wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2026 – 05:34 pm BST

PDB ID	:	5A0Y / pdb_00005a0y
Title	:	METHYL-COENZYME M REDUCTASE FROM METHANOTHERMOBACTER MARBURGENSIS AT 1.1 A RESOLUTION
Authors	:	Wagner, T.; Ermler, U.
Deposited on	:	2015-04-24
Resolution	:	1.10 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:

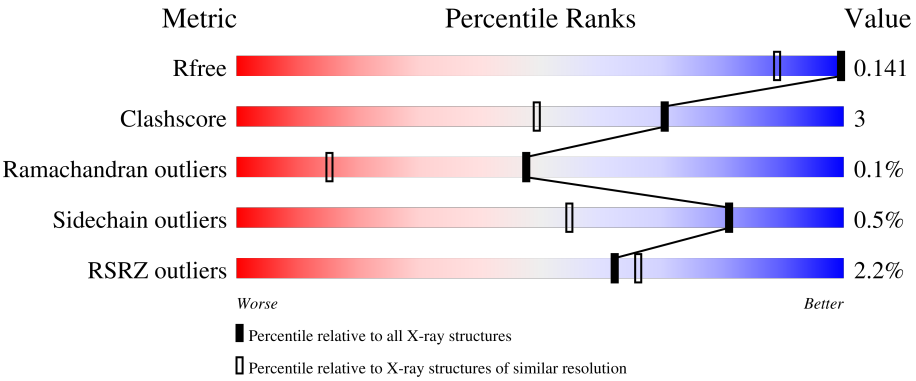
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	550	2% 94% 6%
1	D	550	% 94% 6%
2	B	443	% 94% 5%
2	E	443	2% 94% 6%
3	C	249	6% 92% 7%

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Mol	Chain	Length	Quality of chain
3	F	249	5% 94% 5%

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
10	CL	D	559	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 22747 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 I SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	25	1
			4394	2791	725	858	20			
1	D	548	Total	C	N	O	S	0	22	0
			4376	2783	721	852	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	19	0
			3433	2188	561	663	21			
2	E	442	Total	C	N	O	S	0	21	0
			3436	2197	559	658	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	9	0
			2060	1276	363	410	11			
3	F	248	Total	C	N	O	S	0	7	0
			2053	1273	364	405	11			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

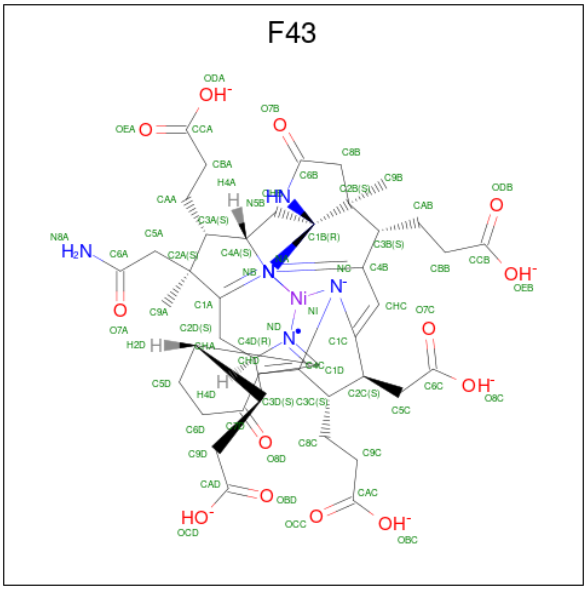
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Mg	0	0
			4	4		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

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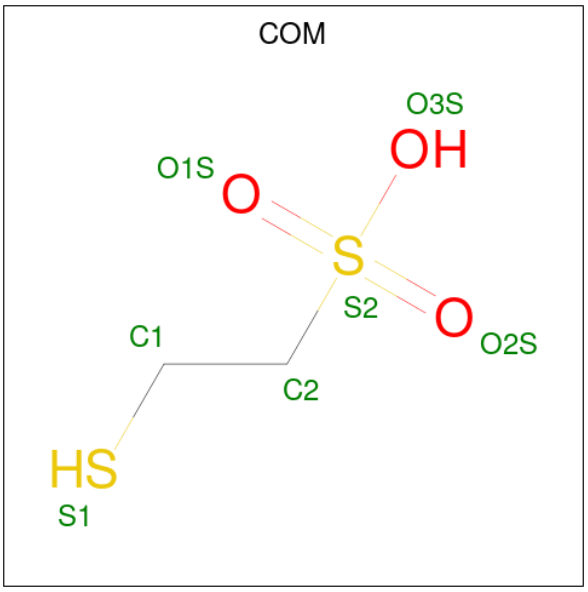
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	3	Total Mg 3 3	0	0
4	E	3	Total Mg 3 3	0	0
4	F	2	Total Mg 2 2	0	0

- Molecule 5 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



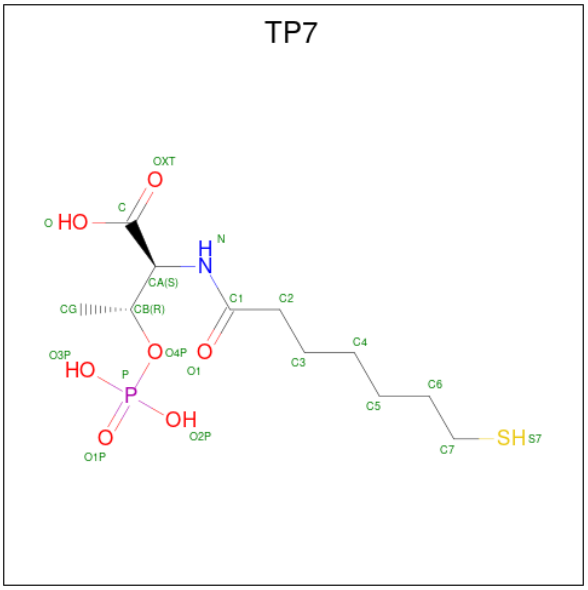
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N Ni O 62 42 6 1 13	0	0
5	D	1	Total C N Ni O 62 42 6 1 13	0	0

- 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 Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$).



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

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total K 1 1	0	0

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Na 1 1	0	0
9	D	1	Total Na 1 1	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0

- Molecule 11 is water.

