



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 10:59 AM UTC

PDB ID : 1E6Y / pdb_00001e6y
Title : Methyl-coenzyme M reductase from Methanosarcina barkeri
Authors : Grabarse, W.; Ermler, U.
Deposited on : 2000-08-23
Resolution : 1.60 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 : **FAILED**
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

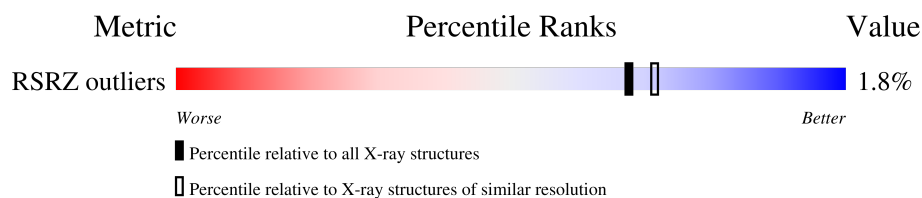
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
RSRZ outliers	180081	4672 (1.60-1.60)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21340 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHYL-COENZYME M REDUCTASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	4	0
			4346	2735	737	846	28			
1	D	568	Total	C	N	O	S	0	3	0
			4348	2738	740	842	28			

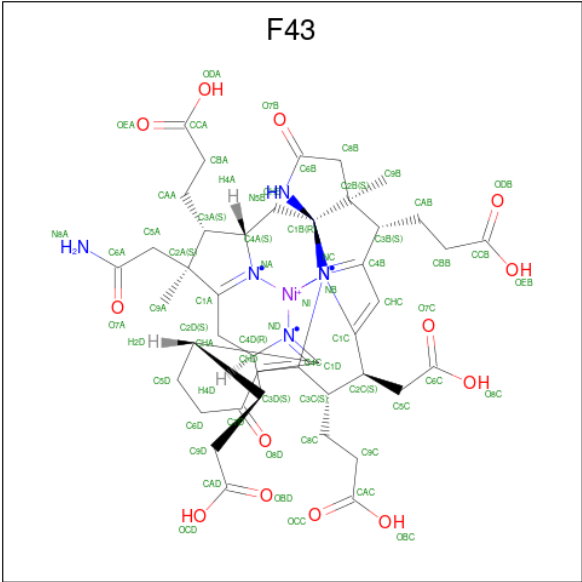
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	4	0
			3176	1987	549	621	19			
2	E	433	Total	C	N	O	S	0	1	0
			3178	1990	550	620	18			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA.

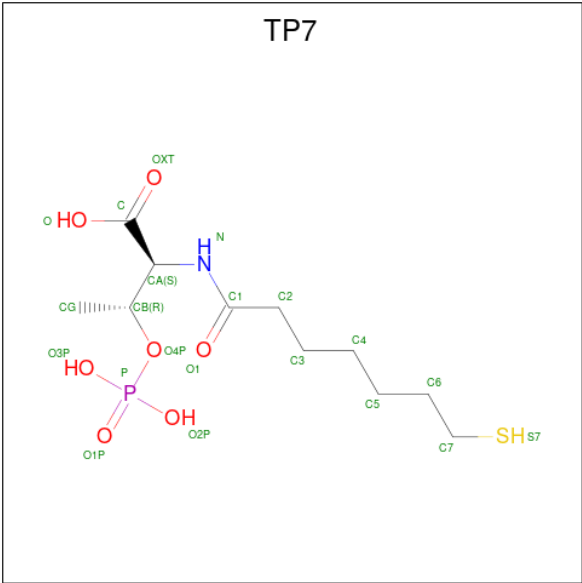
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	0	0
			1947	1202	359	375	11			
3	F	247	Total	C	N	O	S	0	1	0
			1950	1205	359	375	11			

- Molecule 4 is FACTOR 430 (CCD ID: F43) (formula: C₄₂H₅₁N₆NiO₁₃).



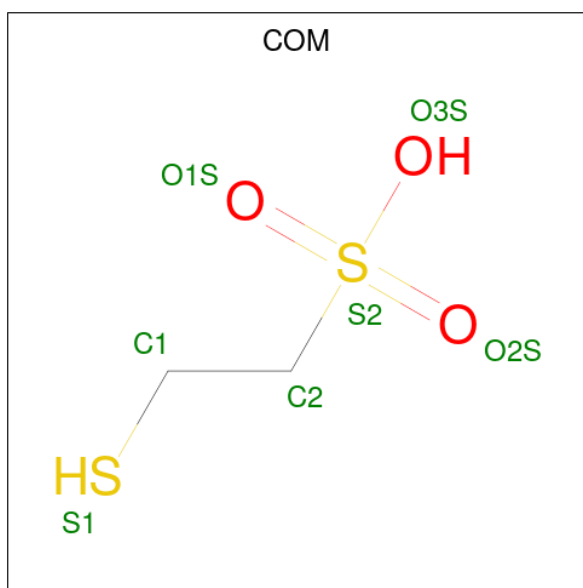
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
4	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 5 is Coenzyme B (CCD ID: TP7) (formula: C₁₁H₂₂NO₇PS).



