wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2024 – 05:51 PM EDT

PDB ID	:	1E6Y
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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

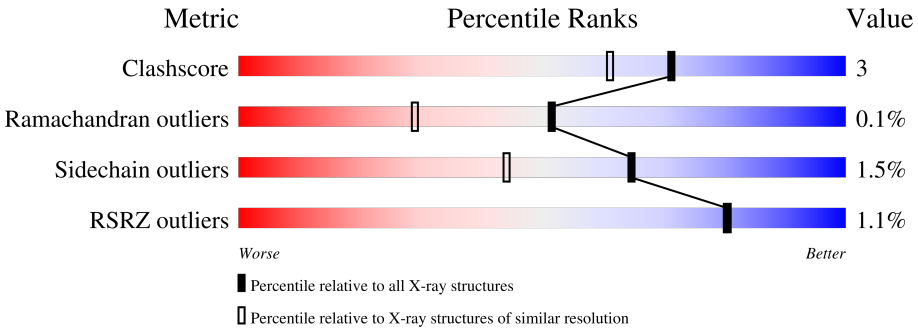
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	569	88% 11%
1	D	569	90% 9%
2	B	433	92% 7%
2	E	433	91% 9%
3	C	247	88% 12%
3	F	247	87% 12%

2 Entry composition (i)

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			

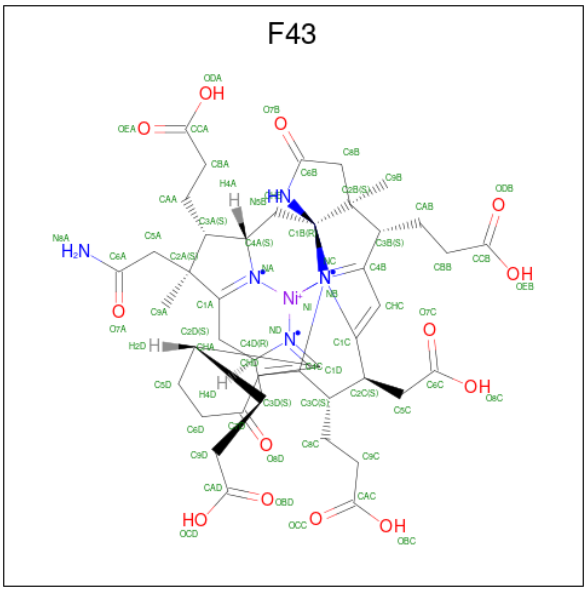
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

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.

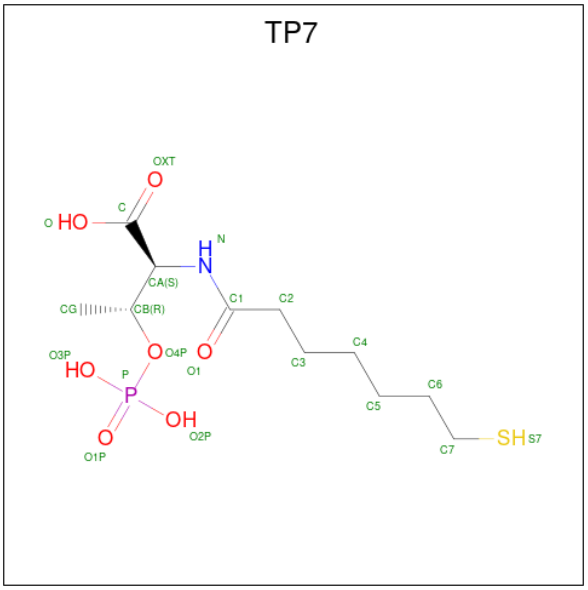
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	0	0
			1947	1202	359	375	11			
3	F	247	Total	C	N	O	S	0	1	0
			1950	1205	359	375	11			

- Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



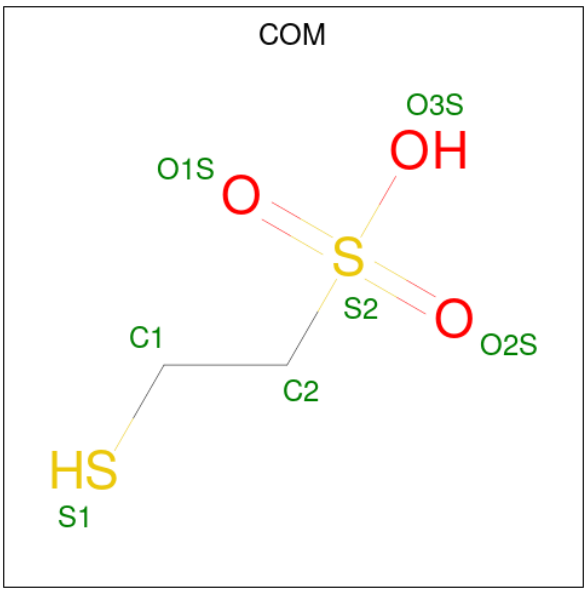
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
4	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 5 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



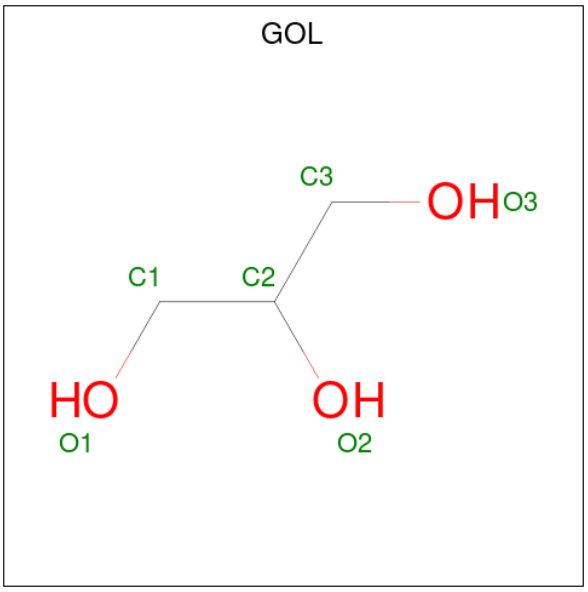
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 8 is water.

