



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 09:43 am BST

PDB ID : 3M30
Title : Structural Insight into Methyl-Coenzyme M Reductase Chemistry using Coenzyme B Analogues
Authors : Cedervall, P.E.; Dey, M.; Ragsdale, S.W.; Wilmot, C.M.
Deposited on : 2010-03-08
Resolution : 1.45 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

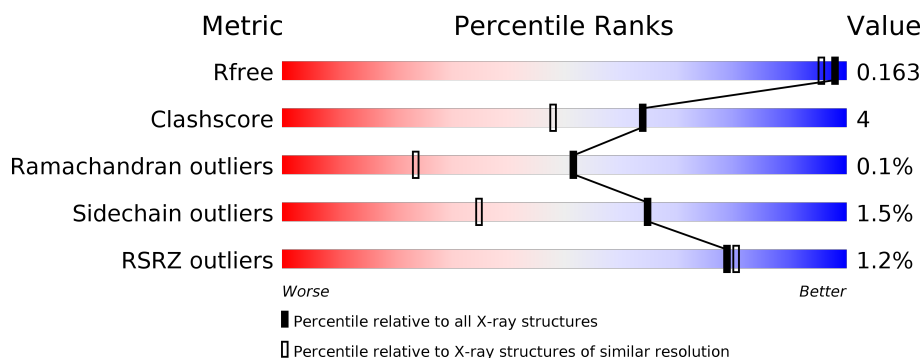
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 86%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 86% 13% . </div> </div>
1	D	549	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 87%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 87% 12% </div> </div>
2	B	442	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 14%, green 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 85% 14% . </div> </div>
2	E	442	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 14% . </div> </div>
3	C	248	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 19%, green 78%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 78% 19% .. </div> </div>
3	F	248	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 19%, green 77%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 77% 19% ... </div> </div>

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
9	ACT	C	1	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 22789 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	548	Total	C	N	O	S	0	33	0
			4469	2822	736	890	21			
1	D	548	Total	C	N	O	S	0	25	0
			4390	2787	722	861	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	30	0
			3505	2238	571	673	23			
2	E	442	Total	C	N	O	S	0	31	0
			3519	2241	573	682	23			

- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	10	0
			2050	1271	359	408	12			
3	F	246	Total	C	N	O	S	0	19	0
			2103	1304	367	420	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

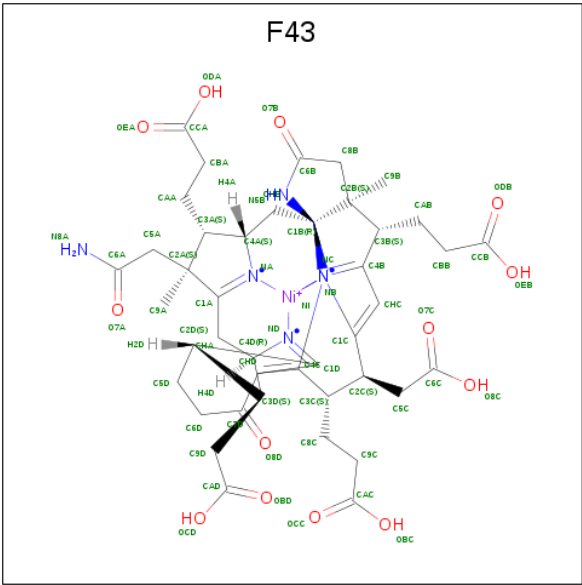
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	E	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		

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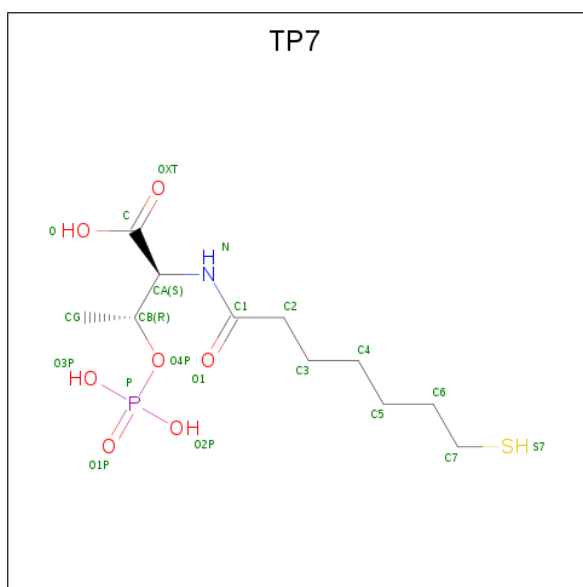
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	2
			2	2		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is FACTOR 430 (three-letter code: F43) (formula: C₄₂H₅₁N₆NiO₁₃).



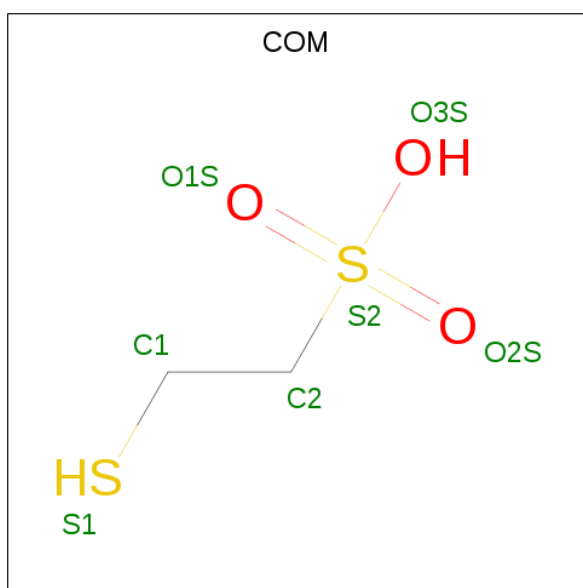
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
5	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 6 is Coenzyme B (three-letter code: TP7) (formula: C₁₁H₂₂NO₇PS).



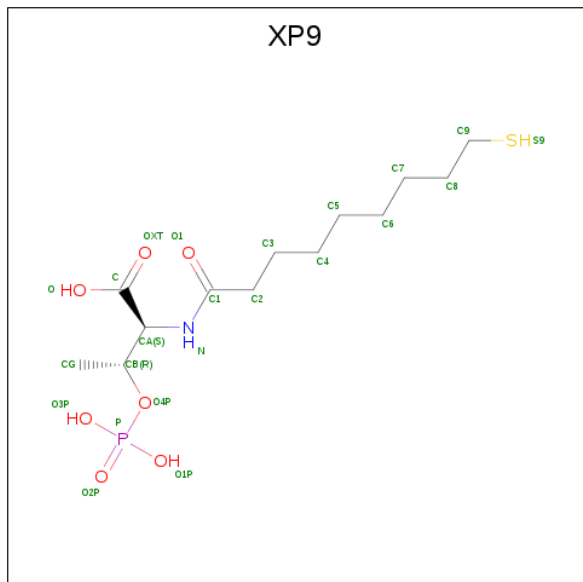
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		
6	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

- Molecule 7 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



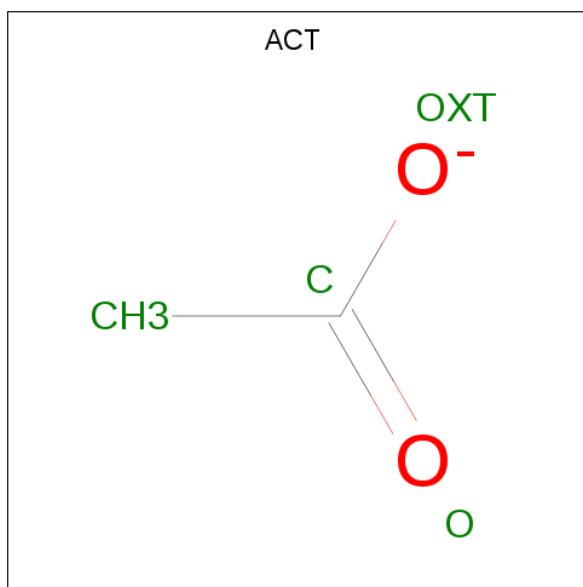
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	2	3	2		
7	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 8 is O-phosphono-N-(9-sulfanylnonanoyl)-L-threonine (three-letter code: XP9) (formula: $C_{13}H_{26}NO_7PS$).