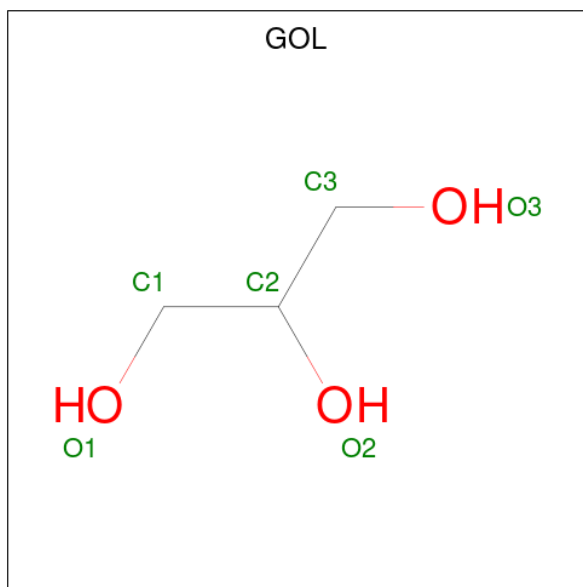
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			7	2	3	2		
6	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	489	Total	O	0	0
			489	489		
8	B	340	Total	O	0	2
			342	342		
8	C	241	Total	O	0	0
			241	241		
8	D	522	Total	O	0	0
			522	522		
8	E	339	Total	O	0	0
			339	339		
8	F	264	Total	O	0	0
			264	264		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.68Å 153.10Å 153.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-1.60) 89.1 (30.00-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 1.60Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.160 , 0.179 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21340	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2047e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	MHS	A	1271	1	10,11,12	1.89	1 (10%)	5,14,16	3.17	2 (40%)
1	AGM	A	1285	1	10,11,12	0.49	0	7,13,15	0.37	0
1	GL3	D	4465	1	2,3,4	2.92	1 (50%)	1,2,4	0.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GL3	A	1465	1	2,3,4	2.96	1 (50%)	1,2,4	0.09	0
3	OCS	F	6065	3	6,8,9	1.40	2 (33%)	7,11,13	1.44	0
3	OCS	C	3065	3	6,8,9	1.53	2 (33%)	7,11,13	1.37	1 (14%)
1	SMC	A	1472	1	5,6,7	0.56	0	3,6,8	0.66	0
1	MHS	D	4271	1	10,11,12	1.91	1 (10%)	5,14,16	3.17	2 (40%)
1	AGM	D	4285	1	10,11,12	0.45	0	7,13,15	0.34	0
1	SMC	D	4472	1	5,6,7	0.57	0	3,6,8	0.62	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
1	MHS	A	1271	1	-	0/5/6/8	0/1/1/1
1	AGM	A	1285	1	-	0/10/11/13	-
1	GL3	D	4465	1	-	1/1/1/2	-
1	GL3	A	1465	1	-	1/1/1/2	-
3	OCS	F	6065	3	-	0/4/7/9	-
3	OCS	C	3065	3	-	0/4/7/9	-
1	SMC	A	1472	1	-	1/3/5/7	-
1	MHS	D	4271	1	-	0/5/6/8	0/1/1/1
1	AGM	D	4285	1	-	0/10/11/13	-
1	SMC	D	4472	1	-	1/3/5/7	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4271	MHS	CM-ND1	5.77	1.58	1.46
1	A	1271	MHS	CM-ND1	5.67	1.57	1.46
1	A	1465	GL3	C-S	-4.18	1.63	1.80
1	D	4465	GL3	C-S	-4.13	1.63	1.80
3	C	3065	OCS	OD1-SG	2.37	1.51	1.45
3	F	6065	OCS	OD1-SG	2.22	1.51	1.45
3	C	3065	OCS	OD3-SG	2.19	1.51	1.45
3	F	6065	OCS	OD3-SG	2.07	1.51	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4271	MHS	ND1-CE1-NE2	-6.39	109.14	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1271	MHS	ND1-CE1-NE2	-6.38	109.14	112.94
1	A	1271	MHS	CD2-NE2-CE1	2.77	108.86	105.24
1	D	4271	MHS	CD2-NE2-CE1	2.72	108.79	105.24
3	C	3065	OCS	OD3-SG-CB	2.15	109.97	106.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1472	SMC	CA-CB-SG-CS
1	A	1465	GL3	S-C-CA-N
1	D	4465	GL3	S-C-CA-N
1	D	4472	SMC	CA-CB-SG-CS