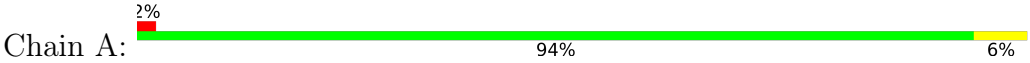
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	685	Total O 685 685	0	0
11	B	553	Total O 553 553	0	0
11	C	287	Total O 287 287	0	0
11	D	571	Total O 571 571	0	0
11	E	444	Total O 444 444	0	0
11	F	254	Total O 254 254	0	0

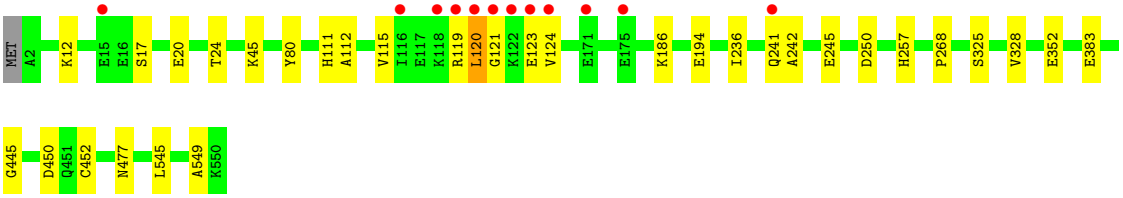
3 Residue-property plots (i)

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 I SUBUNIT ALPHA

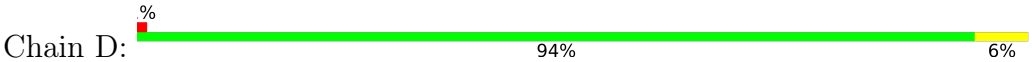
Chain A:

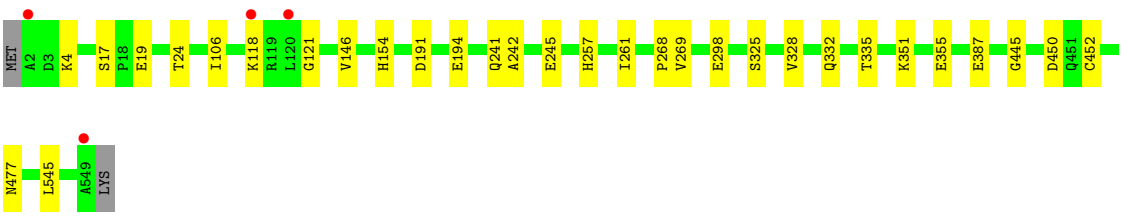




• Molecule 1: METHYL-COENZYME M REDUCTASE I SUBUNIT ALPHA

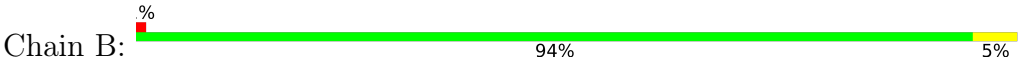
Chain D:

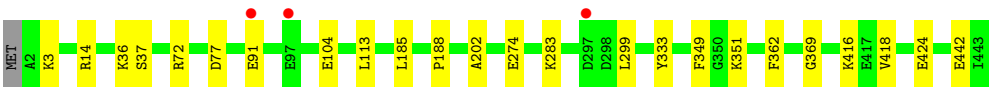




• Molecule 2: METHYL-COENZYME M REDUCTASE I SUBUNIT BETA

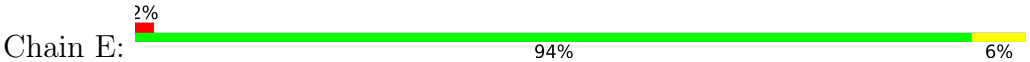
Chain B:

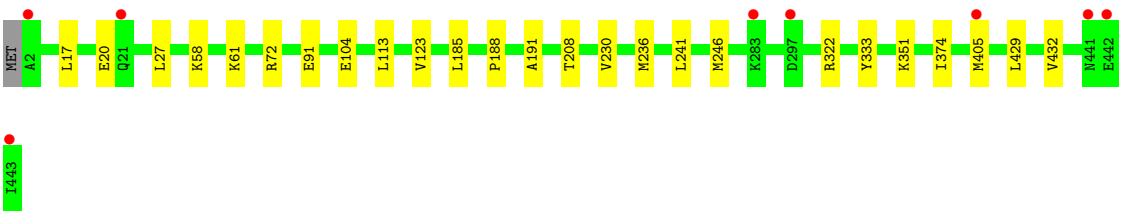




• Molecule 2: METHYL-COENZYME M REDUCTASE I SUBUNIT BETA

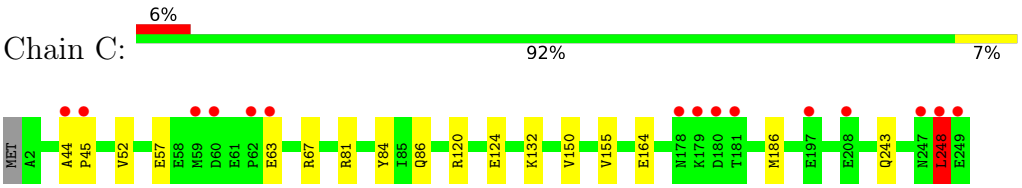
Chain E:





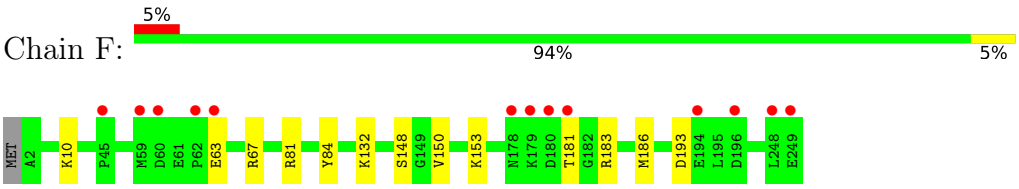
• Molecule 3: METHYL-COENZYME M REDUCTASE I SUBUNIT GAMMA

Chain C:



• Molecule 3: METHYL-COENZYME M REDUCTASE I SUBUNIT GAMMA

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.23Å 118.30Å 122.56Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	48.35 – 1.10 48.35 – 1.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.35-1.10) 92.3 (48.35-1.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.111 , 0.129 0.125 , 0.141	Depositor DCC
R_{free} test set	46960 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	8.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k 0.012 for -h,-l,-k 0.018 for h,-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	22747	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: COM, NA, MGN, K, AGM, SMC, MHS, MG, DYA, CL, GL3, TP7, F43

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	0.72	2/4498 (0.0%)	0.83	3/6106 (0.0%)
1	D	0.71	1/4473 (0.0%)	0.83	3/6070 (0.0%)
2	B	0.69	0/3532	0.78	1/4777 (0.0%)
2	E	0.65	0/3550	0.78	0/4801
3	C	0.72	0/2121	0.89	4/2855 (0.1%)
3	F	0.68	0/2107	0.86	0/2835
All	All	0.70	3/20281 (0.0%)	0.82	11/27444 (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
2	B	0	2
2	E	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	269	VAL	CA-CB	9.16	1.66	1.54
1	A	549	ALA	C-N	-7.64	1.22	1.33
1	A	124	VAL	CA-C	5.30	1.59	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	VAL	N-CA-C	8.58	120.27	107.75
1	D	241	GLN	CA-CB-CG	7.33	128.77	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	248	LEU	N-CA-C	-6.65	104.32	113.56
2	B	3	LYS	CD-CE-NZ	-6.43	91.31	111.90
1	D	477	ASN	CA-CB-CG	5.86	118.46	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	333	TYR	Sidechain
2	B	72	ARG	Sidechain
2	E	333	TYR	Sidechain
2	E	72	ARG	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	4394	0	4234	28	0
1	D	4376	0	4226	25	0
2	B	3433	0	3472	24	0
2	E	3436	0	3503	27	0
3	C	2060	0	2000	25	0
3	F	2053	0	2002	17	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
5	A	62	0	43	1	0
5	D	62	0	43	2	0
6	A	7	0	4	0	0
6	D	7	0	5	0	0
7	A	21	0	19	0	0
7	D	21	0	19	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	1	0	0	0	0
10	A	1	0	0	1	0
10	D	1	0	0	2	0
11	A	685	0	0	19	1
11	B	553	0	0	11	0
11	C	287	0	0	13	1
11	D	571	0	0	12	2
11	E	444	0	0	11	0
11	F	254	0	0	3	2
All	All	22747	0	19570	136	3

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 136 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)
11:D:2503:HOH:O	2:E:351[A]:LYS:NZ	1.70	1.21
1:A:241:GLN:OE1	11:A:2408:HOH:O	1.58	1.20
11:E:2386:HOH:O	3:F:67[A]:ARG:NH2	1.77	1.16
11:A:2585:HOH:O	2:B:351[A]:LYS:NZ	1.76	1.16
2:B:442[A]:GLU:OE1	11:B:2549:HOH:O	1.68	1.09

All (3) 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)
11:C:2220:HOH:O	11:F:2027:HOH:O[1_556]	2.13	0.07
11:D:2167:HOH:O	11:F:2252:HOH:O[2_644]	2.13	0.07
11:A:2273:HOH:O	11:D:2238:HOH:O[2_644]	2.15	0.05

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	566/550 (103%)	548 (97%)	17 (3%)	1 (0%)	43 15
1	D	562/550 (102%)	546 (97%)	15 (3%)	1 (0%)	43 15
2	B	460/443 (104%)	451 (98%)	9 (2%)	0	100 100
2	E	462/443 (104%)	455 (98%)	7 (2%)	0	100 100
3	C	255/249 (102%)	248 (97%)	7 (3%)	0	100 100
3	F	253/249 (102%)	245 (97%)	8 (3%)	0	100 100
All	All	2558/2484 (103%)	2493 (98%)	63 (2%)	2 (0%)	48 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	D	325	SER

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	457/434 (105%)	454 (99%)	3 (1%)	76 45
1	D	454/434 (105%)	454 (100%)	0	100 100
2	B	361/342 (106%)	360 (100%)	1 (0%)	86 62
2	E	363/342 (106%)	363 (100%)	0	100 100
3	C	225/217 (104%)	222 (99%)	3 (1%)	61 24
3	F	223/217 (103%)	219 (98%)	4 (2%)	51 15
All	All	2083/1986 (105%)	2072 (100%)	11 (0%)	81 55

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	148[A]	SER
3	F	148[B]	SER

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Mol	Chain	Res	Type
3	F	186	MET
3	F	150	VAL
3	C	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	441	ASN
2	E	115	GLN
1	D	296	ASN
2	E	421	GLN
1	D	449	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

12 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	MGN	D	400	1	6,9,10	0.58	0	5,12,14	0.53	0
1	SMC	D	452	1	5,6,7	1.15	1 (20%)	2,6,8	1.74	1 (50%)
1	GL3	A	445	1	2,3,4	3.47	1 (50%)	1,2,4	0.63	0
1	GL3	D	445	1	2,3,4	3.16	1 (50%)	1,2,4	0.55	0
1	AGM	D	271	1	10,11,12	0.86	0	6,13,15	0.59	0
1	DYA	D	450	1	7,7,8	1.56	1 (14%)	5,8,10	2.50	3 (60%)
1	DYA	A	450	1	7,7,8	1.67	1 (14%)	5,8,10	2.16	2 (40%)
1	MHS	A	257	1	10,11,12	1.28	1 (10%)	6,14,16	2.73	2 (33%)
1	AGM	A	271	1	10,11,12	0.67	0	6,13,15	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SMC	A	452	1	5,6,7	0.63	0	2,6,8	1.94	1 (50%)
1	MHS	D	257	1	10,11,12	1.09	0	6,14,16	2.19	1 (16%)
1	MGN	A	400	1	6,9,10	1.02	0	5,12,14	0.85	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	MGN	D	400	1	-	0/7/9/12	-
1	SMC	D	452	1	-	1/3/5/7	-
1	GL3	A	445	1	-	0/1/1/2	-
1	GL3	D	445	1	-	0/1/1/2	-
1	AGM	D	271	1	-	2/10/11/13	-
1	DYA	D	450	1	-	3/4/6/8	-
1	DYA	A	450	1	-	3/4/6/8	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	AGM	A	271	1	-	2/10/11/13	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	MGN	A	400	1	-	0/7/9/12	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GL3	C-S	-4.89	1.63	1.80
1	D	445	GL3	C-S	-4.46	1.65	1.80
1	D	450	DYA	CA-N	2.94	1.42	1.35
1	A	450	DYA	CA-N	2.77	1.42	1.35
1	A	257	MHS	CD2-CG	2.14	1.39	1.36