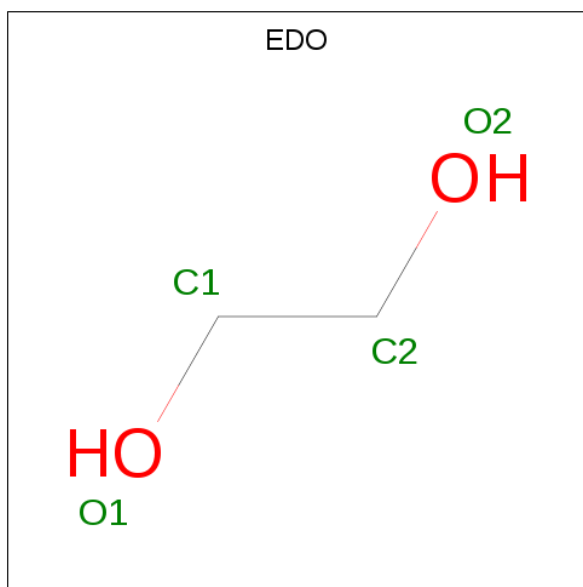
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			46	26	2	14	2	2		
8	D	1	Total	C	N	O	P	S	0	1
			46	26	2	14	2	2		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	1
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

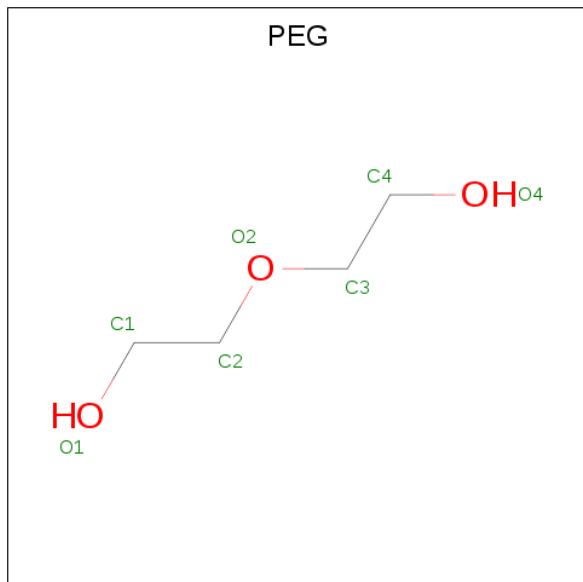


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Zn	0	0
			1	1		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			7	4	3		

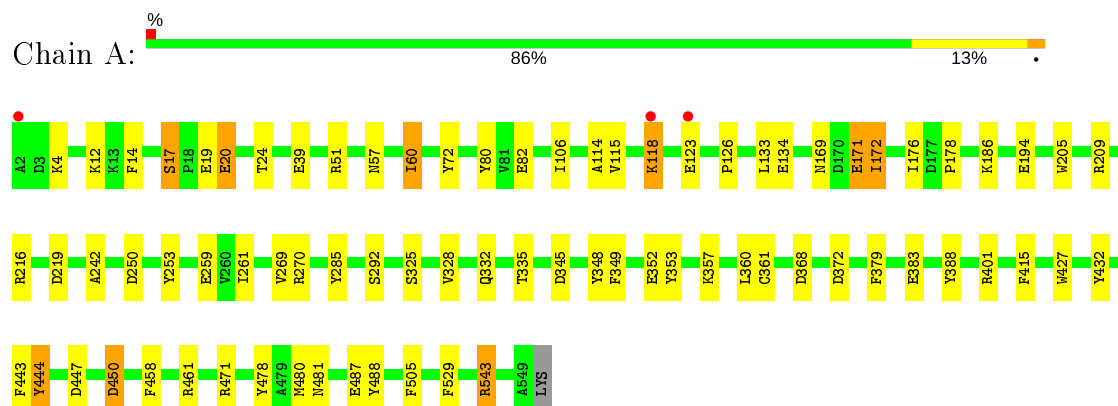
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	507	Total	O	0	30
			519	519		
13	B	451	Total	O	0	26
			472	472		
13	C	251	Total	O	0	11
			259	259		
13	D	502	Total	O	0	15
			511	511		
13	E	405	Total	O	0	15
			415	415		
13	F	252	Total	O	0	9
			256	256		

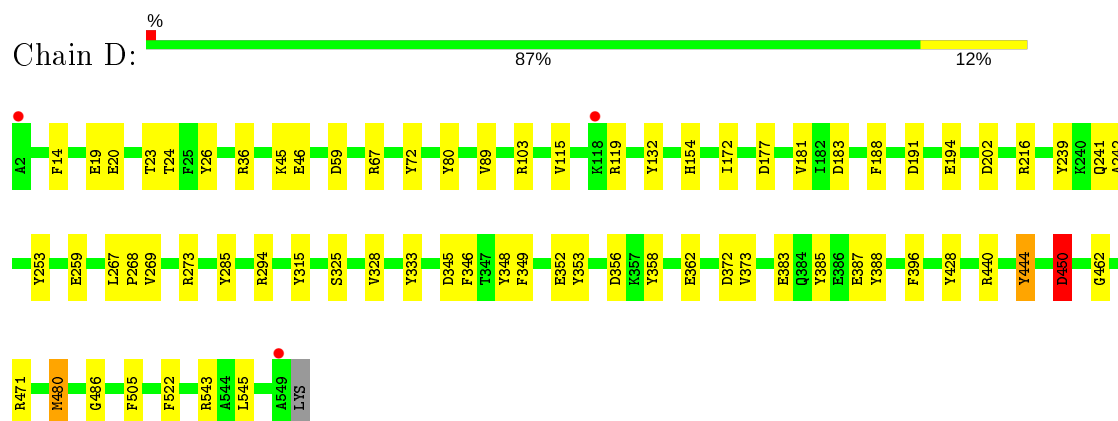
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

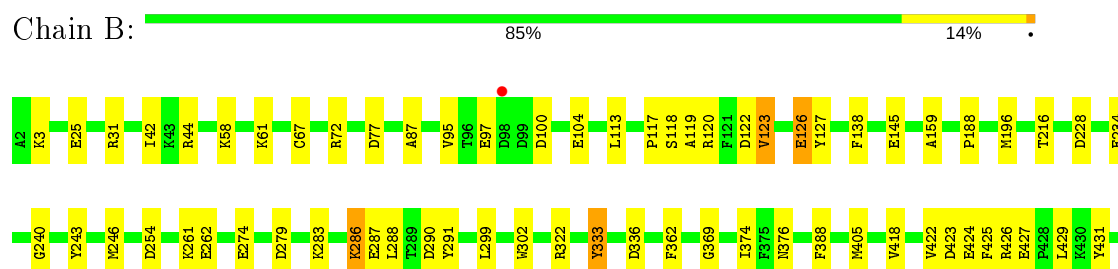
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

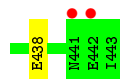
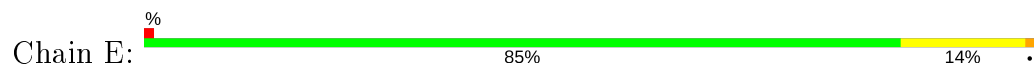


- Molecule 2: Methyl-coenzyme M reductase I subunit beta

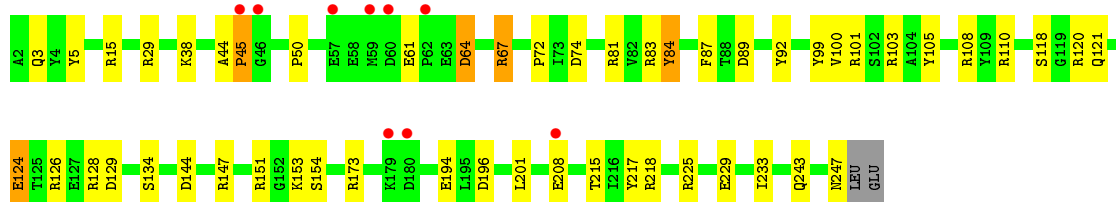
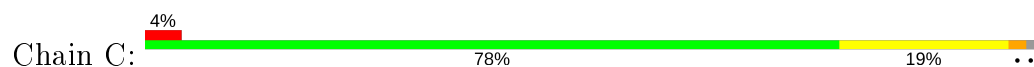




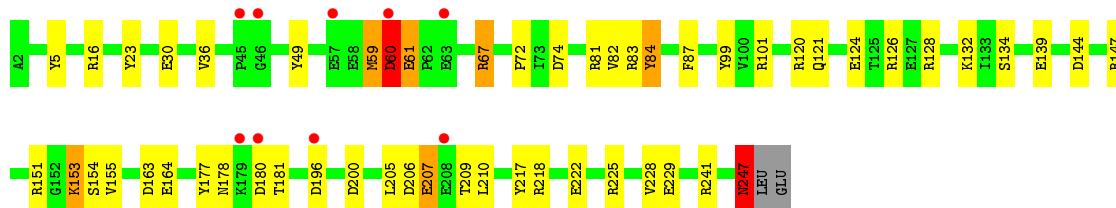
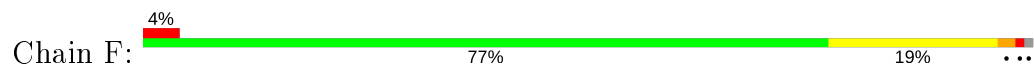
• Molecule 2: Methyl-coenzyme M reductase I subunit beta