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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	$\# Z > 2$
6	COM	A	2572	4	6,6,6	1.69	2 (33%)	8,8,8	1.11	0
7	GOL	A	2573	-	5,5,5	1.09	0	5,5,5	0.50	0
5	TP7	D	5571	-	19,20,20	2.03	4 (21%)	24,26,26	1.24	2 (8%)
5	TP7	A	2571	-	19,20,20	2.01	5 (26%)	24,26,26	1.24	2 (8%)
6	COM	D	5572	4	6,6,6	1.59	1 (16%)	8,8,8	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	F43	D	5570	1,6	63,71,71	3.70	20 (31%)	73,118,118	2.14	21 (28%)
7	GOL	D	5573	-	5,5,5	1.11	0	5,5,5	0.57	0
4	F43	A	2570	1,6	63,71,71	3.68	20 (31%)	73,118,118	2.14	21 (28%)
7	GOL	A	2574	-	5,5,5	0.94	0	5,5,5	0.50	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
6	COM	A	2572	4	-	0/4/4/4	-
7	GOL	A	2573	-	-	1/4/4/4	-
5	TP7	D	5571	-	-	2/24/24/24	-
5	TP7	A	2571	-	-	2/24/24/24	-
6	COM	D	5572	4	-	1/4/4/4	-
4	F43	D	5570	1,6	-	11/28/185/185	-
7	GOL	D	5573	-	-	0/4/4/4	-
4	F43	A	2570	1,6	-	8/28/185/185	-
7	GOL	A	2574	-	-	0/4/4/4	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5570	F43	CHB-C1B	-18.45	1.41	1.53
4	A	2570	F43	CHB-C1B	-18.09	1.41	1.53
4	D	5570	F43	NI-NA	10.87	2.15	1.89
4	A	2570	F43	NI-NA	10.81	2.15	1.89
4	D	5570	F43	CHD-C1D	8.67	1.57	1.43
4	A	2570	F43	CHD-C1D	8.40	1.57	1.43
4	A	2570	F43	NI-NB	8.06	2.08	1.89
4	D	5570	F43	NI-NB	7.95	2.08	1.89
5	A	2571	TP7	C2-C1	-5.88	1.39	1.51
5	D	5571	TP7	C2-C1	-5.83	1.39	1.51
4	A	2570	F43	CHC-C4B	5.73	1.55	1.39
4	D	5570	F43	CHC-C4B	5.42	1.54	1.39
4	A	2570	F43	CAA-C3A	5.32	1.63	1.53
4	D	5570	F43	CAA-C3A	5.24	1.63	1.53
4	A	2570	F43	C4D-ND	5.02	1.56	1.49
4	D	5570	F43	C4B-NB	-4.80	1.19	1.30
4	A	2570	F43	C4B-NB	-4.67	1.20	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5570	F43	C4D-ND	4.61	1.56	1.49
4	A	2570	F43	NI-ND	4.61	2.00	1.89
4	D	5570	F43	NI-ND	4.14	1.99	1.89
4	A	2570	F43	CAB-C3B	3.84	1.63	1.54
4	D	5570	F43	C3D-C4D	-3.70	1.47	1.53
4	D	5570	F43	CAB-C3B	3.67	1.62	1.54
4	A	2570	F43	CHD-C7D	3.64	1.54	1.45
4	D	5570	F43	CHD-C7D	3.54	1.54	1.45
4	A	2570	F43	C3D-C4D	-3.51	1.47	1.53
5	D	5571	TP7	P-O4P	3.36	1.65	1.59
5	D	5571	TP7	C1-N	3.30	1.41	1.34
5	A	2571	TP7	P-O4P	3.12	1.65	1.59
4	D	5570	F43	C4A-NA	-3.08	1.44	1.49
4	D	5570	F43	C5D-C2D	-3.04	1.48	1.53
4	A	2570	F43	C4A-NA	-3.02	1.44	1.49
5	A	2571	TP7	C1-N	3.02	1.40	1.34
4	A	2570	F43	C5D-C2D	-2.92	1.48	1.53
4	A	2570	F43	CHA-C4D	2.77	1.55	1.53
4	D	5570	F43	CHA-C4D	2.68	1.55	1.53
6	A	2572	COM	O2S-S2	2.67	1.52	1.45
6	D	5572	COM	O2S-S2	2.63	1.52	1.45
4	A	2570	F43	C9A-C2A	-2.60	1.50	1.54
4	D	5570	F43	C9D-C3D	-2.60	1.48	1.53
4	D	5570	F43	C9A-C2A	-2.51	1.50	1.54
4	A	2570	F43	C9D-C3D	-2.40	1.49	1.53
4	D	5570	F43	C8B-C2B	-2.30	1.51	1.54
4	A	2570	F43	C8B-C2B	-2.28	1.51	1.54
4	D	5570	F43	C2A-C3A	2.24	1.58	1.54
5	D	5571	TP7	CA-C	2.22	1.56	1.52
4	A	2570	F43	CHB-C4A	2.18	1.54	1.51
6	A	2572	COM	C2-S2	2.17	1.80	1.77
5	A	2571	TP7	CA-C	2.15	1.55	1.52
4	A	2570	F43	C2A-C3A	2.10	1.58	1.54
5	A	2571	TP7	O1-C1	2.09	1.27	1.23
4	D	5570	F43	C3C-C4C	-2.01	1.47	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2570	F43	C3B-C4B-CHC	-5.68	111.24	123.33
4	D	5570	F43	C3B-C4B-CHC	-5.65	111.31	123.33
4	D	5570	F43	C3D-C4D-ND	5.47	110.83	102.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2570	F43	C3D-C4D-ND	5.39	110.70	102.34
4	A	2570	F43	CAB-C3B-C2B	-5.35	107.20	119.00
4	D	5570	F43	CAB-C3B-C2B	-5.33	107.24	119.00
4	A	2570	F43	C4D-ND-C1D	-5.08	100.85	108.46
4	D	5570	F43	C4D-ND-C1D	-4.98	101.00	108.46
4	D	5570	F43	O8D-C7D-C6D	-4.61	113.32	120.87
4	A	2570	F43	O8D-C7D-C6D	-4.57	113.39	120.87
4	A	2570	F43	C2D-C1D-ND	4.15	120.39	110.54
4	D	5570	F43	C2D-C1D-ND	4.14	120.37	110.54
4	A	2570	F43	C6D-C7D-CHD	3.82	123.99	116.94
4	D	5570	F43	C6D-C7D-CHD	3.78	123.91	116.94
4	D	5570	F43	C3A-C2A-C1A	-3.74	96.23	99.97
4	A	2570	F43	C3A-C2A-C1A	-3.66	96.31	99.97
5	D	5571	TP7	O1-C1-N	-3.31	117.35	122.95
5	A	2571	TP7	O1-C1-N	-3.26	117.43	122.95
4	A	2570	F43	C5C-C2C-C3C	-3.02	107.59	115.05
4	A	2570	F43	C2B-C1B-N5B	-2.94	96.11	105.72
4	D	5570	F43	C2B-C1B-N5B	-2.90	96.26	105.72
4	A	2570	F43	C3A-C4A-NA	2.88	106.68	102.30
4	D	5570	F43	C2B-C1B-NB	2.86	106.11	101.86
4	D	5570	F43	C5C-C2C-C3C	-2.85	108.02	115.05
4	D	5570	F43	C3A-C4A-NA	2.81	106.57	102.30
4	A	2570	F43	OEB-CCB-CBB	2.77	122.75	114.00
4	A	2570	F43	C2B-C1B-NB	2.74	105.94	101.86
4	A	2570	F43	C2D-C1D-CHD	-2.73	118.47	121.85
4	A	2570	F43	ODB-CCB-CBB	-2.70	114.52	123.09
4	D	5570	F43	OEB-CCB-CBB	2.70	122.54	114.00
4	D	5570	F43	ODB-CCB-CBB	-2.68	114.58	123.09
4	D	5570	F43	C2D-C1D-CHD	-2.66	118.55	121.85
4	A	2570	F43	C8B-C2B-C1B	2.64	108.26	102.21
4	D	5570	F43	C8B-C2B-C1B	2.64	108.25	102.21
4	A	2570	F43	C5D-C2D-C1D	2.50	113.69	110.43
4	D	5570	F43	CHA-C4D-C3D	-2.45	111.00	117.90
4	A	2570	F43	CHA-C4D-C3D	-2.44	111.01	117.90
5	D	5571	TP7	C4-C3-C2	2.39	121.89	113.13
4	D	5570	F43	C5D-C2D-C1D	2.38	113.54	110.43
4	A	2570	F43	C1B-N5B-C6B	2.38	119.09	112.40
4	D	5570	F43	C1B-N5B-C6B	2.36	119.06	112.40
4	A	2570	F43	OBC-CAC-C9C	2.34	121.38	114.00
4	D	5570	F43	OBC-CAC-C9C	2.33	121.36	114.00
5	A	2571	TP7	C4-C3-C2	2.30	121.59	113.13
4	D	5570	F43	OCC-CAC-C9C	-2.06	116.56	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2570	F43	OCC-CAC-C9C	-2.02	116.68	123.09

