10	1
7	B	811	MLI	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	728/733 (99%)	-0.46	6 (0%) 86 85	16, 30, 58, 88	0
1	B	729/733 (99%)	-0.40	2 (0%) 94 93	15, 28, 53, 92	0
All	All	1457/1466 (99%)	-0.43	8 (0%) 91 90	15, 29, 55, 92	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	PRO	4.0
1	A	732	LEU	2.9
1	B	320	ASP	2.9
1	A	361	PRO	2.7
1	A	363	GLU	2.7
1	A	127	GLU	2.7
1	A	320	ASP	2.3
1	B	319	ILE	2.1

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,

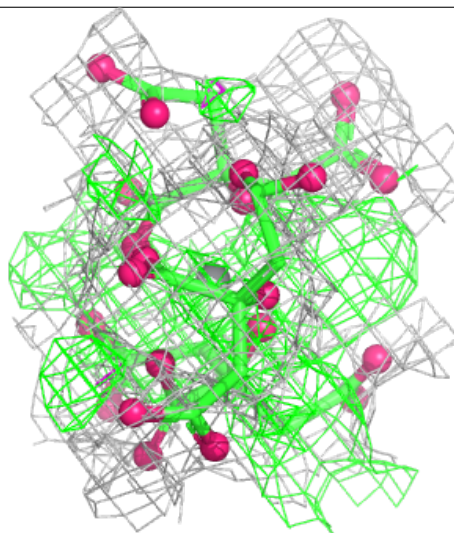
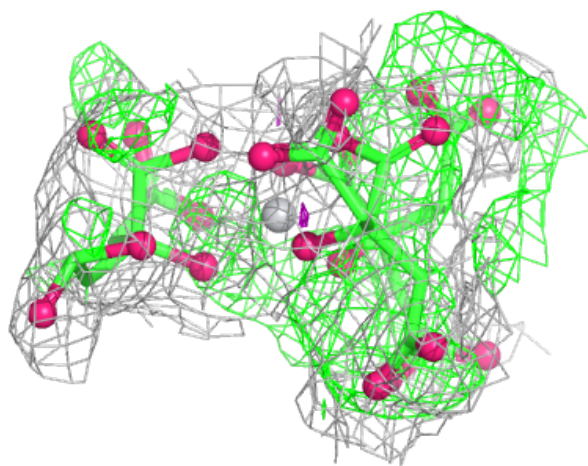
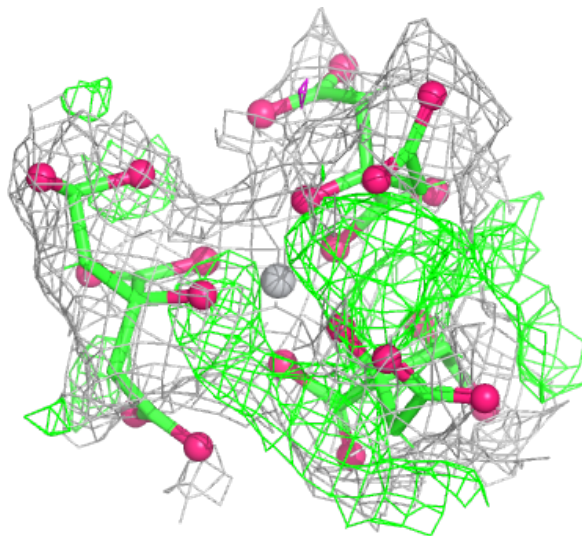
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MLI	B	810	7/7	0.72	0.57	57,70,84,85	0
8	PEG	B	807	7/7	0.72	0.40	63,84,105,105	0
6	UW8	B	804	40/40	0.77	0.17	60,87,102,104	0
7	MLI	B	805	7/7	0.77	0.12	74,84,92,92	0
7	MLI	B	811	7/7	0.81	0.35	53,70,97,97	0
7	MLI	B	809	7/7	0.81	0.39	54,65,73,79	0
8	PEG	B	808	7/7	0.81	0.52	54,79,95,100	0
8	PEG	B	812	7/7	0.85	0.23	35,60,85,85	0
7	MLI	B	806	7/7	0.86	0.30	41,56,73,73	0
5	CL	A	805	1/1	0.90	0.09	53,53,53,53	0
5	CL	A	804	1/1	0.98	0.11	54,54,54,54	0
4	NI	A	803	1/1	0.99	0.12	20,20,20,20	0
2	SF4	A	801	8/8	0.99	0.11	21,23,25,26	0
2	SF4	B	801	8/8	0.99	0.12	16,18,20,21	0
3	UWE	A	802	3/3	0.99	0.11	18,18,23,26	0
4	NI	B	803	1/1	1.00	0.12	16,16,16,16	0
3	UWE	B	802	3/3	1.00	0.12	12,12,20,23	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.