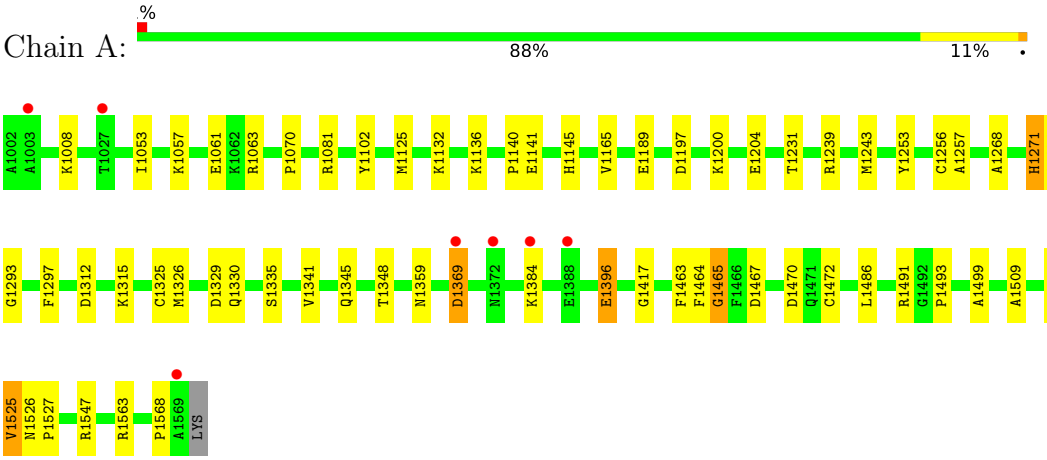
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	489	Total O 489 489	0	0
8	B	340	Total O 342 342	0	2
8	C	241	Total O 241 241	0	0
8	D	522	Total O 522 522	0	0
8	E	339	Total O 339 339	0	0
8	F	264	Total O 264 264	0	0

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.

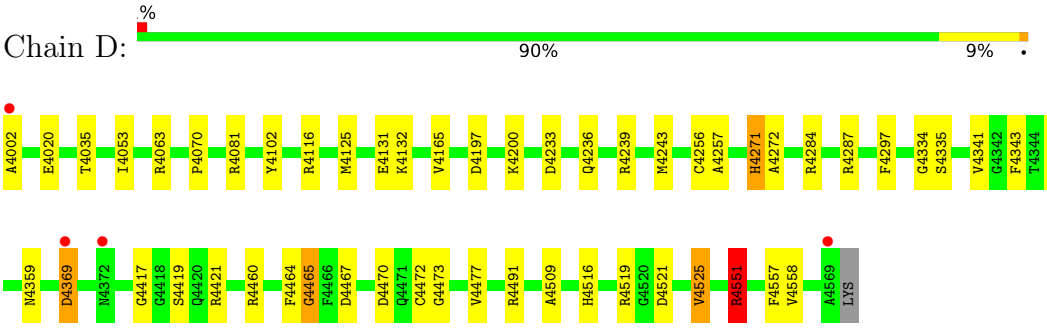
• Molecule 1: METHYL-COENZYME M REDUCTASE SUBUNIT ALPHA

Chain A:



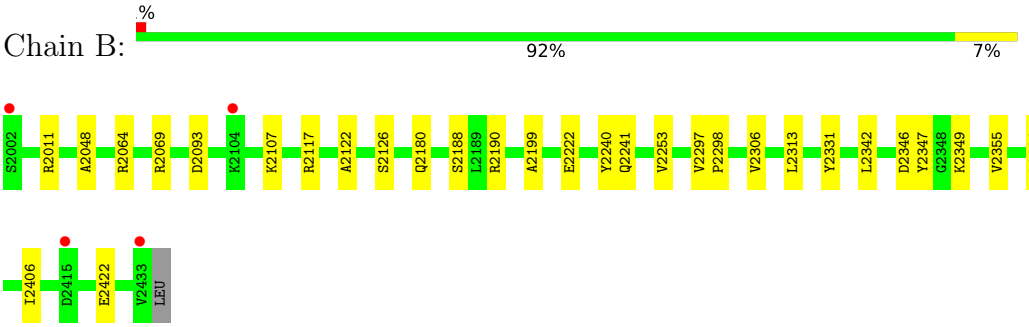
• Molecule 1: METHYL-COENZYME M REDUCTASE SUBUNIT ALPHA

Chain D:



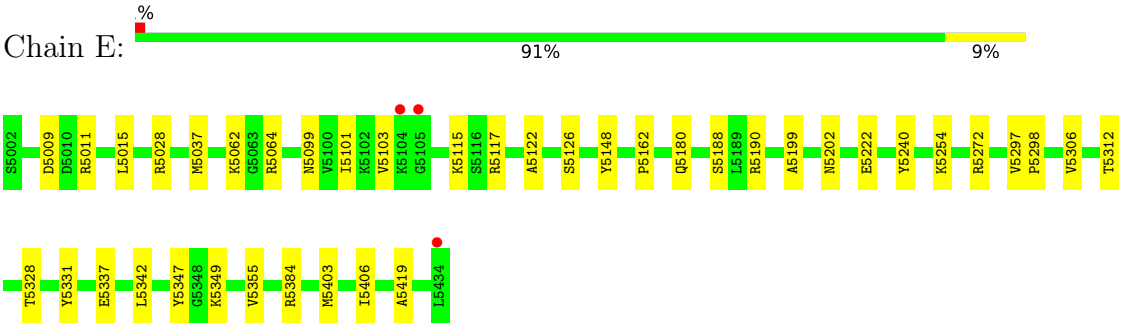
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain B:



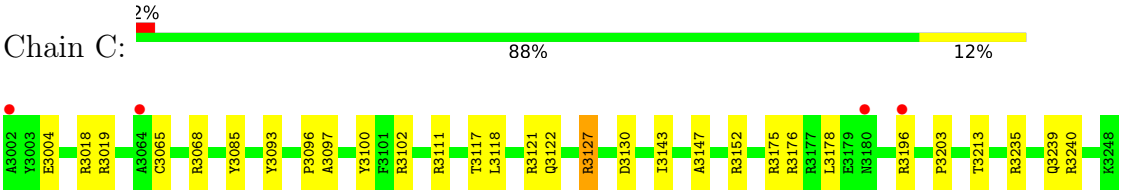
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain E:



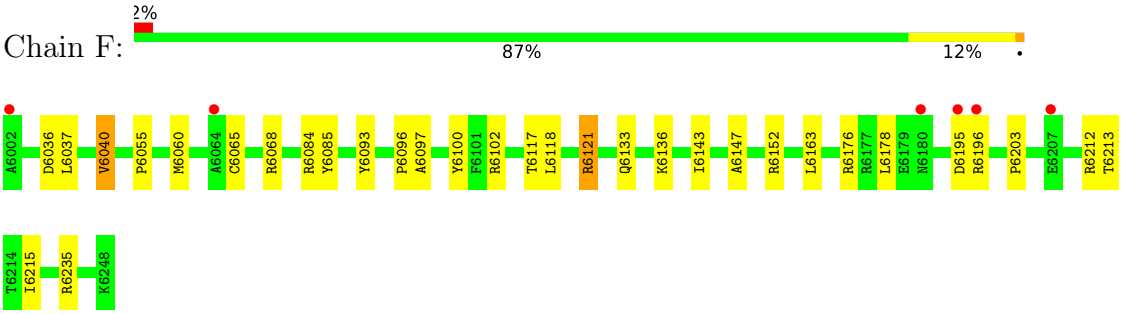
• Molecule 3: METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA

Chain C:



• Molecule 3: METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA

Chain F:



4 Data and refinement statistics (i)

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 22.25 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-1.60) 89.2 (22.25-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 1.60Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.160 , 0.179 0.159 , (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 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SMC, GL3, OCS, AGM, COM, F43, TP7, MHS, GOL

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	0.31	0/4423	0.68	9/5988 (0.2%)
1	D	0.64	6/4418 (0.1%)	1.95	26/5979 (0.4%)
2	B	0.29	0/3244	0.61	8/4390 (0.2%)
2	E	0.30	0/3231	0.65	8/4372 (0.2%)
3	C	0.31	0/1976	0.85	17/2666 (0.6%)
3	F	0.32	0/1983	1.85	15/2676 (0.6%)
All	All	0.41	6/19275 (0.0%)	1.24	83/26071 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
2	B	0	2
2	E	0	3
3	C	0	1
3	F	0	1
All	All	0	11

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4551[A]	ARG	CZ-NH2	22.62	1.62	1.33
1	D	4551[B]	ARG	CZ-NH2	22.62	1.62	1.33
1	D	4551[A]	ARG	NE-CZ	10.05	1.46	1.33
1	D	4551[B]	ARG	NE-CZ	10.05	1.46	1.33
1	D	4551[A]	ARG	CG-CD	-8.02	1.31	1.51

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4551[A]	ARG	NH1-CZ-NH2	-85.30	25.57	119.40
1	D	4551[B]	ARG	NH1-CZ-NH2	-85.30	25.57	119.40
3	F	6040[A]	VAL	CG1-CB-CG2	-59.08	16.37	110.90
3	F	6040[B]	VAL	CG1-CB-CG2	-59.08	16.37	110.90
1	D	4551[A]	ARG	NE-CZ-NH2	-44.85	97.87	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1396[A]	GLU	Sidechain
1	A	1396[B]	GLU	Sidechain
2	B	2331	TYR	Sidechain
2	B	2347	TYR	Sidechain
3	C	3093	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4346	0	4191	39	0
1	D	4348	0	4205	50	0
2	B	3176	0	3161	17	0
2	E	3178	0	3170	22	0
3	C	1947	0	1888	9	0
3	F	1950	0	1894	13	0
4	A	62	0	43	6	0
4	D	62	0	43	5	0
5	A	21	0	19	2	0
5	D	21	0	19	1	0
6	A	7	0	5	1	0
6	D	7	0	5	0	0
7	A	12	0	16	0	0
7	D	6	0	8	0	0
8	A	489	0	0	5	0
8	B	342	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	241	0	0	1	0
8	D	522	0	0	4	0
8	E	339	0	0	4	0
8	F	264	0	0	2	0
All	All	21340	0	18667	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 131 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:D:4551[B]:ARG:NH2	1:D:4551[B]:ARG:CZ	1.69	1.56
1:D:4551[B]:ARG:CD	1:D:4551[B]:ARG:CG	1.76	1.55
1:D:4551[B]:ARG:CG	1:D:4551[B]:ARG:NE	1.87	1.38
1:D:4551[B]:ARG:CD	1:D:4551[B]:ARG:CB	2.38	1.01
1:D:4551[B]:ARG:HE	1:D:4551[B]:ARG:HG2	1.24	1.01

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/569 (100%)	546 (96%)	19 (3%)	1 (0%)	47	26
1	D	565/569 (99%)	546 (97%)	18 (3%)	1 (0%)	47	26
2	B	434/433 (100%)	428 (99%)	6 (1%)	0	100	100
2	E	432/433 (100%)	426 (99%)	6 (1%)	0	100	100
3	C	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
3	F	245/247 (99%)	237 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2486/2498 (100%)	2422 (97%)	62 (2%)	2 (0%)	51 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1525	VAL
1	D	4525	VAL

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	446/443 (101%)	436 (98%)	10 (2%)	52 27
1	D	445/443 (100%)	436 (98%)	9 (2%)	55 31
2	B	335/332 (101%)	333 (99%)	2 (1%)	86 77
2	E	333/332 (100%)	331 (99%)	2 (1%)	86 77
3	C	201/201 (100%)	197 (98%)	4 (2%)	55 31
3	F	202/201 (100%)	198 (98%)	4 (2%)	55 31
All	All	1962/1952 (100%)	1931 (98%)	31 (2%)	65 41

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3178	LEU
3	F	6176	ARG
1	D	4131	GLU
3	F	6195	ASP
1	D	4551[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	3239	GLN
1	D	4019	GLN
3	F	6133	GLN
2	E	5402	GLN
2	B	2241	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)

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	D	4271	1	7,11,12	1.81	1 (14%)	6,14,16	1.29	1 (16%)
3	OCS	F	6065	3	7,8,9	1.24	2 (28%)	6,11,13	1.68	3 (50%)
1	AGM	A	1285	1	10,11,12	0.49	0	6,13,15	0.33	0
1	GL3	A	1465	1	2,3,4	3.52	1 (50%)	1,2,4	0.12	0
1	SMC	A	1472	1	5,6,7	0.61	0	2,6,8	0.53	0
1	AGM	D	4285	1	10,11,12	0.46	0	6,13,15	0.25	0
1	SMC	D	4472	1	5,6,7	0.60	0	2,6,8	0.52	0
1	MHS	A	1271	1	7,11,12	1.82	1 (14%)	6,14,16	1.35	1 (16%)
1	GL3	D	4465	1	2,3,4	3.47	1 (50%)	1,2,4	0.03	0
3	OCS	C	3065	3	7,8,9	1.34	2 (28%)	6,11,13	1.70	2 (33%)

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	D	4271	1	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCS	F	6065	3	-	0/4/7/9	-
1	AGM	A	1285	1	-	0/10/11/13	-
1	GL3	A	1465	1	-	1/1/1/2	-
1	SMC	A	1472	1	-	1/3/5/7	-
1	AGM	D	4285	1	-	0/10/11/13	-
1	SMC	D	4472	1	-	1/3/5/7	-
1	MHS	A	1271	1	-	0/5/6/8	0/1/1/1
1	GL3	D	4465	1	-	1/1/1/2	-
3	OCS	C	3065	3	-	0/4/7/9	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1465	GL3	C-S	-4.97	1.63	1.80
1	D	4465	GL3	C-S	-4.91	1.63	1.80
1	D	4271	MHS	CM-ND1	4.57	1.58	1.47
1	A	1271	MHS	CM-ND1	4.49	1.57	1.47
3	C	3065	OCS	OD1-SG	2.29	1.51	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3065	OCS	OD3-SG-CB	2.55	109.97	106.94
3	F	6065	OCS	OD2-SG-CB	2.43	109.61	105.74
3	C	3065	OCS	OD2-SG-CB	2.20	109.25	105.74
1	D	4271	MHS	NE2-CE1-ND1	-2.10	109.14	112.26
1	A	1271	MHS	NE2-CE1-ND1	-2.10	109.14	112.26