There are no chirality outliers.

All (25) torsion outliers are listed below:

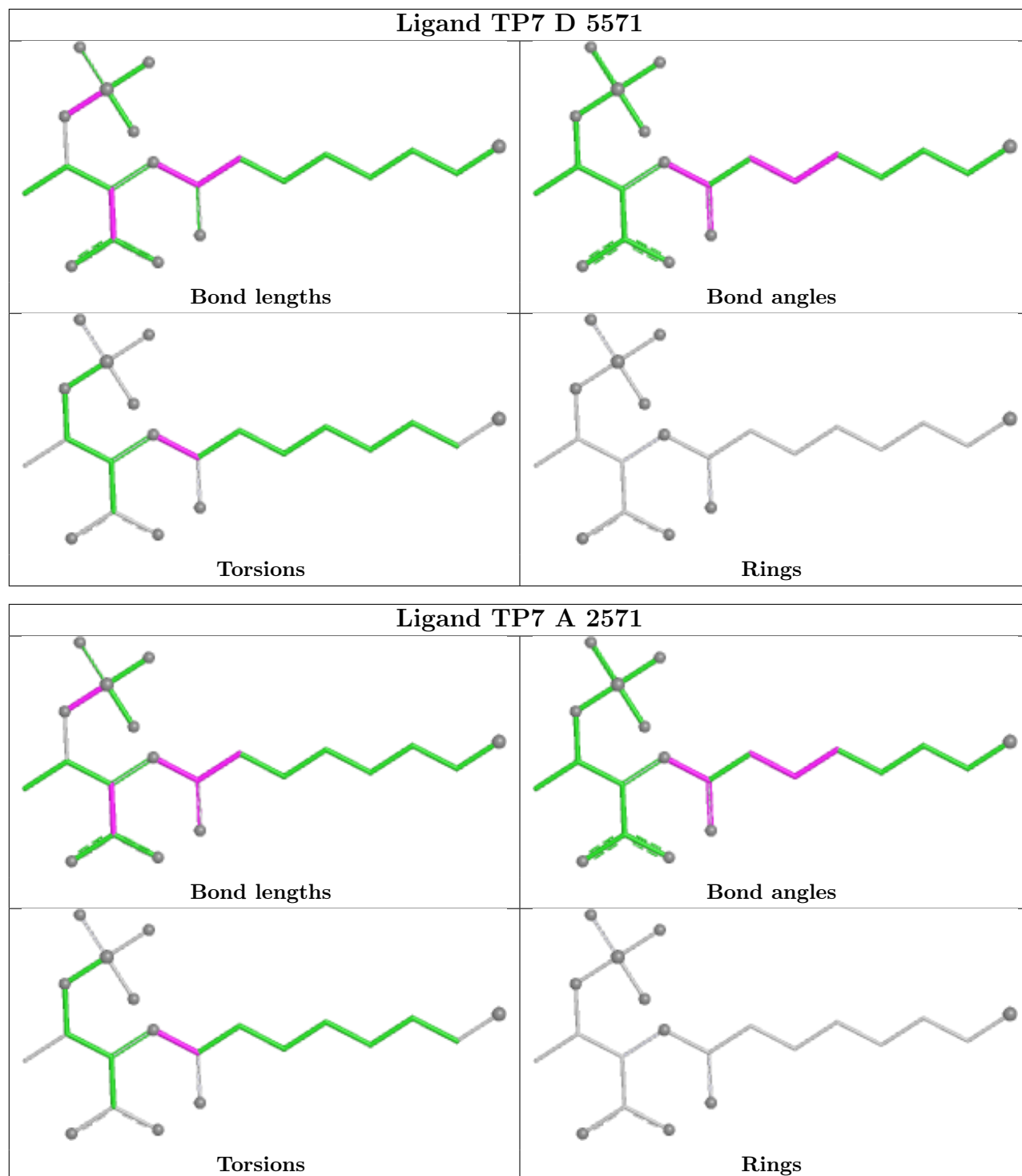
Mol	Chain	Res	Type	Atoms
4	A	2570	F43	C3A-CAA-CBA-CCA
4	D	5570	F43	C3A-CAA-CBA-CCA
5	D	5571	TP7	O1-C1-N-CA
5	D	5571	TP7	C2-C1-N-CA
5	A	2571	TP7	O1-C1-N-CA
7	A	2573	GOL	O2-C2-C3-O3
5	A	2571	TP7	C2-C1-N-CA
4	D	5570	F43	CAA-CBA-CCA-ODA
4	D	5570	F43	CAB-CBB-CCB-OEB
4	A	2570	F43	CAA-CBA-CCA-OEA
4	A	2570	F43	CAB-CBB-CCB-OEB
4	D	5570	F43	CAA-CBA-CCA-OEA
4	D	5570	F43	C8C-C9C-CAC-OBC
4	A	2570	F43	C8C-C9C-CAC-OBC
4	D	5570	F43	CAB-CBB-CCB-ODB
4	A	2570	F43	C8C-C9C-CAC-OCC
4	D	5570	F43	C8C-C9C-CAC-OCC
4	A	2570	F43	CAB-CBB-CCB-ODB
4	A	2570	F43	CAA-CBA-CCA-ODA
4	D	5570	F43	C3D-C9D-CAD-OCD
6	D	5572	COM	C1-C2-S2-O2S
4	A	2570	F43	C3D-C9D-CAD-OCD
4	D	5570	F43	C2C-C5C-C6C-O7C
4	D	5570	F43	C2C-C5C-C6C-O8C
4	D	5570	F43	C3D-C9D-CAD-ODB