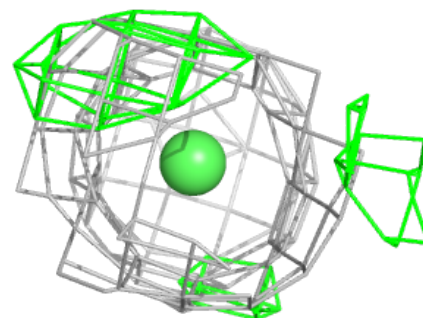
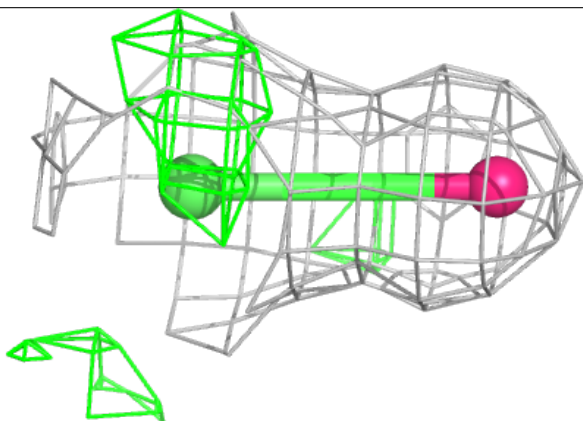
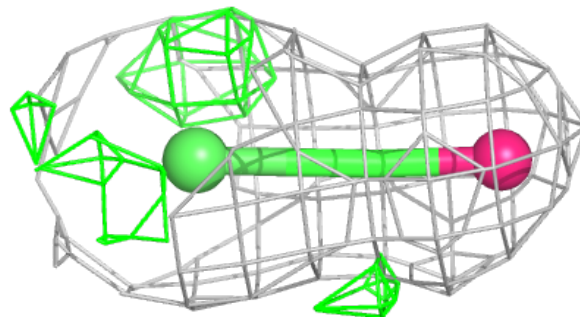
Electron density around UW8 B 804:

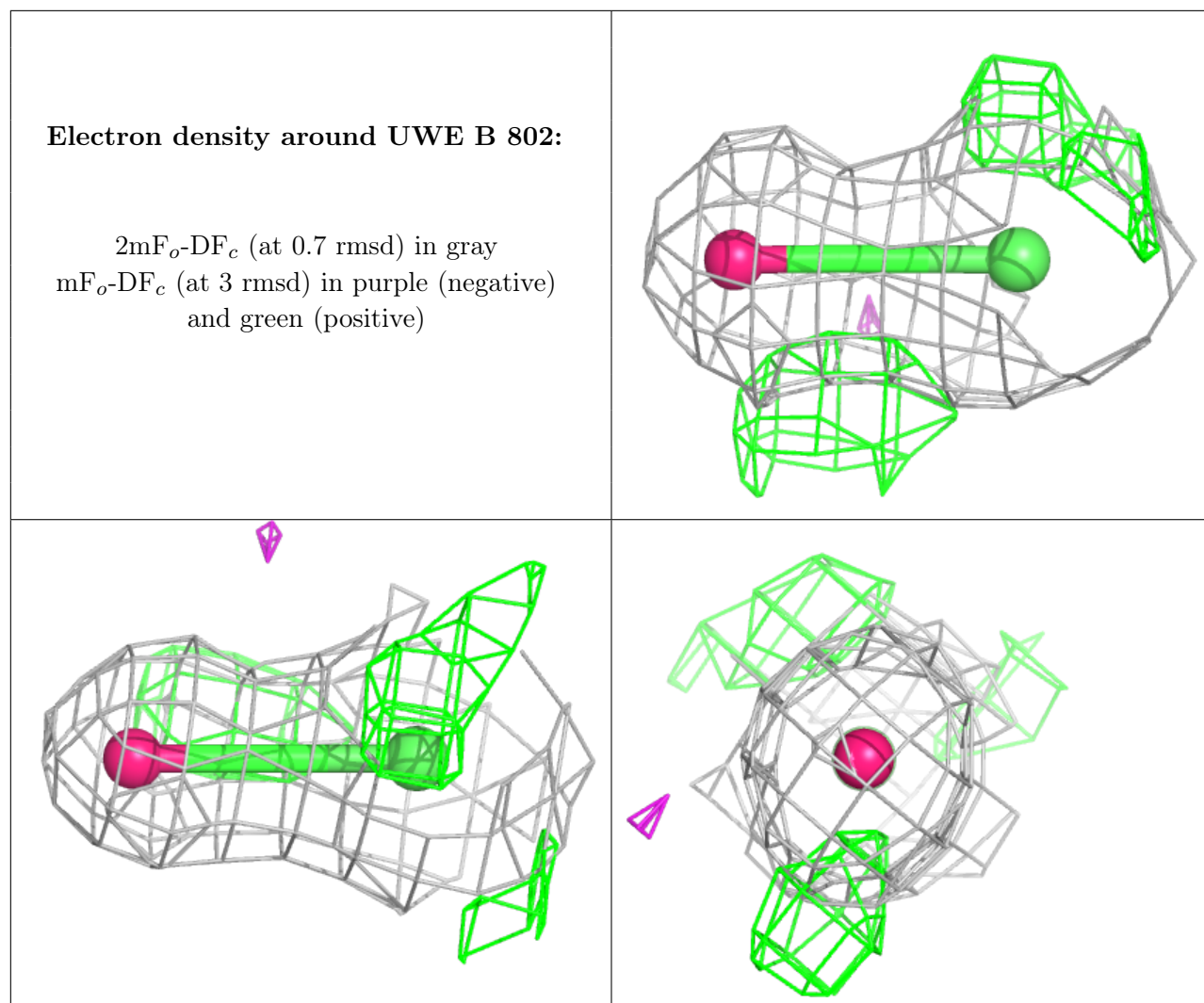
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UWE A 802:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.