• Molecule 3: Methyl-coenzyme M reductase I subunit gamma



• Molecule 3: Methyl-coenzyme M reductase I subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	20.07 – 1.45 19.89 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.07-1.45) 97.1 (19.89-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.136 , 0.164 0.135 , 0.163	Depositor DCC
R_{free} test set	20161 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.008 for -h,-l,-k 0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22789	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PEG, SMC, ACT, MG, F43, MGN, TP7, XP9, AGM, EDO, GL3, COM, MHS

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	1.50	20/4572 (0.4%)	1.36	28/6206 (0.5%)
1	D	1.54	24/4505 (0.5%)	1.38	33/6116 (0.5%)
2	B	1.50	16/3628 (0.4%)	1.34	24/4904 (0.5%)
2	E	1.50	13/3633 (0.4%)	1.30	27/4910 (0.5%)
3	C	1.58	13/2109 (0.6%)	1.48	33/2841 (1.2%)
3	F	1.59	22/2179 (1.0%)	1.45	22/2933 (0.8%)
All	All	1.53	108/20626 (0.5%)	1.37	167/27910 (0.6%)

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	1	1
1	D	1	1
2	B	0	1
All	All	2	3

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	19	GLU	CD-OE1	9.52	1.36	1.25
3	F	139	GLU	CD-OE2	7.28	1.33	1.25
1	D	269	VAL	CA-CB	6.91	1.69	1.54
1	D	14	PHE	CD2-CE2	6.55	1.52	1.39
3	C	153	LYS	CE-NZ	6.43	1.65	1.49

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	147	ARG	NE-CZ-NH1	13.21	126.91	120.30
3	F	147	ARG	NE-CZ-NH1	12.33	126.47	120.30
2	B	44	ARG	NE-CZ-NH1	12.19	126.39	120.30
3	C	120	ARG	NE-CZ-NH1	9.91	125.25	120.30
3	F	147	ARG	NE-CZ-NH2	-8.87	115.87	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	450	ASP	CA
1	D	450	ASP	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	ARG	Sidechain
2	B	333	TYR	Sidechain
1	D	480	MET	Peptide

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	4469	0	4240	32	0
1	D	4390	0	4228	25	0
2	B	3505	0	3572	39	0
2	E	3519	0	3563	37	0
3	C	2050	0	1984	25	0
3	F	2103	0	2051	27	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	62	0	43	1	0
5	D	62	0	43	1	0
6	A	21	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	21	0	19	0	0
7	A	7	0	5	0	0
7	D	7	0	5	0	0
8	A	46	0	46	1	0
8	D	46	0	46	3	0
9	A	4	0	3	0	0
9	C	4	0	3	10	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
10	C	4	0	6	0	0
10	D	4	0	6	1	0
10	F	8	0	12	4	0
11	A	1	0	0	0	0
12	C	7	0	10	0	0
13	A	519	0	0	9	0
13	B	472	0	0	19	0
13	C	259	0	0	5	0
13	D	511	0	0	7	0
13	E	415	0	0	14	0
13	F	256	0	0	11	0
All	All	22789	0	19916	170	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 4.

The worst 5 of 170 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)
3:C:81:ARG:CG	9:C:1:ACT:H1	1.62	1.28
3:C:81:ARG:CD	9:C:1:ACT:H1	1.69	1.21
3:C:81:ARG:HD3	9:C:1:ACT:CH3	1.73	1.19
2:B:322[B]:ARG:NH2	3:C:67[B]:ARG:HG3	1.65	1.10
2:B:58[B]:LYS:HD2	13:B:3633:HOH:O	1.53	1.06

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	574/549 (105%)	556 (97%)	17 (3%)	1 (0%)	47	22
1	D	566/549 (103%)	549 (97%)	16 (3%)	1 (0%)	47	22
2	B	471/442 (107%)	461 (98%)	10 (2%)	0	100	100
2	E	472/442 (107%)	462 (98%)	10 (2%)	0	100	100
3	C	254/248 (102%)	246 (97%)	8 (3%)	0	100	100
3	F	263/248 (106%)	254 (97%)	8 (3%)	1 (0%)	34	13
All	All	2600/2478 (105%)	2528 (97%)	69 (3%)	3 (0%)	51	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	60	ASP
1	D	325	SER
1	A	325	SER

5.3.2 Protein sidechains ⓘ

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	466/434 (107%)	454 (97%)	12 (3%)	46	13
1	D	458/434 (106%)	456 (100%)	2 (0%)	91	80
2	B	371/341 (109%)	365 (98%)	6 (2%)	62	31
2	E	372/341 (109%)	365 (98%)	7 (2%)	57	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	224/216 (104%)	220 (98%)	4 (2%)	59	26
3	F	232/216 (107%)	224 (97%)	8 (3%)	37	6
All	All	2123/1982 (107%)	2084 (98%)	39 (2%)	65	26

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	287	GLU
3	C	208	GLU
3	F	207[A]	GLU
3	C	45	PRO
3	C	61	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	121	GLN
3	F	247	ASN
2	E	21	GLN
1	A	241	GLN
3	F	121	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	SMC	A	452	1	5,6,7	1.23	0	2,6,8	2.27	1 (50%)
1	MHS	A	257	1	7,11,12	2.13	2 (28%)	6,14,16	4.28	3 (50%)
1	GL3	A	445	1	2,3,4	2.44	1 (50%)	1,2,4	0.20	0
1	GL3	D	445	1	2,3,4	2.43	1 (50%)	1,2,4	0.36	0
1	MHS	D	257	1	7,11,12	1.52	1 (14%)	6,14,16	3.81	3 (50%)
1	SMC	D	452	1	5,6,7	1.23	1 (20%)	2,6,8	1.99	1 (50%)
1	MGN	A	400	1	6,9,10	1.07	0	5,12,14	0.60	0
1	MGN	D	400	1	6,9,10	1.43	1 (16%)	5,12,14	0.43	0
1	AGM	D	271	1	10,11,12	1.78	1 (10%)	6,13,15	1.45	1 (16%)
1	AGM	A	271	1	10,11,12	1.33	2 (20%)	6,13,15	1.99	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	SMC	A	452	1	-	1/3/5/7	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	GL3	A	445	1	-	1/1/1/2	-
1	GL3	D	445	1	-	1/1/1/2	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	SMC	D	452	1	-	1/3/5/7	-
1	MGN	A	400	1	-	0/7/9/12	-
1	MGN	D	400	1	-	0/7/9/12	-
1	AGM	D	271	1	-	1/10/11/13	-
1	AGM	A	271	1	-	1/10/11/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	271	AGM	CB-CA	4.25	1.59	1.53
1	A	257	MHS	CE1-NE2	4.06	1.44	1.34
1	A	445	GL3	C-S	-3.46	1.68	1.80
1	D	445	GL3	C-S	-3.42	1.68	1.80
1	D	257	MHS	CE1-NE2	3.20	1.42	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	NE2-CE1-ND1	-9.49	98.17	112.26
1	D	257	MHS	NE2-CE1-ND1	-7.21	101.55	112.26
1	D	257	MHS	CM-ND1-CG	4.15	129.96	124.44
1	A	257	MHS	CD2-NE2-CE1	3.63	111.44	105.78
1	D	257	MHS	CD2-NE2-CE1	3.49	111.23	105.78