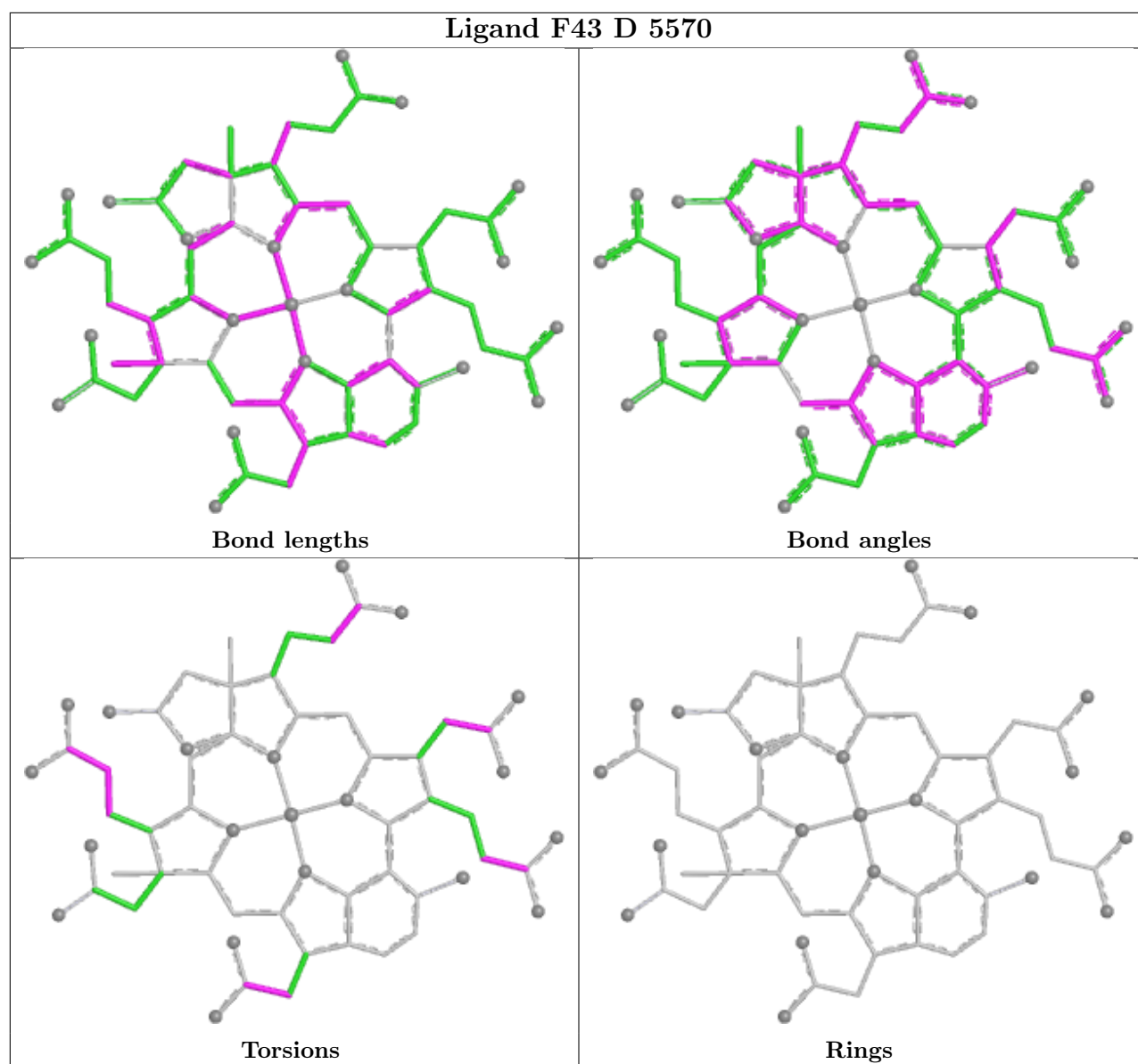
There are no ring outliers.