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	D	4472	SMC	CA-CB-SG-CS
1	A	1465	GL3	S-C-CA-N
1	D	4465	GL3	S-C-CA-N

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	4271	MHS	1	0
1	A	1465	GL3	1	0
1	A	1472	SMC	1	0
1	D	4472	SMC	1	0
1	A	1271	MHS	1	0
1	D	4465	GL3	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 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	$\#\|Z\| > 2$
4	F43	A	2570	1,6	61,71,71	3.85	20 (32%)	64,118,118	2.11	15 (23%)
5	TP7	A	2571	-	19,20,20	2.03	5 (26%)	24,26,26	1.23	2 (8%)
4	F43	D	5570	1,6	61,71,71	3.87	21 (34%)	64,118,118	2.10	16 (25%)
7	GOL	D	5573	-	5,5,5	1.05	0	5,5,5	0.55	0
6	COM	A	2572	4	6,6,6	1.66	2 (33%)	7,8,8	1.35	1 (14%)
6	COM	D	5572	4	6,6,6	1.56	1 (16%)	7,8,8	1.39	1 (14%)
7	GOL	A	2574	-	5,5,5	0.89	0	5,5,5	0.48	0
5	TP7	D	5571	-	19,20,20	2.05	4 (21%)	24,26,26	1.23	2 (8%)
7	GOL	A	2573	-	5,5,5	1.02	0	5,5,5	0.49	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
4	F43	A	2570	1,6	-	10/28/185/185	-
5	TP7	A	2571	-	-	2/24/24/24	-
4	F43	D	5570	1,6	-	10/28/185/185	-
7	GOL	D	5573	-	-	0/4/4/4	-
6	COM	A	2572	4	-	0/4/4/4	-
6	COM	D	5572	4	-	2/4/4/4	-
7	GOL	A	2574	-	-	0/4/4/4	-
5	TP7	D	5571	-	-	2/24/24/24	-
7	GOL	A	2573	-	-	1/4/4/4	-

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5570	F43	CHB-C1B	-18.14	1.41	1.53
4	A	2570	F43	CHB-C1B	-17.79	1.41	1.53
4	D	5570	F43	NI-NA	12.09	2.15	1.89
4	A	2570	F43	NI-NA	12.02	2.15	1.89
4	D	5570	F43	CHD-C1D	10.48	1.57	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2570	F43	C4D-ND-C1D	-5.83	100.85	108.51
4	D	5570	F43	C4D-ND-C1D	-5.71	101.00	108.51
4	A	2570	F43	CAB-C3B-C2B	-5.62	107.20	119.09
4	D	5570	F43	CAB-C3B-C2B	-5.60	107.24	119.09
4	A	2570	F43	C3B-C4B-CHC	-5.60	111.24	123.32

There are no chirality outliers.

5 of 27 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	A	2571	TP7	O1-C1-N-CA
5	D	5571	TP7	C2-C1-N-CA

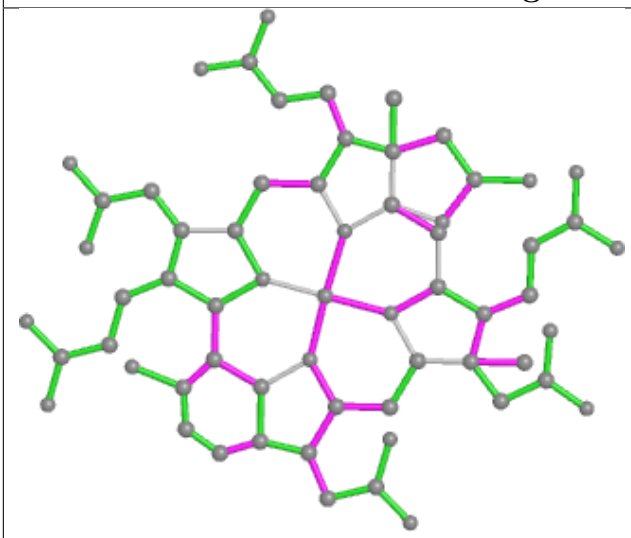
There are no ring outliers.

5 monomers are involved in 15 short contacts:

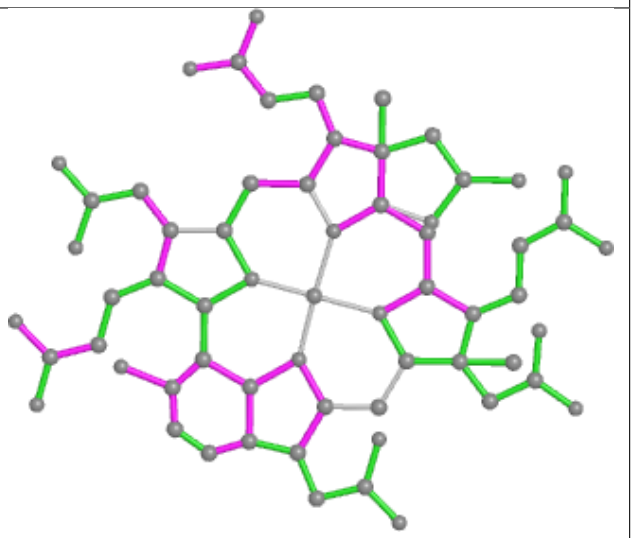
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2570	F43	6	0
5	A	2571	TP7	2	0
4	D	5570	F43	5	0
6	A	2572	COM	1	0
5	D	5571	TP7	1	0

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 then 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.