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	MHS	ND1-CE1-NE2	-6.01	109.42	112.93
1	D	257	MHS	ND1-CE1-NE2	-4.91	110.06	112.93
1	D	450	DYA	O-C-CA	-3.83	120.53	125.39
1	A	450	DYA	O-C-CA	-3.51	120.92	125.39
1	D	450	DYA	CA-CB-CG	-2.94	119.66	126.82

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	450	DYA	O-C-CA-CB
1	A	450	DYA	CA-CB-CG-OD1
1	A	452	SMC	CA-CB-SG-CS
1	D	450	DYA	O-C-CA-CB
1	D	450	DYA	CA-CB-CG-OD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 21 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	F43	A	554	1,6	61,71,71	2.20	5 (8%)	64,118,118	1.05	3 (4%)
6	COM	D	555	5	6,6,6	0.70	0	7,8,8	0.65	0
5	F43	D	552	1,6	61,71,71	2.21	6 (9%)	64,118,118	1.26	10 (15%)
6	COM	A	555	5	6,6,6	1.19	1 (16%)	7,8,8	1.08	0
7	TP7	D	556	-	19,20,20	0.80	1 (5%)	24,26,26	0.76	0
7	TP7	A	557	-	19,20,20	0.63	0	24,26,26	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	F43	A	554	1,6	-	5/28/185/185	-
6	COM	D	555	5	-	0/4/4/4	-
5	F43	D	552	1,6	-	7/28/185/185	-
6	COM	A	555	5	-	0/4/4/4	-
7	TP7	D	556	-	-	0/24/24/24	-
7	TP7	A	557	-	-	1/24/24/24	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	554	F43	NI-NA	10.27	2.11	1.89
5	D	552	F43	NI-NA	9.85	2.10	1.89
5	A	554	F43	NI-NB	9.51	2.10	1.89
5	D	552	F43	NI-NB	9.17	2.09	1.89
5	A	554	F43	NI-ND	7.69	2.06	1.89

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	552	F43	O8D-C7D-C6D	-3.00	115.95	120.86
5	A	554	F43	O8D-C7D-C6D	-2.84	116.21	120.86
5	D	552	F43	C3D-C4D-ND	2.54	106.29	102.34
5	A	554	F43	C2B-C1B-NB	2.37	105.39	101.84
5	D	552	F43	C2C-C5C-C6C	-2.32	109.41	114.04

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	552	F43	C3A-CAA-CBA-CCA
5	A	554	F43	C3A-CAA-CBA-CCA
5	D	552	F43	C2C-C5C-C6C-O8C
5	D	552	F43	C2C-C5C-C6C-O7C
5	A	554	F43	CAB-CBB-CCB-ODB

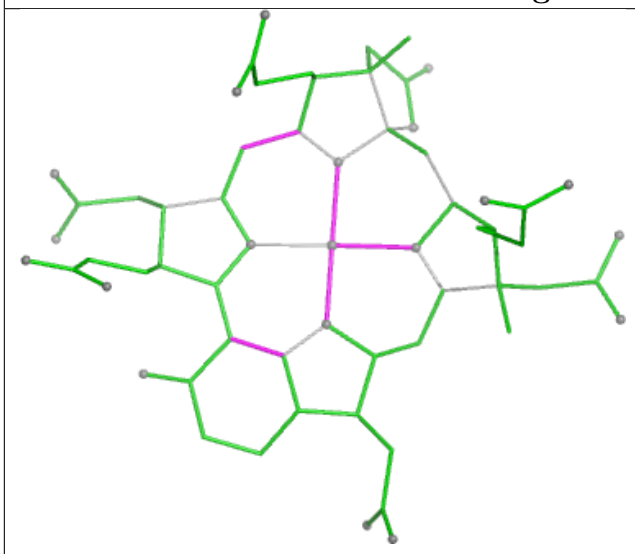
There are no ring outliers.

2 monomers are involved in 3 short contacts:

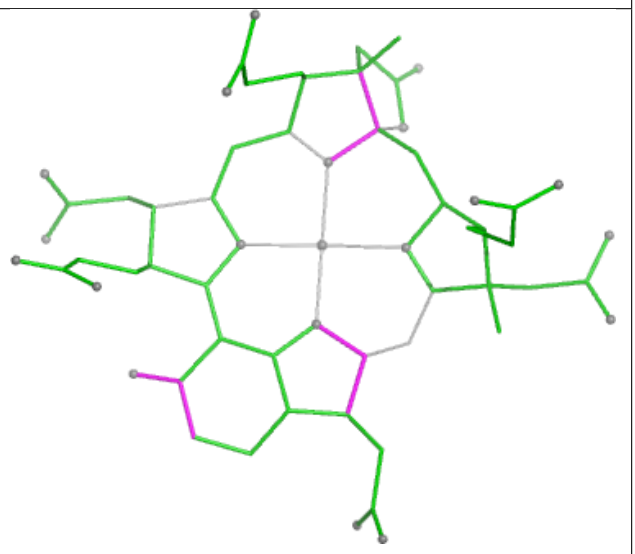
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	554	F43	1	0
5	D	552	F43	2	0

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.