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	SMC	CA-CB-SG-CS
1	D	452	SMC	CA-CB-SG-CS
1	A	445	GL3	S-C-CA-N
1	D	445	GL3	S-C-CA-N
1	D	271	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 10 are monoatomic - leaving 19 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	$\# Z > 2$
10	EDO	C	251	-	3,3,3	0.56	0	2,2,2	0.50	0
5	F43	D	552	1,7	46,71,71	3.07	12 (26%)	48,118,118	2.18	14 (29%)
10	EDO	D	556	-	3,3,3	0.48	0	2,2,2	0.58	0
9	ACT	C	1	-	1,3,3	1.65	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	XP9	A	555[C]	-	18,22,22	0.77	0	20,28,28	0.91	1 (5%)
10	EDO	F	252	-	3,3,3	0.76	0	2,2,2	0.23	0
7	COM	A	554	5	6,6,6	1.39	1 (16%)	7,8,8	1.85	3 (42%)
8	XP9	A	555[B]	-	18,22,22	0.82	0	20,28,28	1.25	2 (10%)
8	XP9	D	555[B]	-	18,22,22	0.78	1 (5%)	20,28,28	1.13	2 (10%)
6	TP7	D	553[A]	-	16,20,20	1.02	1 (6%)	18,26,26	1.02	2 (11%)
8	XP9	D	555[C]	-	18,22,22	0.80	1 (5%)	20,28,28	0.92	1 (5%)
6	TP7	A	553[A]	-	16,20,20	1.08	1 (6%)	18,26,26	1.04	1 (5%)
9	ACT	A	556[B]	4	1,3,3	1.04	0	0,3,3	0.00	-
10	EDO	F	251	-	3,3,3	0.64	0	2,2,2	0.58	0
10	EDO	B	446	-	3,3,3	0.53	0	2,2,2	0.31	0
12	PEG	C	252	-	6,6,6	0.57	0	5,5,5	0.94	0
7	COM	D	554	5	6,6,6	0.83	0	7,8,8	1.21	1 (14%)
10	EDO	A	557	-	3,3,3	0.79	0	2,2,2	0.70	0
5	F43	A	1	1,7	46,71,71	3.01	10 (21%)	48,118,118	1.62	11 (22%)

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
10	EDO	C	251	-	-	0/1/1/1	-
5	F43	D	552	1,7	-	1/18/185/185	-
10	EDO	D	556	-	-	1/1/1/1	-
5	F43	A	1	1,7	-	1/18/185/185	-
8	XP9	A	555[C]	-	-	3/22/26/26	-
10	EDO	F	252	-	-	1/1/1/1	-
7	COM	A	554	5	-	0/4/4/4	-
8	XP9	A	555[B]	-	-	3/22/26/26	-
8	XP9	D	555[B]	-	-	4/22/26/26	-
6	TP7	D	553[A]	-	-	1/20/24/24	-
8	XP9	D	555[C]	-	-	1/22/26/26	-
6	TP7	A	553[A]	-	-	2/20/24/24	-
10	EDO	A	557	-	-	1/1/1/1	-
10	EDO	F	251	-	-	1/1/1/1	-
10	EDO	B	446	-	-	1/1/1/1	-
7	COM	D	554	5	-	0/4/4/4	-
12	PEG	C	252	-	-	1/4/4/4	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	NI-NB	11.01	2.13	1.89
5	D	552	F43	NI-NA	10.57	2.12	1.89
5	A	1	F43	NI-NA	10.49	2.12	1.89
5	D	552	F43	NI-NB	10.19	2.11	1.89
5	A	1	F43	NI-ND	8.77	2.08	1.89

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	552	F43	O8D-C7D-C6D	-6.98	109.42	120.86
5	D	552	F43	C4B-CHC-C1C	5.63	135.06	125.84
5	D	552	F43	C6D-C7D-CHD	5.09	126.53	116.95
5	D	552	F43	C5D-C2D-C1D	3.92	115.72	110.45
5	A	1	F43	O8D-C7D-C6D	-3.90	114.48	120.86

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	553[A]	TP7	CB-O4P-P-O3P
5	D	552	F43	C3A-CAA-CBA-CCA
5	A	1	F43	C3A-CAA-CBA-CCA
8	A	555[B]	XP9	C6-C7-C8-C9
8	A	555[B]	XP9	C3-C4-C5-C6

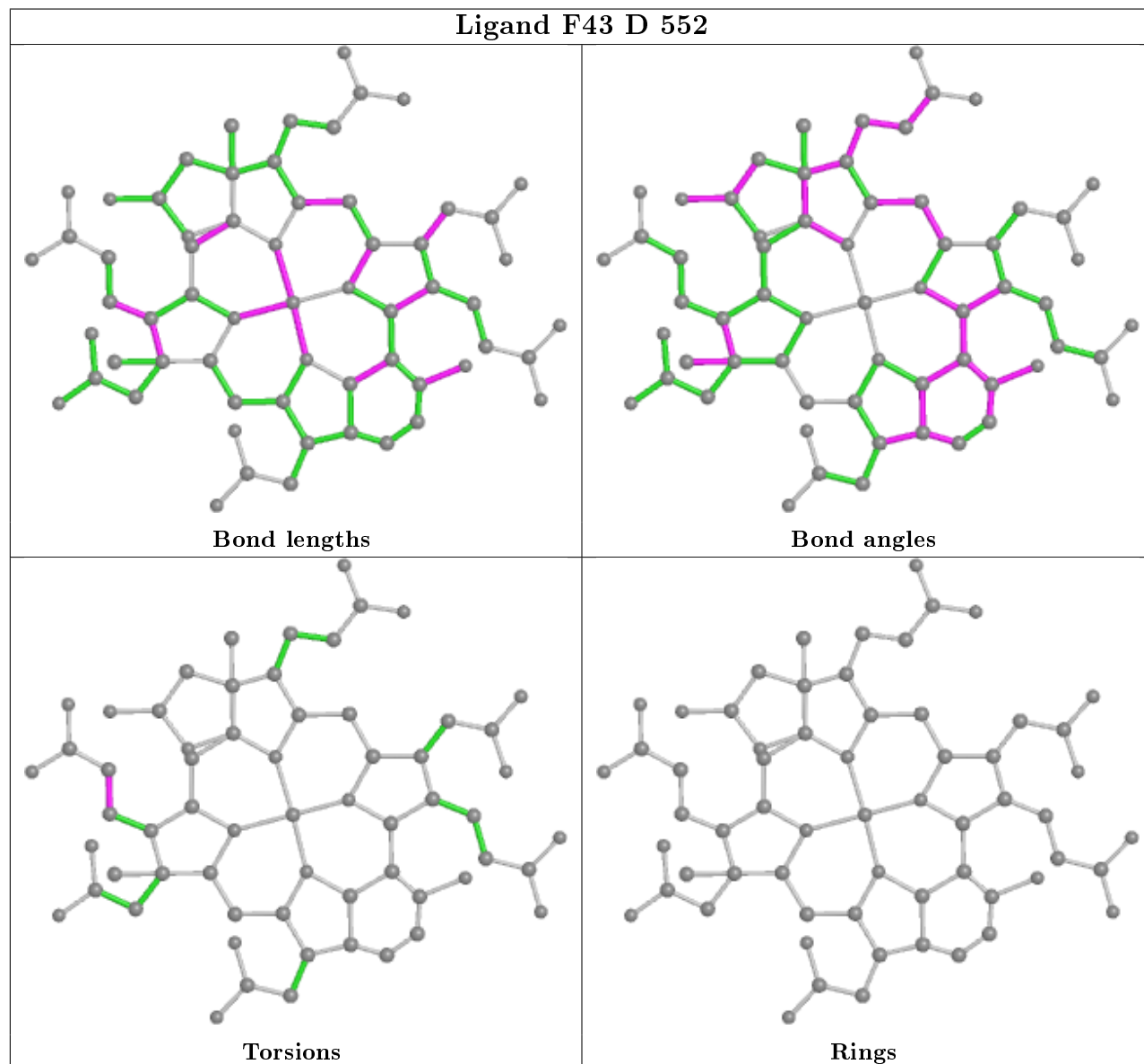
There are no ring outliers.