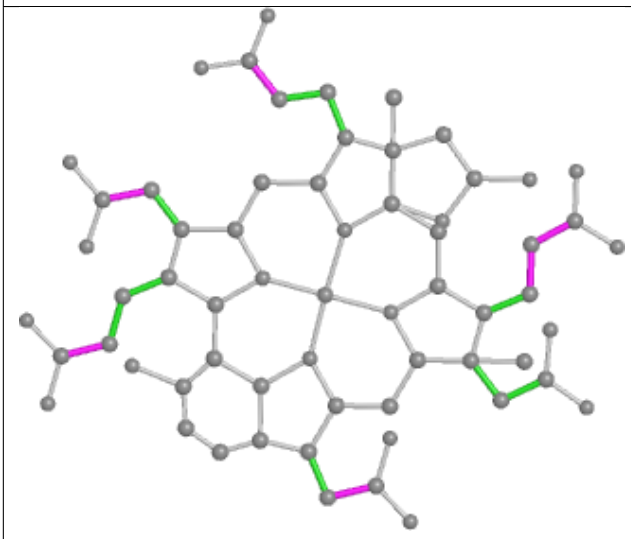
Ligand F43 A 2570



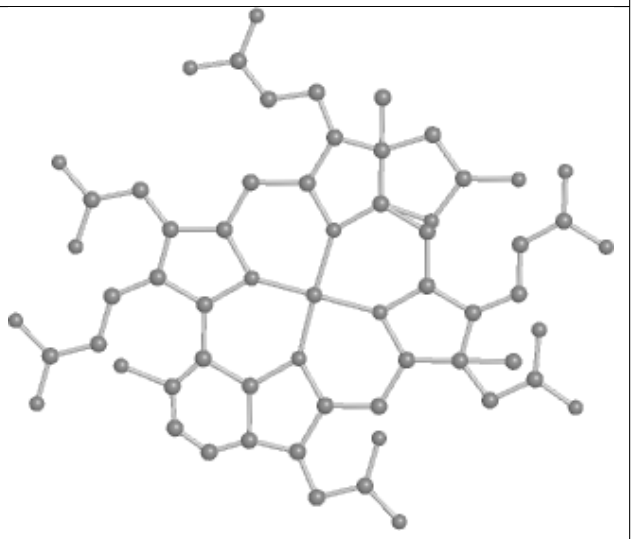
Bond lengths



Bond angles

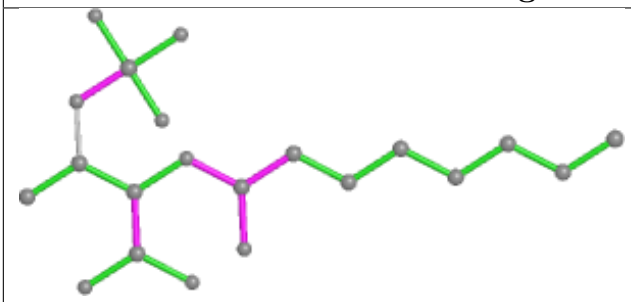


Torsions

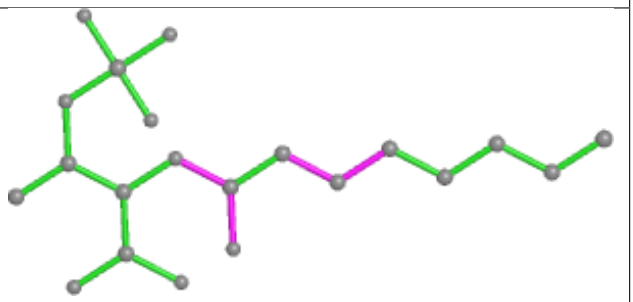


Rings

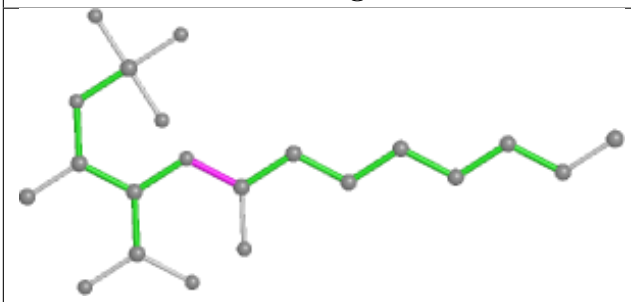
Ligand TP7 A 2571



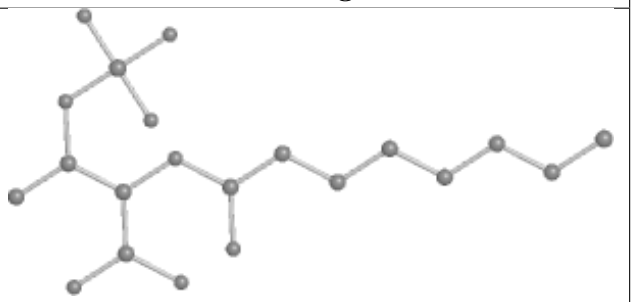
Bond lengths



Bond angles

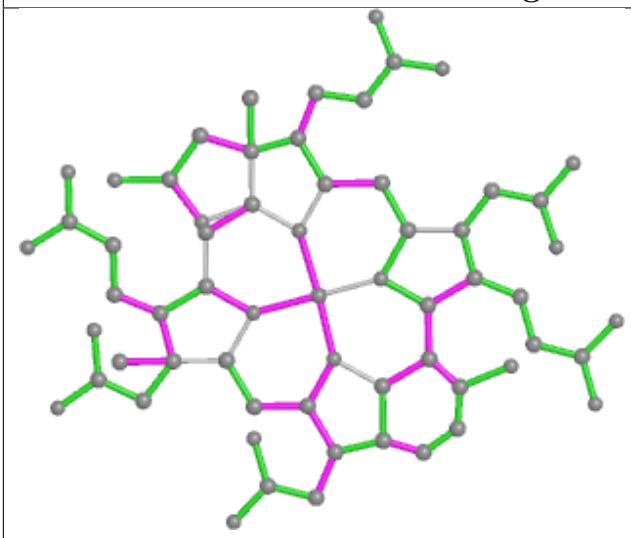


Torsions

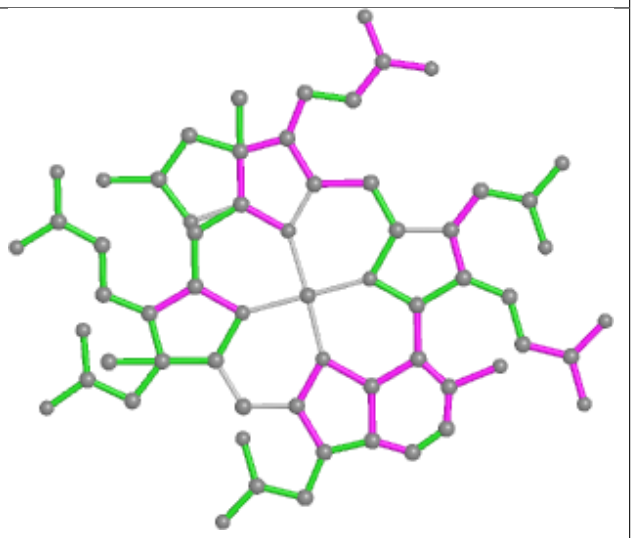


Rings

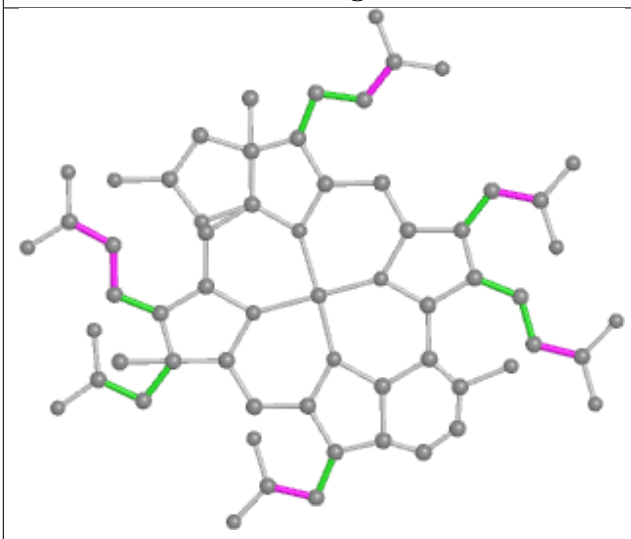
Ligand F43 D 5570



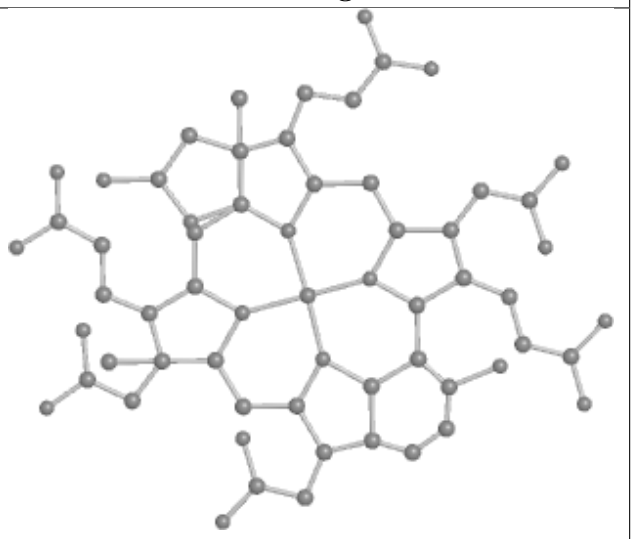
Bond lengths



Bond angles

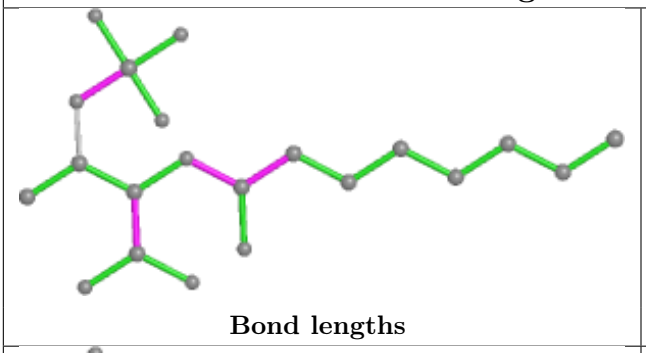


Torsions

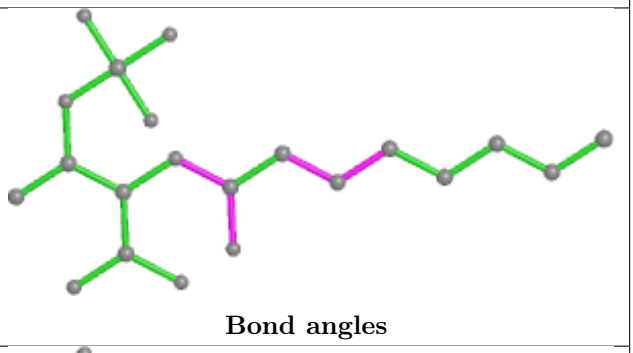


Rings

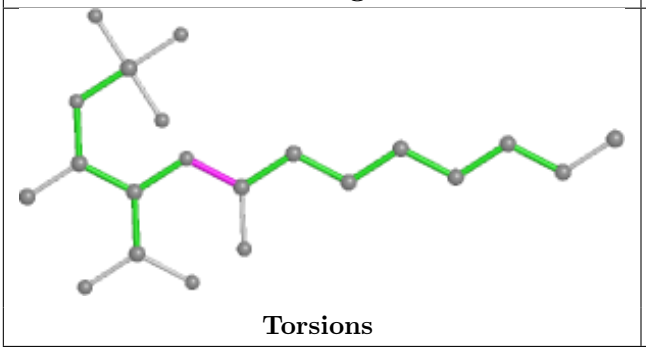
Ligand TP7 D 5571



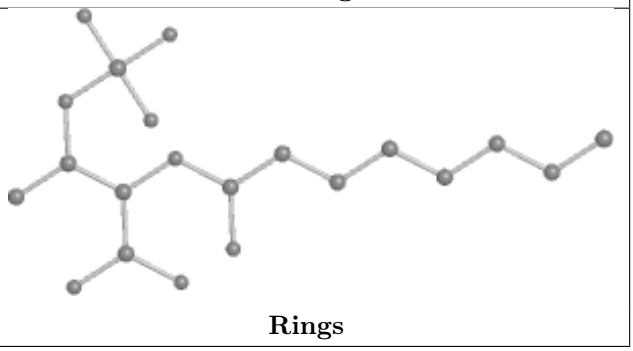
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.51	7 (1%)	79	78	7, 12, 22, 36	0
1	D	564/569 (99%)	-0.54	4 (0%)	87	87	7, 11, 20, 36	0
2	B	432/433 (99%)	-0.47	4 (0%)	84	84	8, 12, 24, 42	0