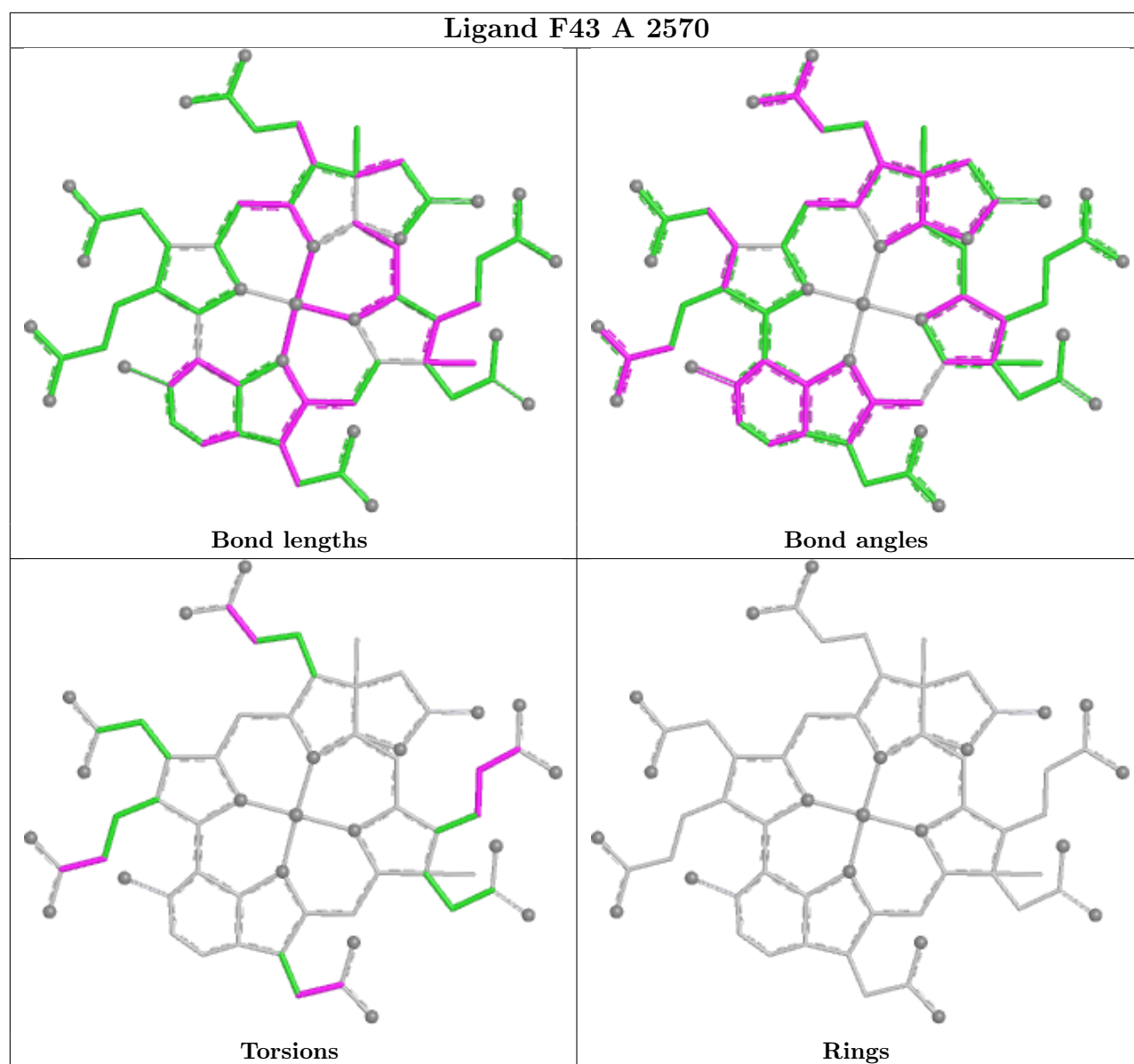
No monomer is involved in short contacts.

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.