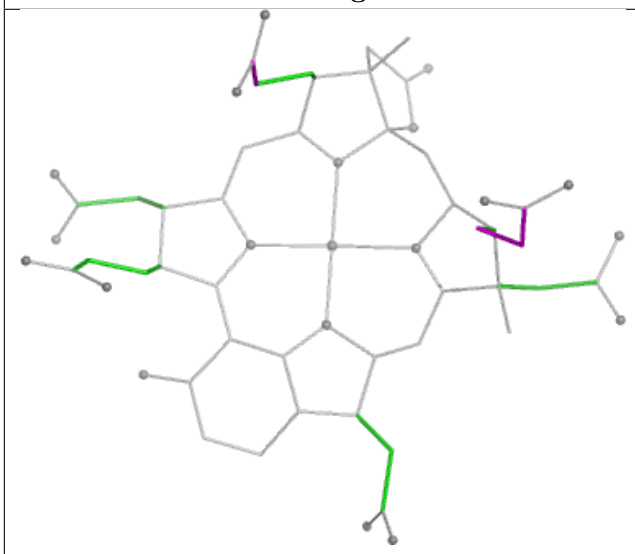
Ligand F43 A 554



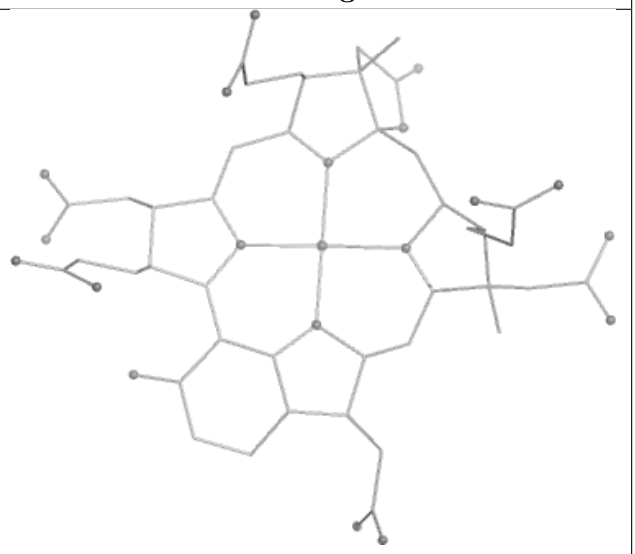
Bond lengths



Bond angles

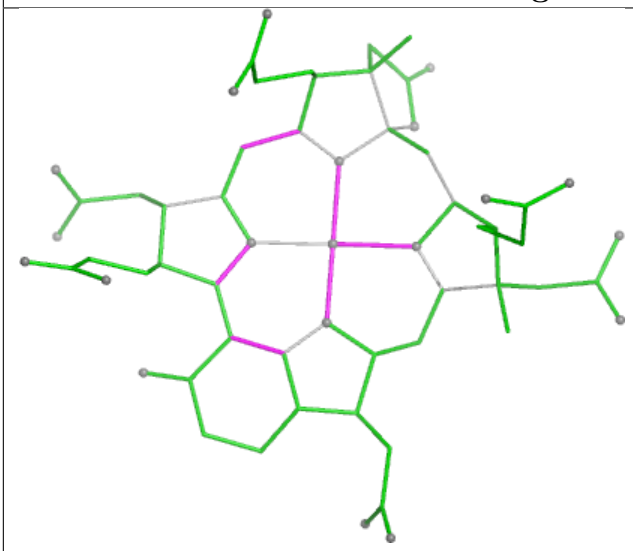


Torsions

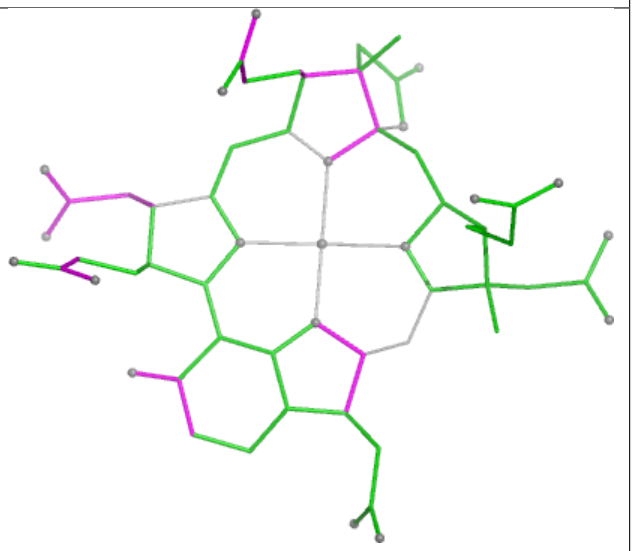


Rings

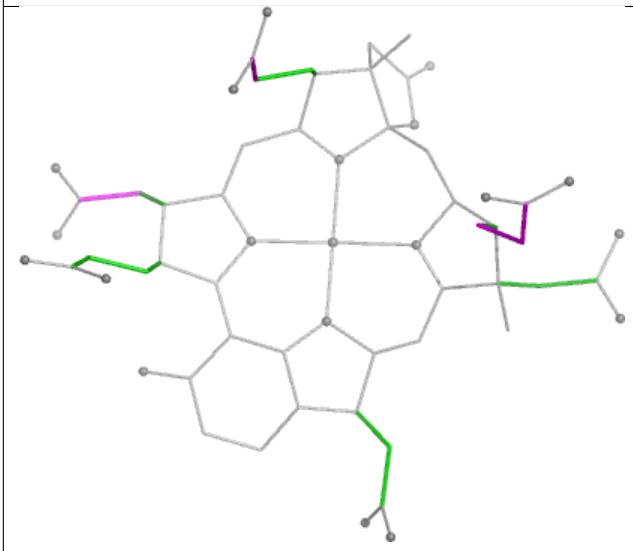
Ligand F43 D 552



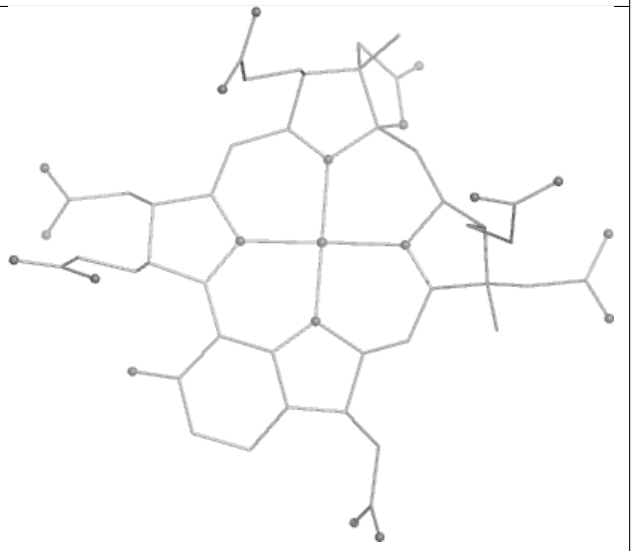
Bond lengths



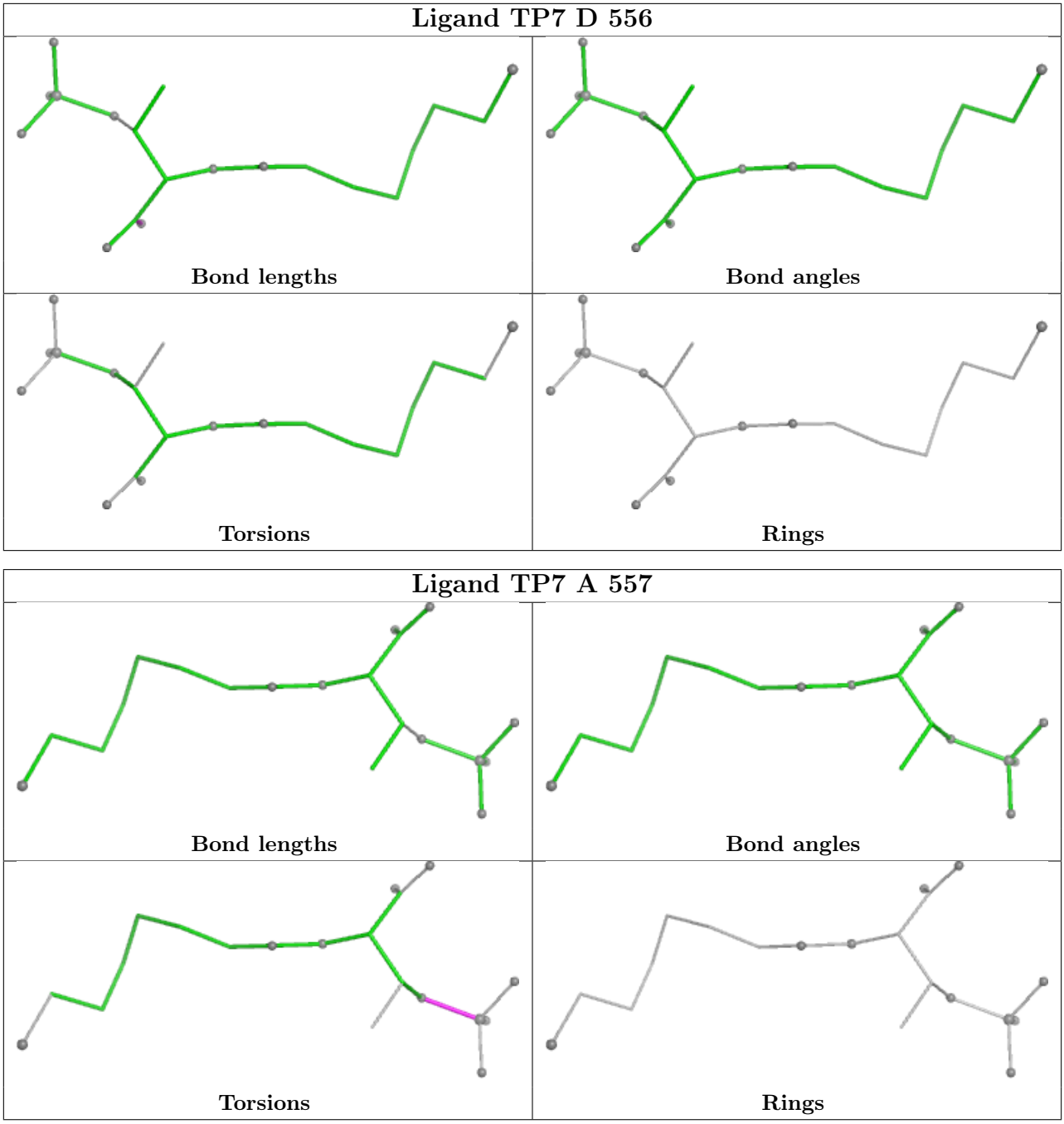
Bond angles



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	543/550 (98%)	-0.41	12 (2%)	62	66	4, 9, 21, 53	27 (4%)
1	D	542/550 (98%)	-0.42	4 (0%)	84	88	4, 9, 20, 73	22 (4%)
2	B	442/443 (99%)	-0.28	3 (0%)	84	88	4, 12, 21, 48	19 (4%)
2	E	442/443 (99%)	-0.23	8 (1%)	67	72	5, 12, 24, 52	21 (4%)
3	C	248/249 (99%)	0.06	15 (6%)	27	31	6, 15, 38, 61	9 (3%)
3	F	248/249 (99%)	0.05	13 (5%)	33	36	6, 15, 40, 83	7 (2%)
All	All	2465/2484 (99%)	-0.26	55 (2%)	62	66	4, 11, 25, 83	105 (4%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	7.4
3	C	248	LEU	7.1
1	A	122	LYS	6.6
1	A	123	GLU	5.2
1	D	2	ALA	4.7