2	E	433/433 (100%)	-0.50	3 (0%)	87	87	8, 12, 22, 37	0
3	C	246/247 (99%)	-0.34	4 (1%)	72	71	9, 15, 24, 35	0
3	F	246/247 (99%)	-0.40	6 (2%)	59	56	10, 14, 24, 39	0
All	All	2485/2498 (99%)	-0.48	28 (1%)	80	80	7, 12, 23, 42	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4569	ALA	9.3
1	A	1569	ALA	8.3
3	C	3002	ALA	6.1
3	C	3064	ALA	4.8
2	B	2433	VAL	4.4

6.2 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, 95^{th} 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	0.95	0.10	19,24,26,26	0
1	MHS	A	1271	11/12	0.97	0.05	9,10,12,12	0
1	MHS	D	4271	11/12	0.97	0.06	10,11,12,13	0
3	OCS	F	6065	9/10	0.97	0.07	18,22,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	AGM	D	4285	12/13	0.98	0.08	6,7,8,8	0
1	AGM	A	1285	12/13	0.98	0.07	6,7,8,8	0
1	GL3	A	1465	4/5	0.99	0.05	9,9,9,9	0
1	GL3	D	4465	4/5	0.99	0.05	8,8,8,8	0
1	SMC	D	4472	7/8	0.99	0.05	9,10,10,10	0
1	SMC	A	1472	7/8	0.99	0.05	9,9,10,11	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