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	564/569 (99%)	-0.33	11 (1%) 65 69	7, 12, 22, 36	4 (0%)
1	D	564/569 (99%)	-0.40	6 (1%) 78 82	7, 11, 20, 36	3 (0%)
2	B	432/433 (99%)	-0.28	10 (2%) 61 64	8, 12, 24, 42	4 (0%)
2	E	433/433 (100%)	-0.35	7 (1%) 70 74	8, 12, 22, 37	1 (0%)
3	C	246/247 (99%)	-0.12	5 (2%) 65 69	9, 15, 24, 35	0
3	F	246/247 (99%)	-0.19	5 (2%) 65 69	10, 14, 24, 39	1 (0%)
All	All	2485/2498 (99%)	-0.31	44 (1%) 67 71	7, 12, 23, 42	13 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2433	VAL	6.4
1	A	1569	ALA	5.3
1	D	4569	ALA	4.5
2	B	2002	SER	4.1
1	D	4002	ALA	4.0
3	C	3064	ALA	3.8
3	C	3002	ALA	3.6
3	F	6196	ARG	3.5
1	A	1369	ASP	3.2
3	F	6195	ASP	3.2
2	E	5434	LEU	3.2
1	A	1028	GLY	3.1
1	D	4369	ASP	3.1
2	B	2103	VAL	3.0
3	C	3196	ARG	3.0
1	A	1004	ASP	3.0
1	A	1204	GLU	2.8
3	F	6064	ALA	2.8
1	A	1002	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	5103	VAL	2.6
2	B	2104	LYS	2.6
2	B	2412	LEU	2.6
2	B	2283	LYS	2.5
1	D	4567	ILE	2.5
1	D	4372	ASN	2.5
2	E	5104	LYS	2.5
3	F	6207	GLU	2.4
1	A	1027	THR	2.3
2	B	2431	ALA	2.3
2	E	5431	ALA	2.3
1	A	1388	GLU	2.3
2	E	5202	ASN	2.3
3	F	6002	ALA	2.2
1	A	1372	ASN	2.2
2	E	5416	VAL	2.1
1	A	1061	GLU	2.1
2	B	2432	GLY	2.1
3	C	3195	ASP	2.1
3	C	3004	GLU	2.1
2	B	2418	GLY	2.1
2	B	2416	VAL	2.1
1	D	4141	GLU	2.1
1	A	1003	ALA	2.0
2	E	5433	VAL	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
3	OCS	C	3065	9/10	0.94	0.09	19,24,26,26	0
3	OCS	F	6065	9/10	0.95	0.09	18,22,25,25	0
1	MHS	D	4271	11/12	0.96	0.06	10,11,12,13	0
1	AGM	A	1285	12/13	0.97	0.04	6,7,8,8	0
1	MHS	A	1271	11/12	0.97	0.05	9,10,12,12	0
1	AGM	D	4285	12/13	0.98	0.04	6,7,8,8	0
1	SMC	D	4472	7/8	0.98	0.05	9,10,10,10	0
1	SMC	A	1472	7/8	0.98	0.04	9,9,10,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	GL3	A	1465	4/5	0.99	0.04	9,9,9,9	0
1	GL3	D	4465	4/5	0.99	0.04	8,8,8,8	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

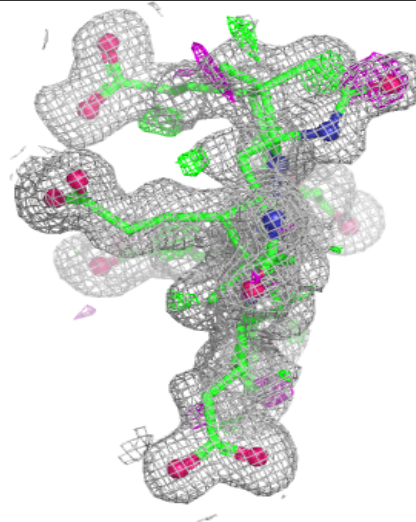
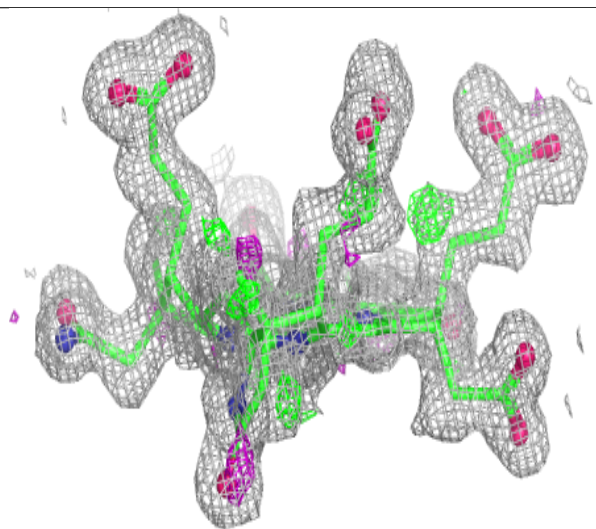
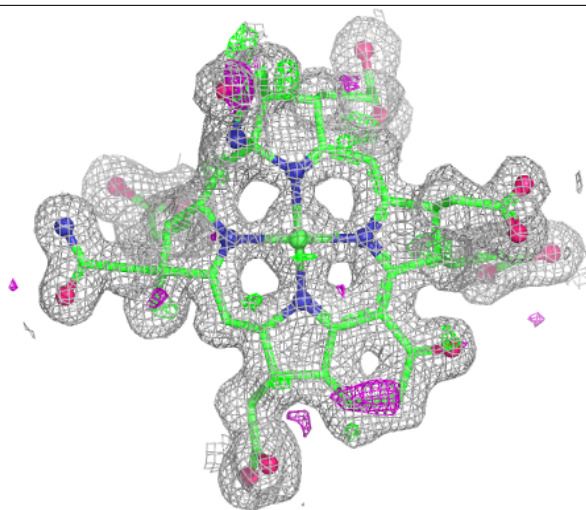
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	D	5573	6/6	0.69	0.20	30,32,33,35	0
7	GOL	A	2574	6/6	0.72	0.23	36,38,39,40	0
7	GOL	A	2573	6/6	0.73	0.19	33,34,35,37	0
6	COM	D	5572	7/7	0.94	0.11	16,17,17,18	0
6	COM	A	2572	7/7	0.94	0.10	15,16,17,18	0
4	F43	D	5570	62/62	0.97	0.07	8,10,12,13	0
4	F43	A	2570	62/62	0.97	0.07	8,10,11,14	0
5	TP7	D	5571	21/21	0.98	0.04	7,9,10,12	0
5	TP7	A	2571	21/21	0.98	0.05	8,8,10,12	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.