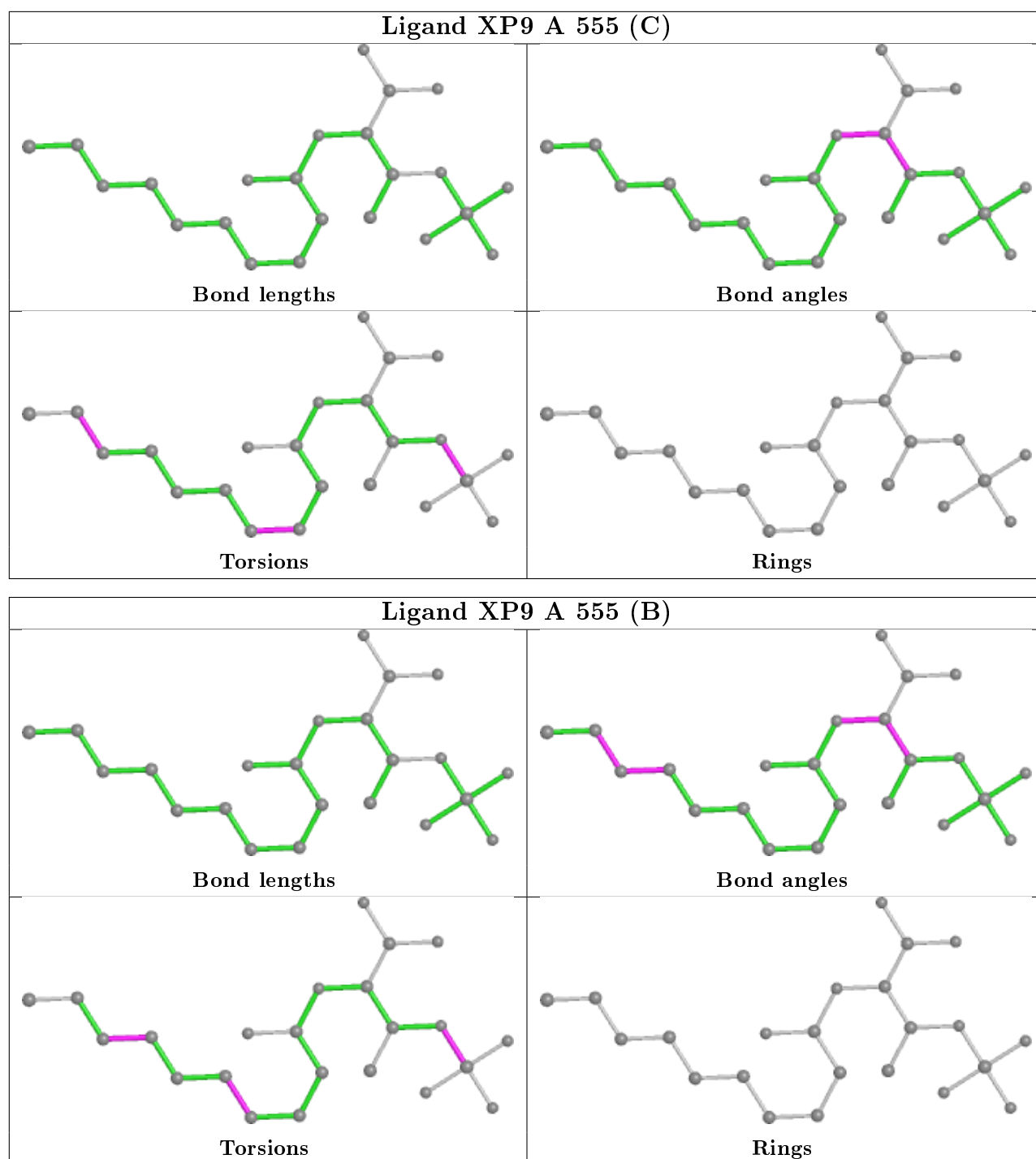
9 monomers are involved in 23 short contacts:

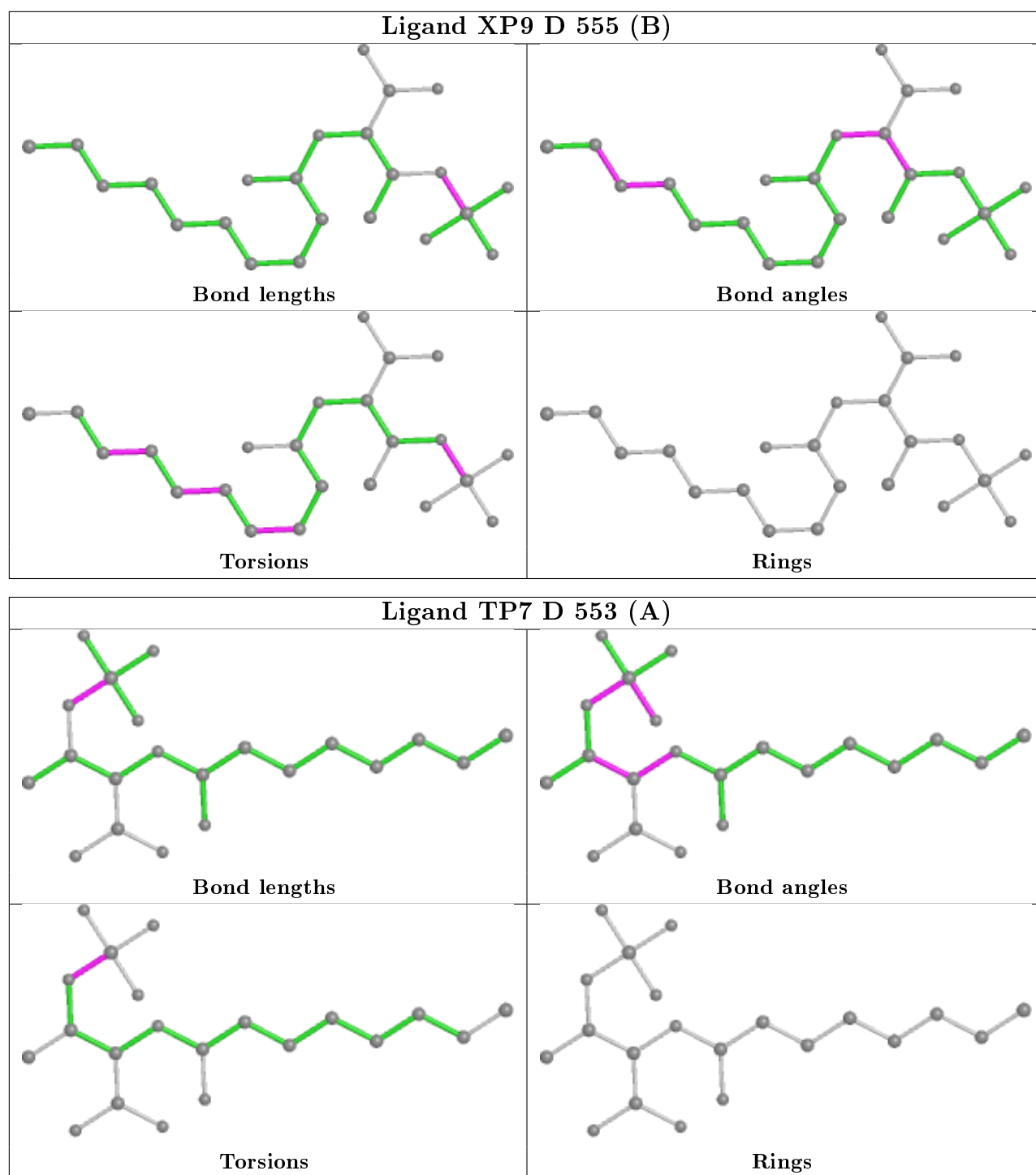
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	552	F43	1	0
10	D	556	EDO	1	0
9	C	1	ACT	10	0
10	F	252	EDO	3	0
8	A	555[B]	XP9	1	0
8	D	555[B]	XP9	3	0
6	A	553[A]	TP7	2	0
10	F	251	EDO	1	0
5	A	1	F43	1	0

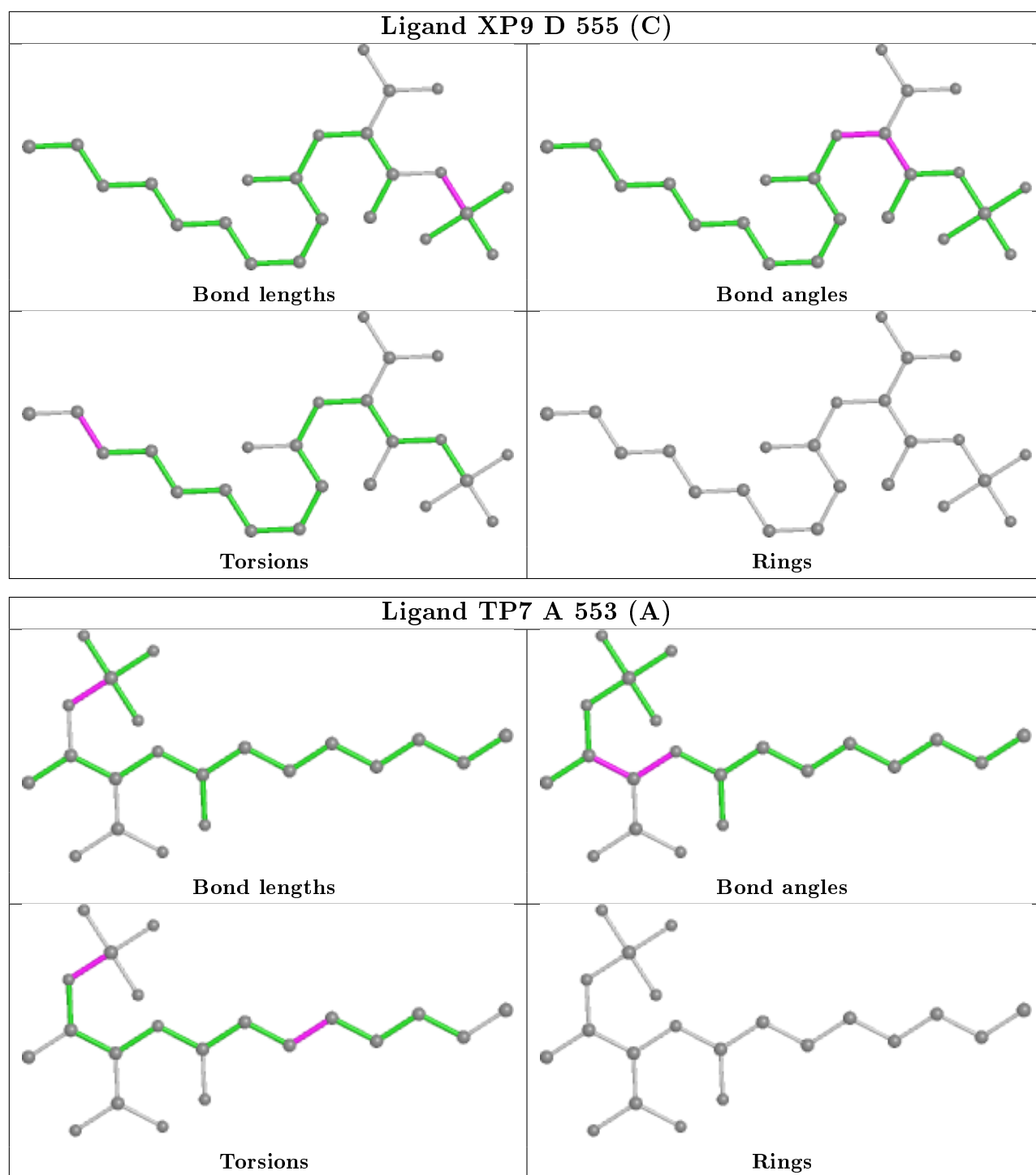
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