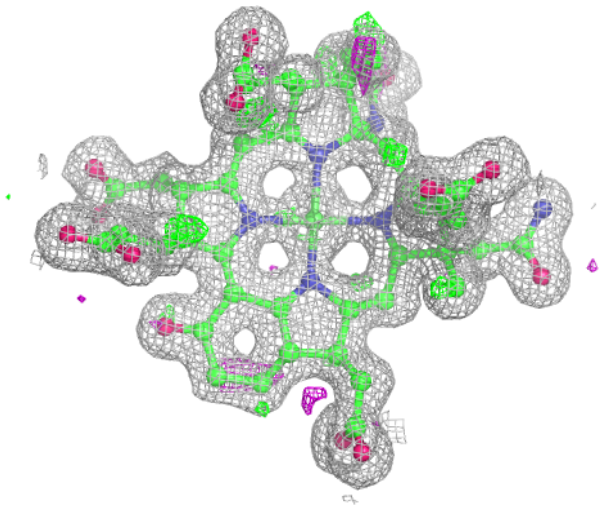
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

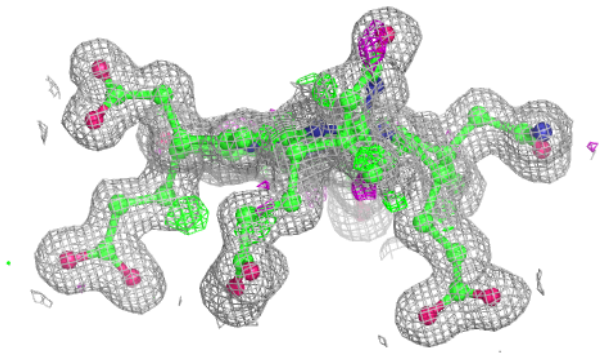
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	A	2574	6/6	0.68	0.25	36,38,39,40	0
7	GOL	D	5573	6/6	0.71	0.25	30,32,33,35	0
7	GOL	A	2573	6/6	0.77	0.20	33,34,35,37	0
6	COM	D	5572	7/7	0.94	0.11	16,17,17,18	0
6	COM	A	2572	7/7	0.95	0.10	15,16,17,18	0
4	F43	D	5570	62/62	0.98	0.07	8,10,12,13	0
5	TP7	A	2571	21/21	0.98	0.07	8,8,10,12	0
5	TP7	D	5571	21/21	0.98	0.07	7,9,10,12	0
4	F43	A	2570	62/62	0.98	0.07	8,10,11,14	0

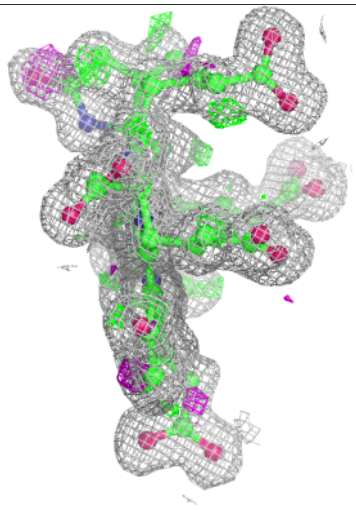
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