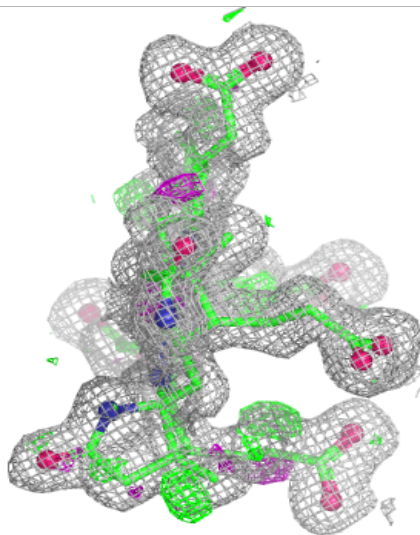
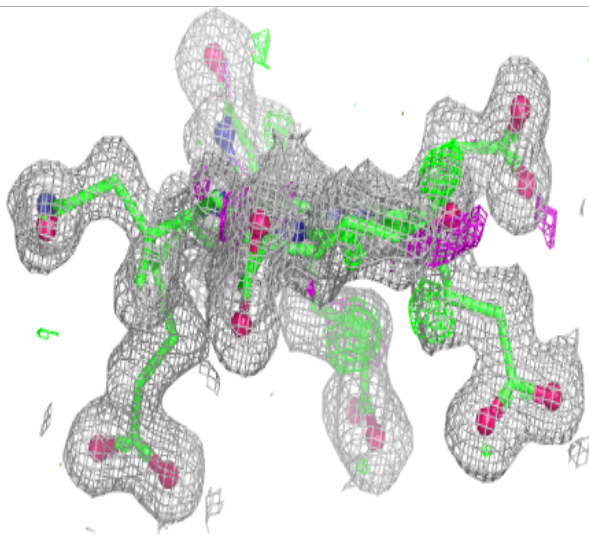
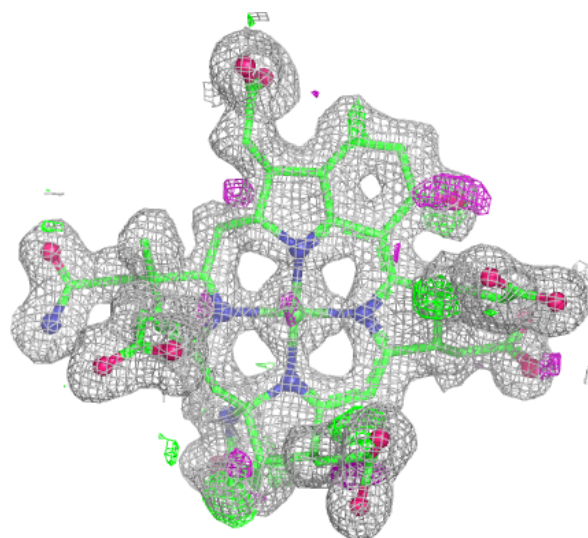
Electron density around F43 D 5570:

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



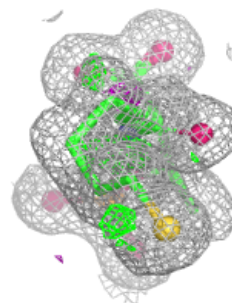
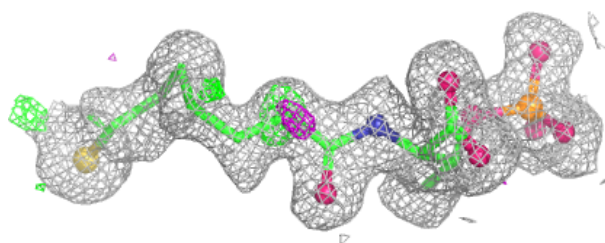
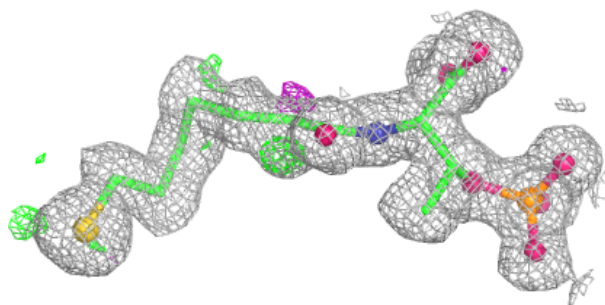
Electron density around F43 A 2570:

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

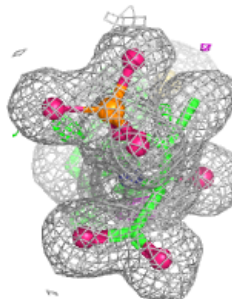
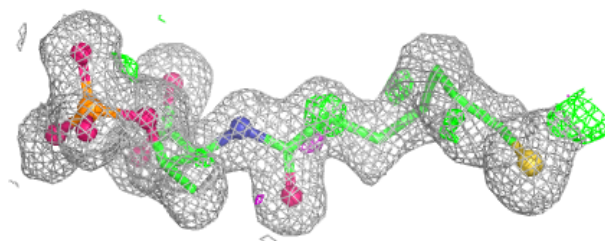
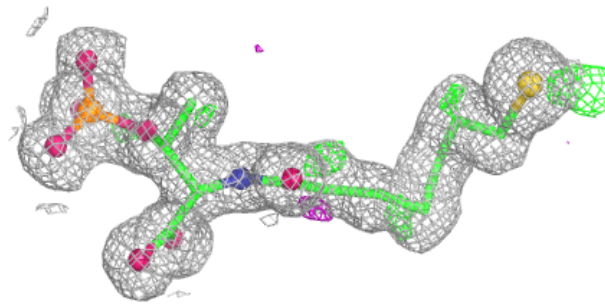


Electron density around TP7 D 5571:

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

**Electron density around TP7 A 2571:**

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



5.5 Other polymers ⓘ

There are no such residues in this entry.