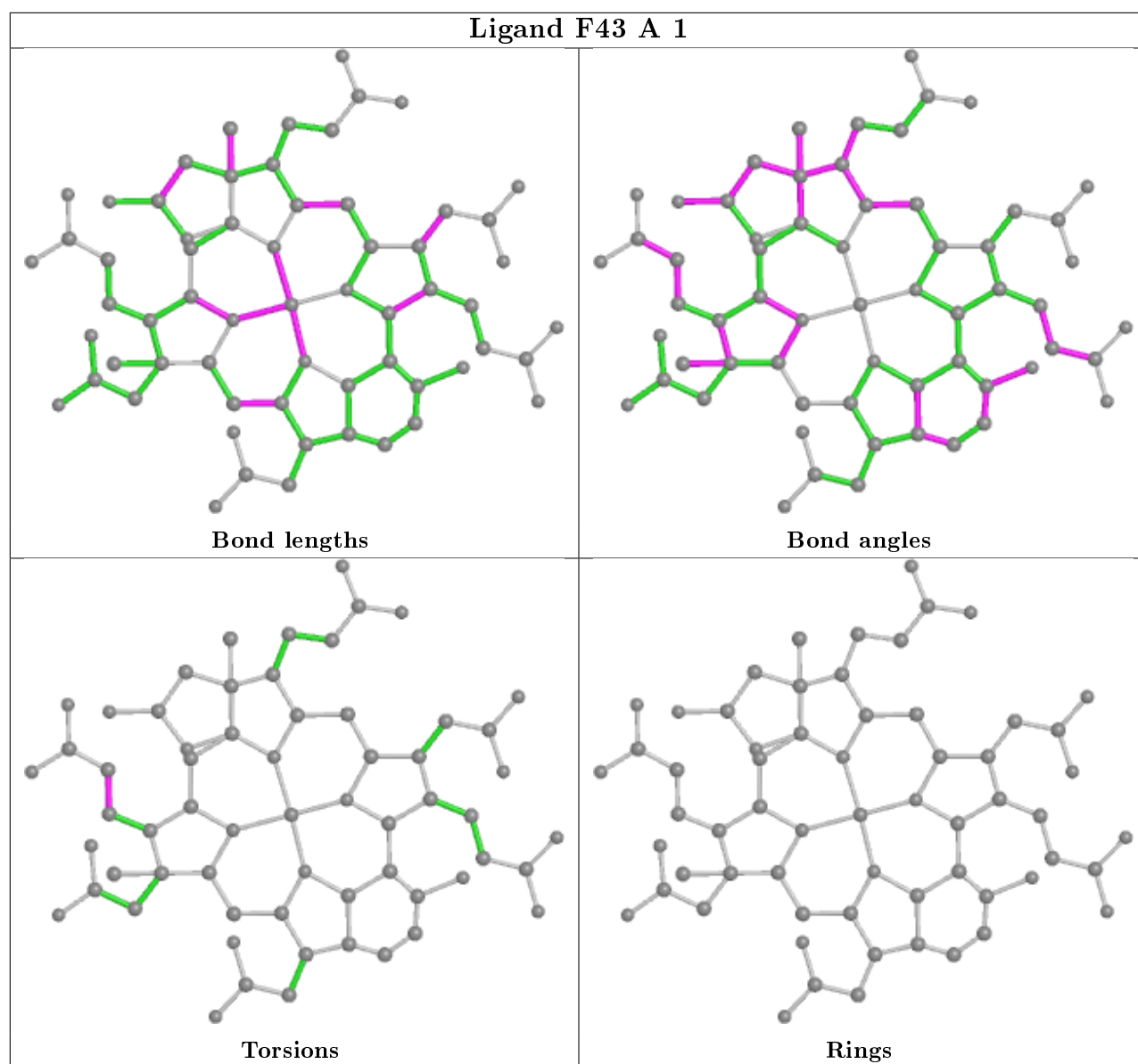
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/549 (98%)	-0.68	3 (0%) 89 91	5, 9, 20, 34	0
1	D	543/549 (98%)	-0.68	3 (0%) 89 91	5, 9, 20, 38	0
2	B	442/442 (100%)	-0.69	1 (0%) 95 95	6, 11, 20, 39	0
2	E	442/442 (100%)	-0.61	4 (0%) 84 86	7, 12, 24, 42	0
3	C	246/248 (99%)	-0.45	9 (3%) 41 44	8, 13, 30, 49	0
3	F	246/248 (99%)	-0.38	9 (3%) 41 44	8, 14, 30, 53	0
All	All	2462/2478 (99%)	-0.62	29 (1%) 79 80	5, 11, 23, 53	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	5.4
3	C	60	ASP	5.2
3	F	45	PRO	4.8
3	C	45	PRO	4.8
1	D	549	ALA	4.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	AGM	D	271	12/13	0.97	0.06	5,6,7,9	0
1	MHS	D	257	11/12	0.98	0.05	8,10,12,13	0
1	MGN	A	400	10/11	0.98	0.05	5,7,8,8	0
1	MGN	D	400	10/11	0.98	0.05	6,7,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MHS	A	257	11/12	0.98	0.04	9,11,13,18	0
1	AGM	A	271	12/13	0.98	0.05	5,6,7,8	0
1	SMC	A	452	7/8	0.99	0.06	6,7,8,10	0
1	SMC	D	452	7/8	0.99	0.05	7,7,10,11	0
1	GL3	A	445	4/5	0.99	0.06	5,6,7,7	0
1	GL3	D	445	4/5	1.00	0.06	5,6,6,7	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	A	557	4/4	0.76	0.11	35,35,36,43	0
12	PEG	C	252	7/7	0.83	0.12	37,38,44,44	0
10	EDO	F	252	4/4	0.84	0.15	35,39,40,44	0
9	ACT	C	1	4/4	0.87	0.20	27,29,30,33	4
10	EDO	C	251	4/4	0.87	0.13	36,39,40,43	0
10	EDO	F	251	4/4	0.88	0.11	34,34,36,39	0
10	EDO	D	556	4/4	0.90	0.09	33,36,41,41	0
10	EDO	B	446	4/4	0.93	0.09	42,42,43,44	0
4	MG	B	444	1/1	0.96	0.14	26,26,26,26	0
4	MG	A	551[A]	1/1	0.97	0.21	20,20,20,20	1
4	MG	B	445	1/1	0.97	0.32	34,34,34,34	0
4	MG	F	250	1/1	0.97	0.07	15,15,15,15	0
8	XP9	A	555[C]	23/23	0.98	0.06	5,8,8,10	23
8	XP9	A	555[B]	23/23	0.98	0.06	6,7,9,11	23
6	TP7	D	553[A]	21/21	0.98	0.06	7,8,9,12	21
4	MG	C	250	1/1	0.98	0.08	15,15,15,15	0
6	TP7	A	553[A]	21/21	0.98	0.05	7,8,10,13	21
9	ACT	A	556[B]	4/4	0.98	0.07	13,15,16,17	4
8	XP9	D	555[B]	23/23	0.98	0.07	6,7,10,12	23
8	XP9	D	555[C]	23/23	0.98	0.07	6,8,9,11	23
4	MG	A	552[B]	1/1	0.98	0.10	12,12,12,12	1
4	MG	D	1	1/1	0.98	0.14	21,21,21,21	0