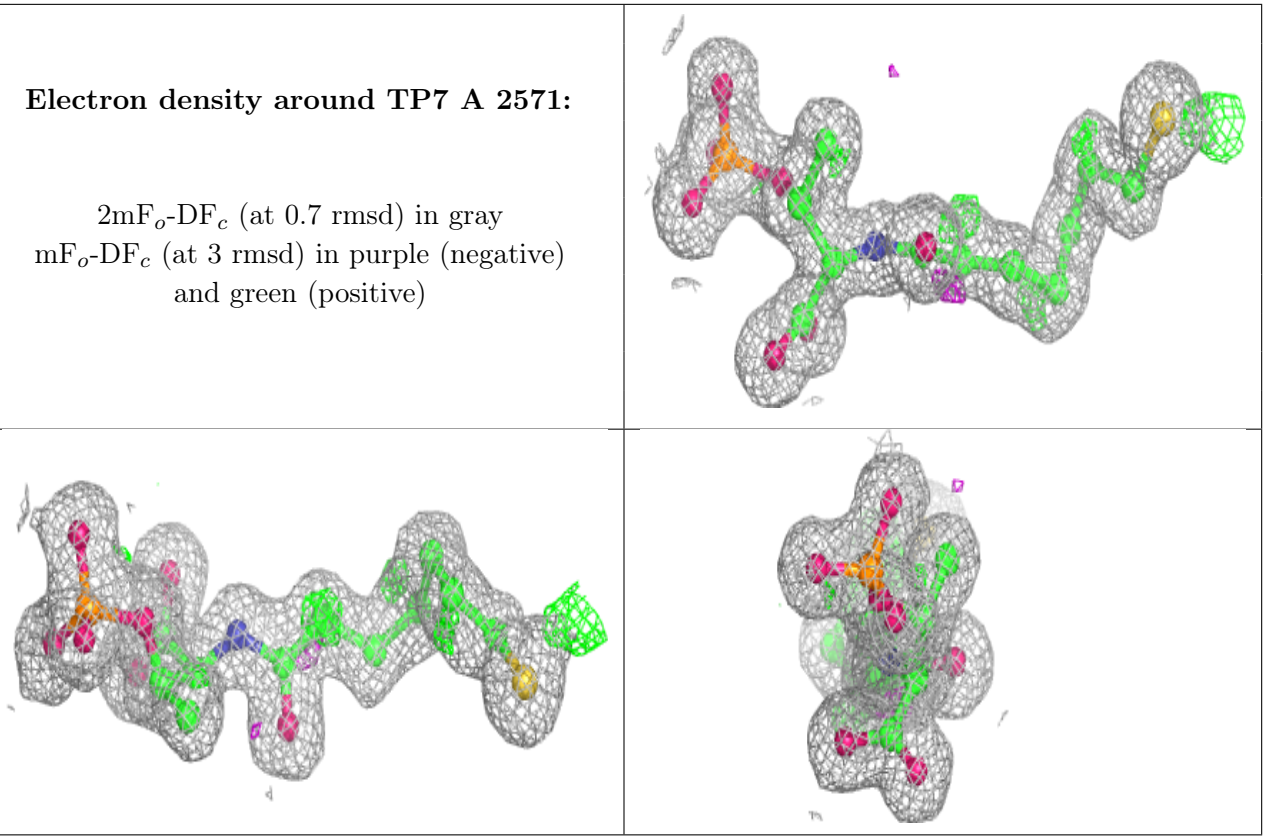






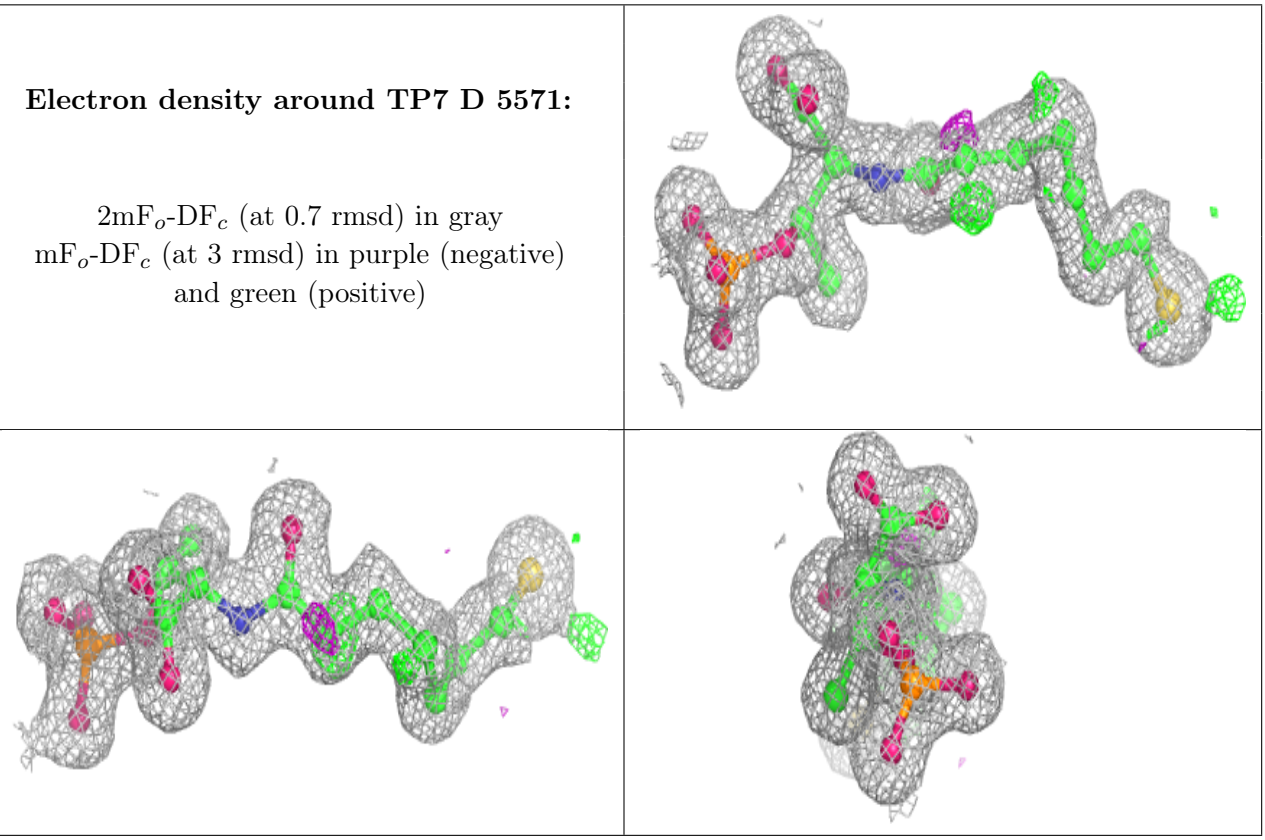
Electron density around TP7 A 2571:

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



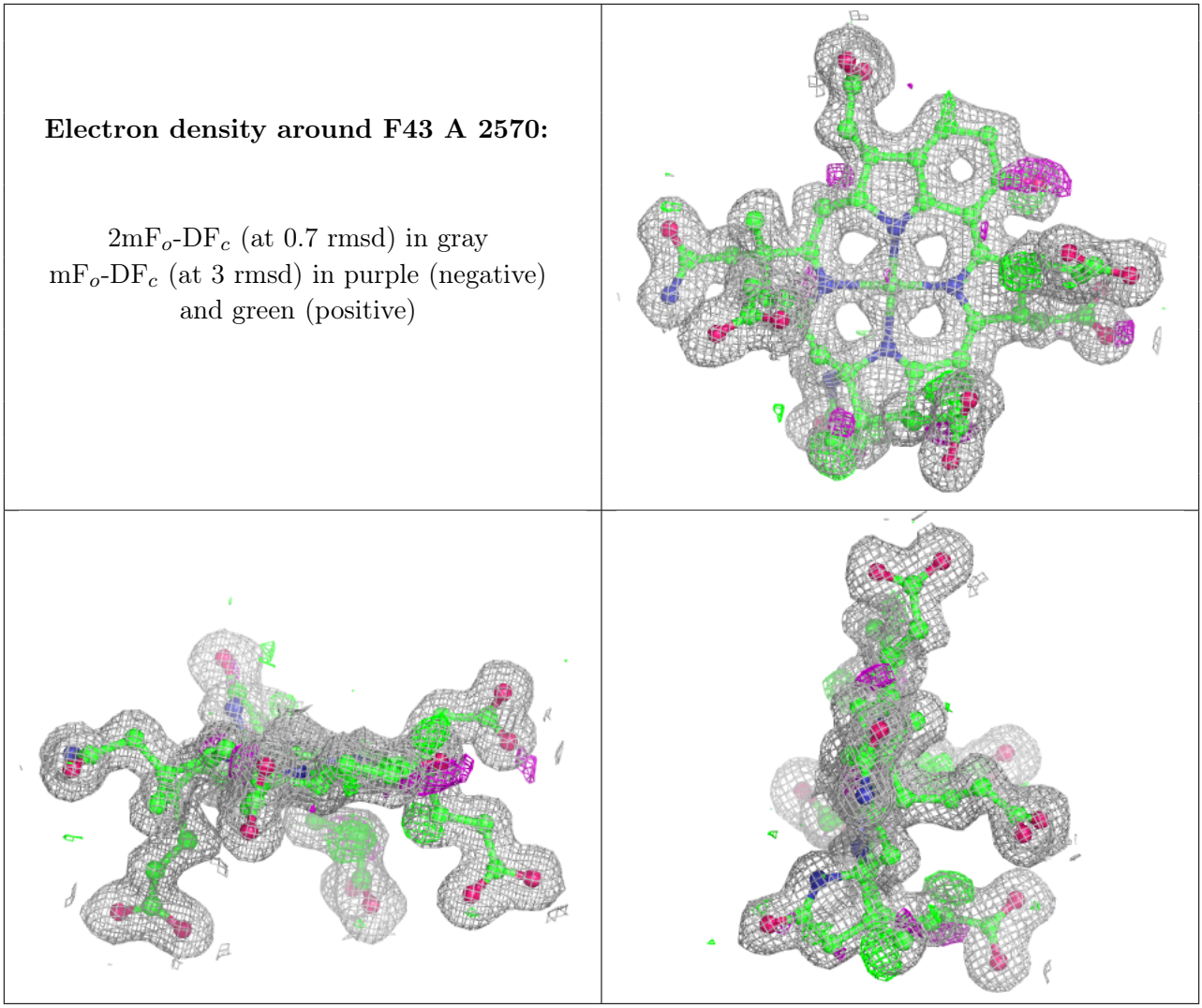
Electron density around TP7 D 5571:

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



Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.