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
1	MHS	A	257	11/12	0.98	0.05	10,11,15,17	0
1	MHS	D	257	11/12	0.98	0.05	9,11,13,16	0
1	MGN	A	400	10/11	0.99	0.03	7,8,8,8	0
1	DYA	A	450	8/9	0.99	0.02	7,8,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SMC	A	452	7/8	0.99	0.04	7,8,9,9	0
1	AGM	A	271	12/13	0.99	0.03	5,6,7,7	0
1	AGM	D	271	12/13	0.99	0.03	5,6,6,7	0
1	MGN	D	400	10/11	0.99	0.03	6,6,7,8	0
1	DYA	D	450	8/9	0.99	0.03	7,7,9,10	0
1	GL3	D	445	4/5	1.00	0.02	6,6,6,6	0
1	GL3	A	445	4/5	1.00	0.03	7,7,7,8	0
1	SMC	D	452	7/8	1.00	0.03	7,7,9,10	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	MG	E	446	1/1	0.93	0.30	34,34,34,34	0
4	MG	D	560	1/1	0.94	0.10	22,22,22,22	1
4	MG	B	445	1/1	0.94	0.09	20,20,20,20	1
10	CL	A	565	1/1	0.94	0.13	24,24,24,24	1
10	CL	D	559	1/1	0.94	0.13	25,25,25,25	1
4	MG	E	445	1/1	0.97	0.06	16,16,16,16	1
4	MG	D	557	1/1	0.98	0.12	21,21,21,21	0
4	MG	F	251	1/1	0.98	0.04	15,15,15,15	1
4	MG	B	444	1/1	0.98	0.10	25,25,25,25	0
4	MG	A	563	1/1	0.98	0.19	23,23,23,23	0
4	MG	E	444	1/1	0.99	0.21	24,24,24,24	0
4	MG	A	562	1/1	0.99	0.20	18,18,18,18	0
4	MG	C	251	1/1	0.99	0.06	12,12,12,12	1
4	MG	D	551	1/1	0.99	0.20	20,20,20,20	0
6	COM	A	555	7/7	0.99	0.05	9,10,11,12	0
6	COM	D	555	7/7	0.99	0.04	8,10,10,10	0
7	TP7	A	557	21/21	0.99	0.04	7,8,8,9	0
7	TP7	D	556	21/21	0.99	0.04	6,8,8,8	0
9	NA	D	558	1/1	0.99	0.10	14,14,14,14	0
4	MG	A	551	1/1	0.99	0.18	18,18,18,18	0

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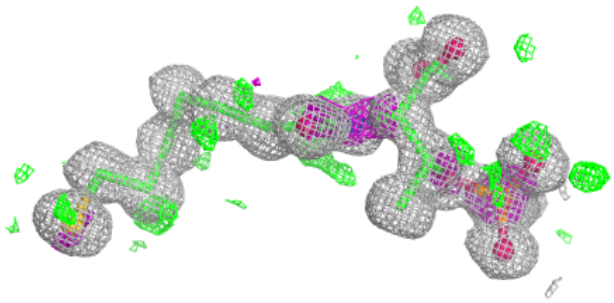
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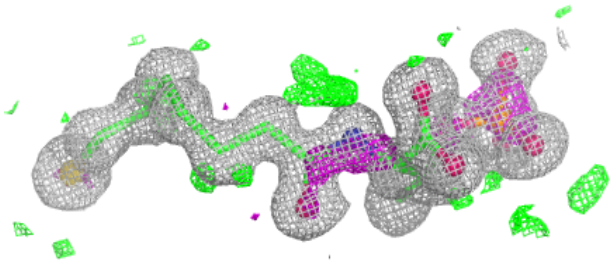
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	553	1/1	0.99	0.04	11,11,11,11	1
5	F43	D	552	62/62	1.00	0.03	6,7,10,13	0
8	K	A	561	1/1	1.00	0.06	9,9,9,9	0
9	NA	A	564	1/1	1.00	0.05	15,15,15,15	0
4	MG	F	250	1/1	1.00	0.05	16,16,16,16	0
4	MG	C	250	1/1	1.00	0.04	16,16,16,16	0
5	F43	A	554	62/62	1.00	0.03	5,6,9,12	0

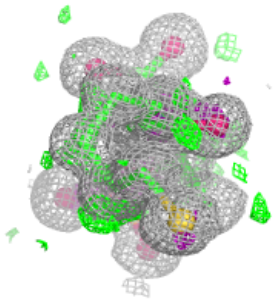
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TP7 A 557:

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

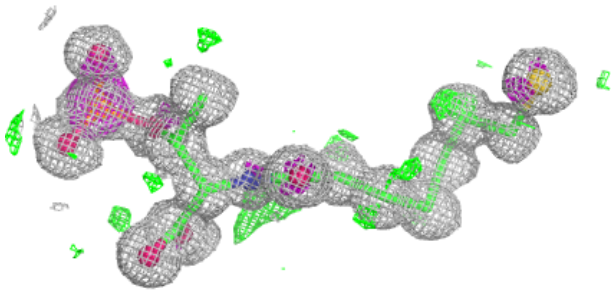


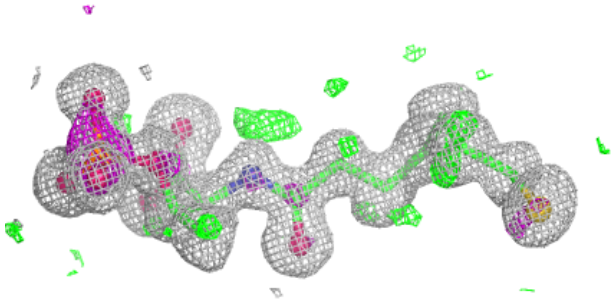


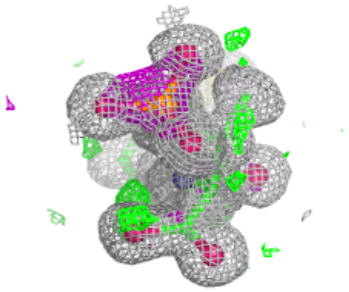


Electron density around TP7 D 556:

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

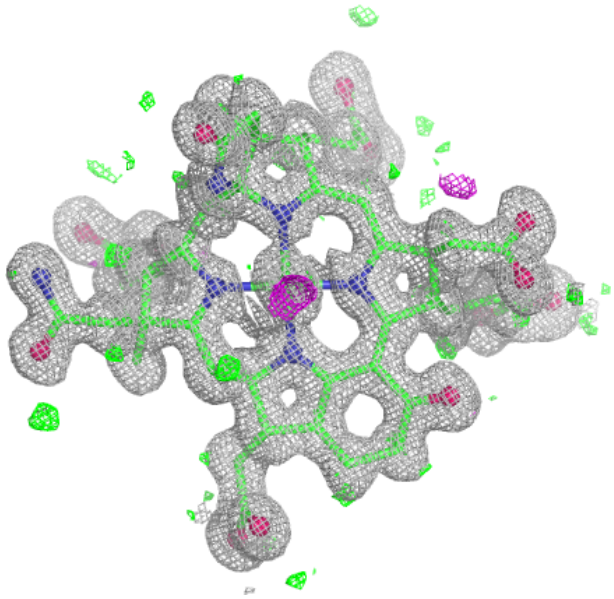


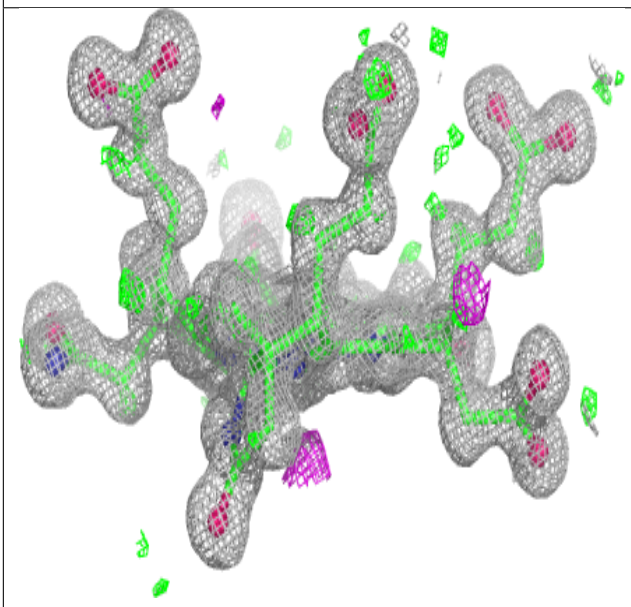


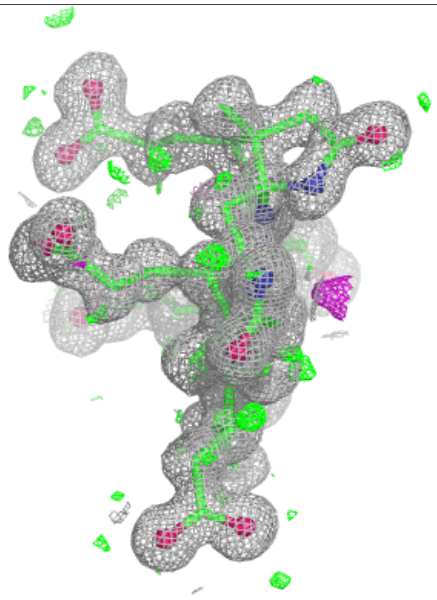


Electron density around F43 D 552:

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

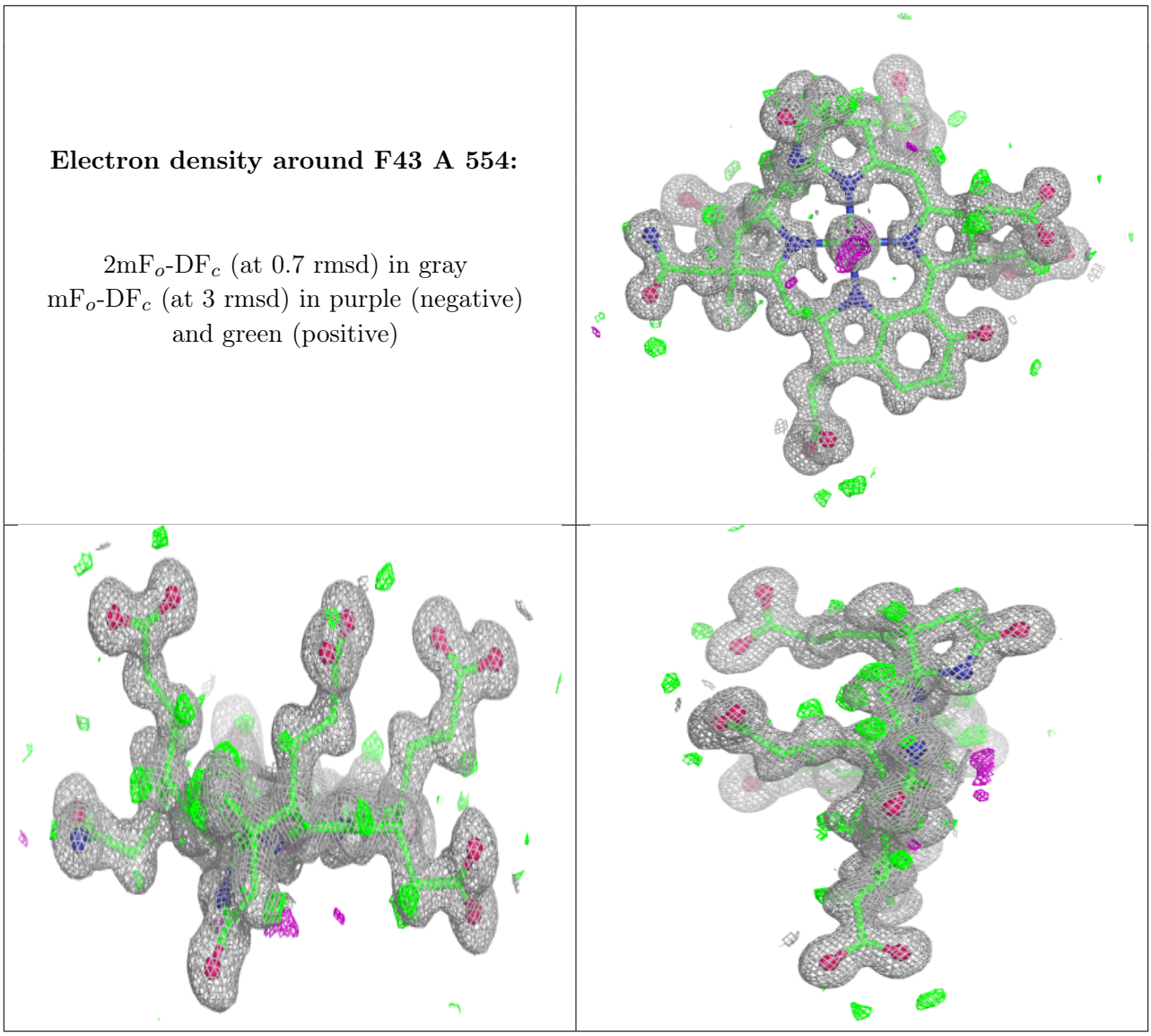






Electron density around F43 A 554:

$2mF_o$-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.