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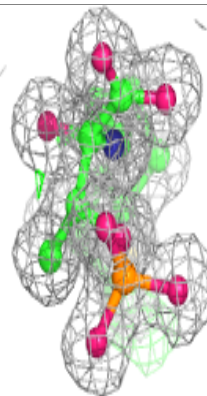
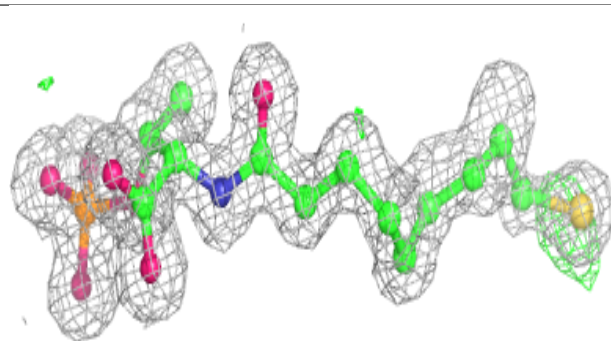
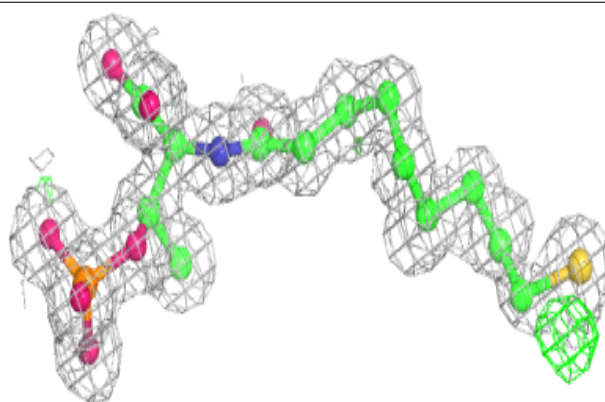
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	D	551	1/1	0.99	0.24	24,24,24,24	0
4	MG	E	444	1/1	0.99	0.18	21,21,21,21	0
5	F43	D	552	62/62	0.99	0.05	4,7,9,12	0
5	F43	A	1	62/62	0.99	0.05	5,7,10,13	0
7	COM	D	554	7/7	0.99	0.06	9,10,12,13	0
7	COM	A	554	7/7	0.99	0.04	9,9,12,12	7
11	ZN	A	558	1/1	1.00	0.03	10,10,10,10	1

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

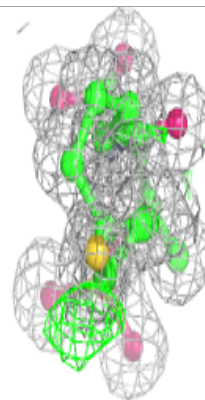
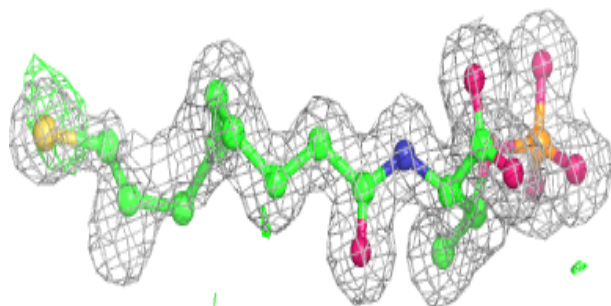
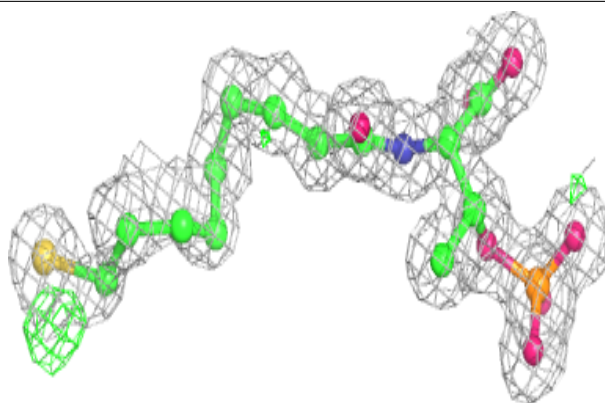
Electron density around XP9 A 555 (C):

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

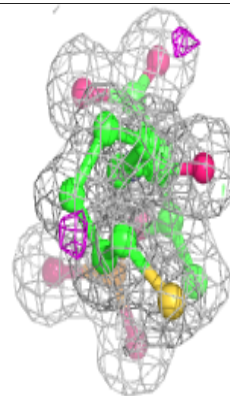
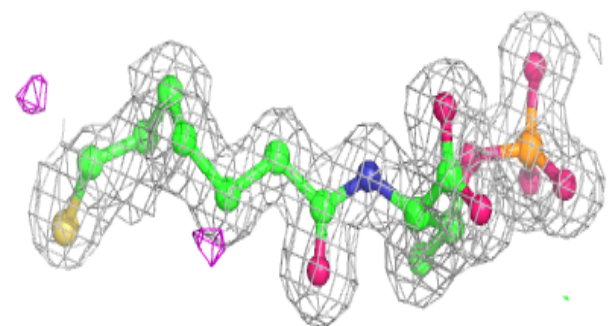
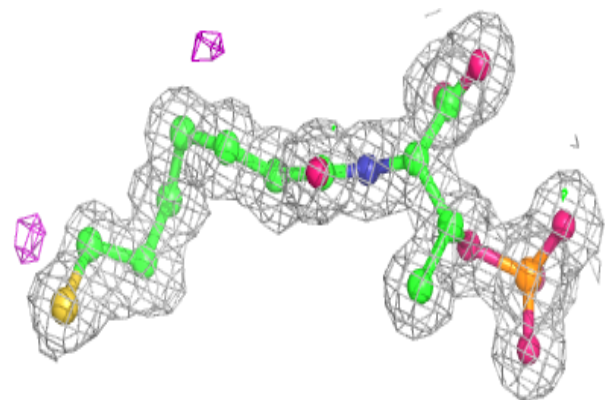


Electron density around XP9 A 555 (B):

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

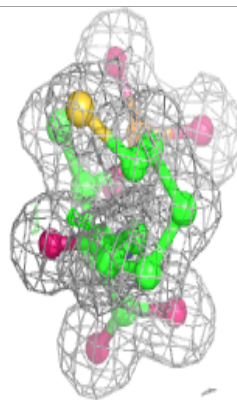
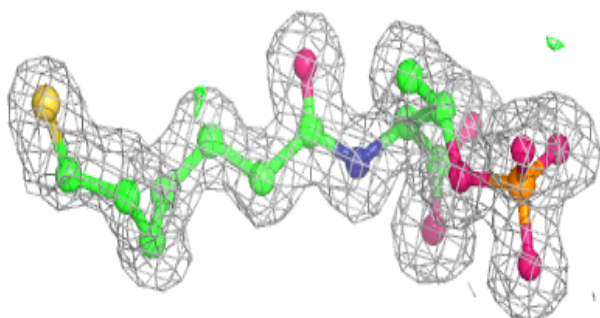
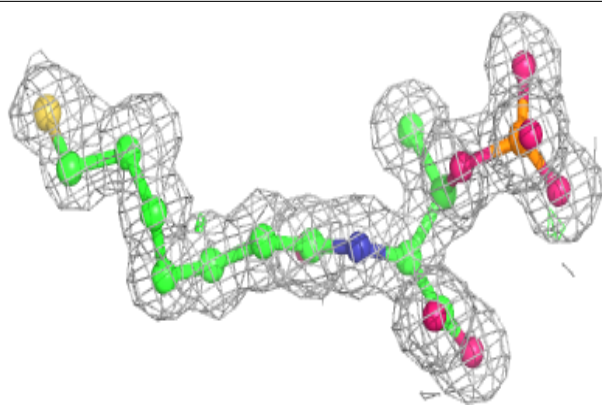
**Electron density around TP7 D 553 (A):**

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

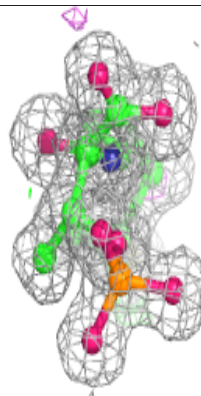
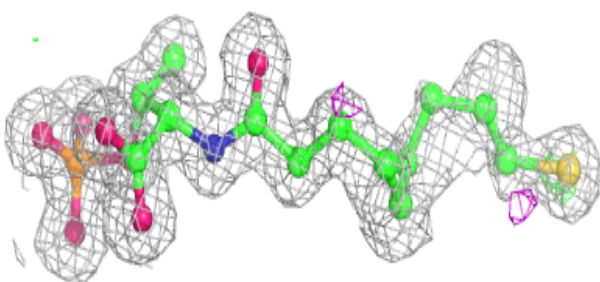
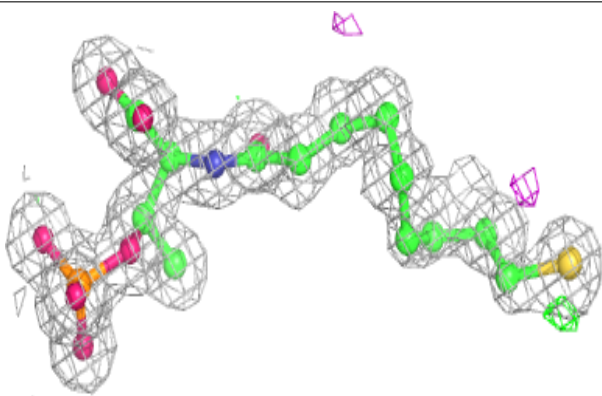


Electron density around TP7 A 553 (A):

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

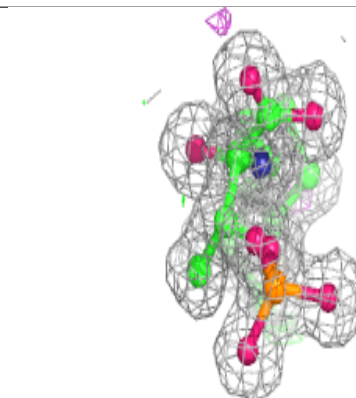
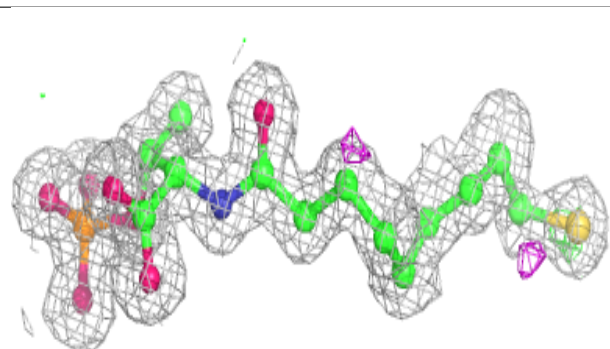
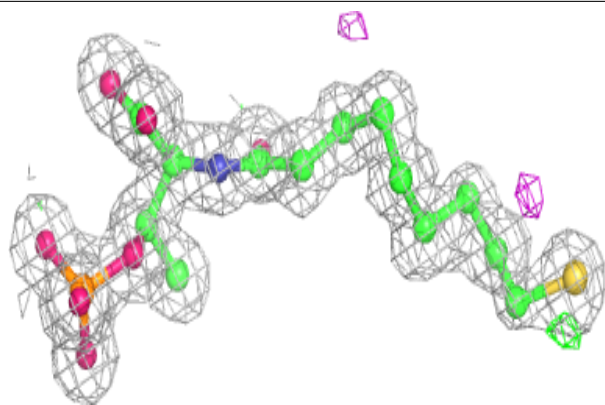
**Electron density around XP9 D 555 (B):**

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



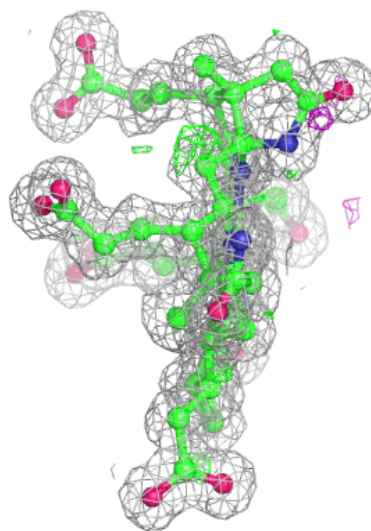
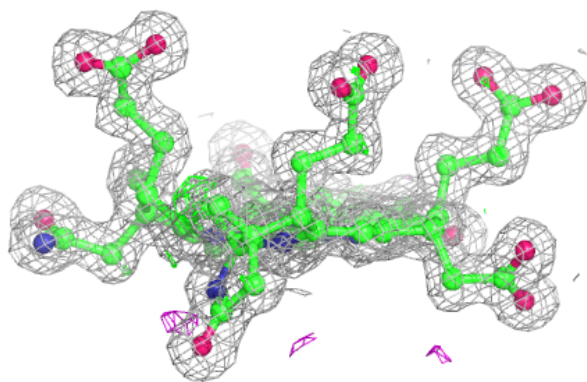
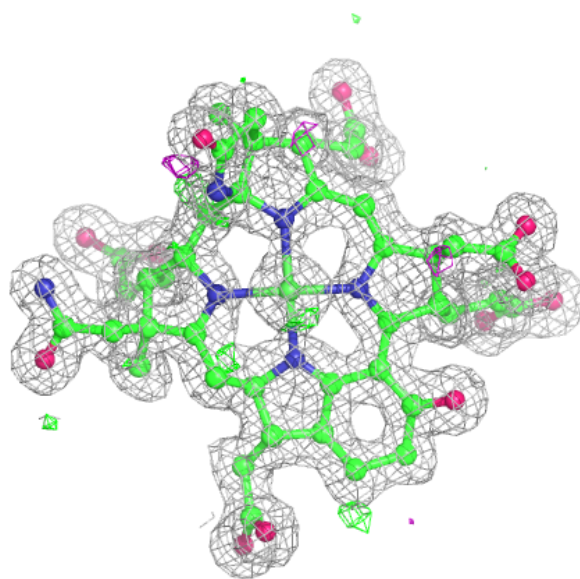
Electron density around XP9 D 555 (C):

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



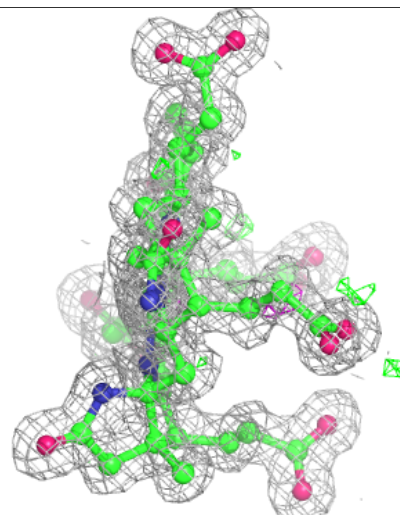
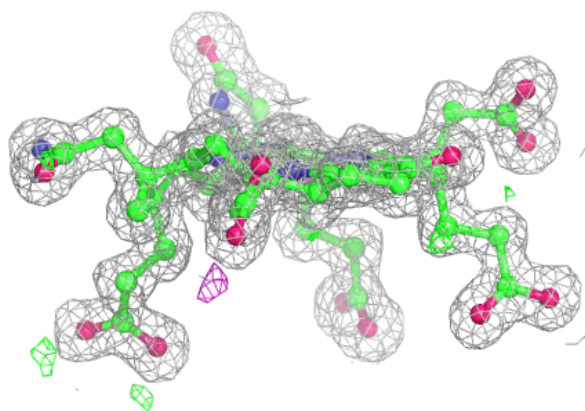
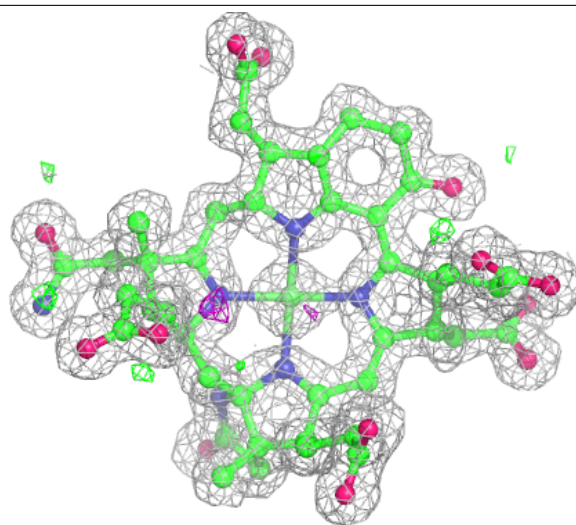
Electron density around F43 D 552:

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



Electron density around F43 A 1:

$2mF_o-DF_c$ (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.