



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 19, 2025 – 08:30 AM EDT

PDB ID : 3M32
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 : 1.35 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

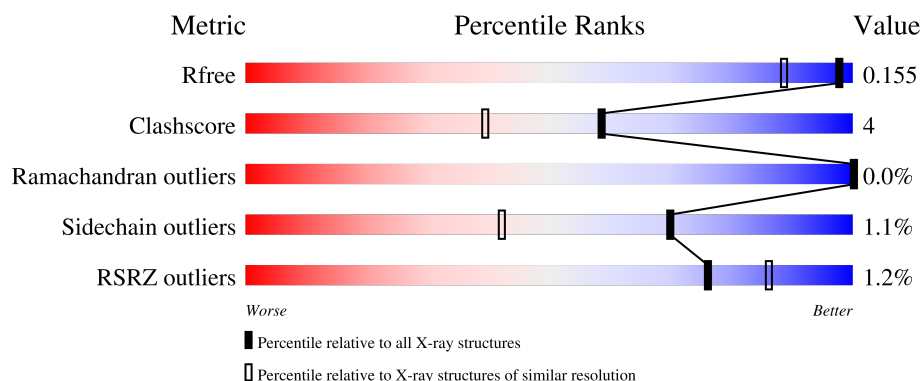
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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}	164625	1089 (1.36-1.36)
Clashscore	180529	1157 (1.36-1.36)
Ramachandran outliers	177936	1146 (1.36-1.36)
Sidechain outliers	177891	1146 (1.36-1.36)
RSRZ outliers	164620	1088 (1.36-1.36)

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

Mol	Chain	Length	Quality of chain
1	A	549	<div> <div style="width: 83%;"></div> <div style="width: 15%;"></div> <div style="width: 2%;"></div> </div> <div>83% 15% .</div>
1	D	549	<div> <div style="width: 83%;"></div> <div style="width: 16%;"></div> <div style="width: 1%;"></div> </div> <div>83% 16% .</div>
2	B	442	<div> <div style="width: 82%;"></div> <div style="width: 16%;"></div> <div style="width: 2%;"></div> </div> <div>82% 16% .</div>
2	E	442	<div> <div style="width: 84%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div> <div>84% 15% .</div>
3	C	248	<div> <div style="width: 80%;"></div> <div style="width: 18%;"></div> <div style="width: 2%;"></div> </div> <div>80% 18% .</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	248	<div><div></div><div>3%</div><div>72%</div><div>25%</div><div>..</div></div>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 22665 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	28	0
			4431	2801	735	874	21			
1	D	548	Total	C	N	O	S	0	22	0
			4380	2779	727	853	21			

- 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	24	0
			3462	2211	560	668	23			
2	E	442	Total	C	N	O	S	0	25	0
			3471	2216	564	668	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	10	0
			2056	1276	360	407	13			
3	F	246	Total	C	N	O	S	0	20	0
			2113	1309	372	418	14			

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

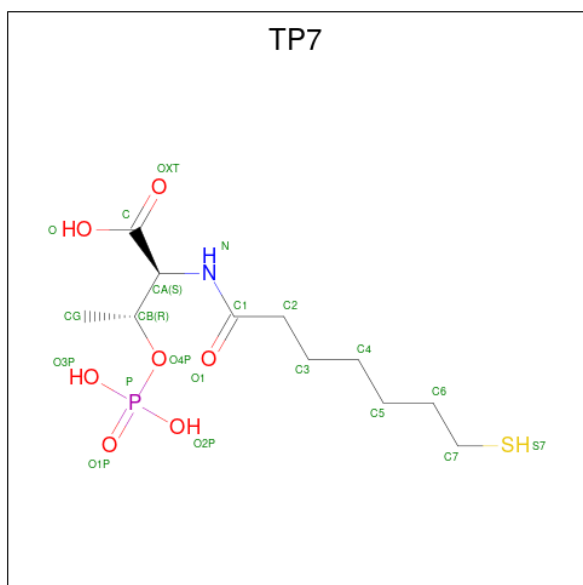
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	2
			2	2		
4	B	2	Total	Mg	0	1
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	D	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

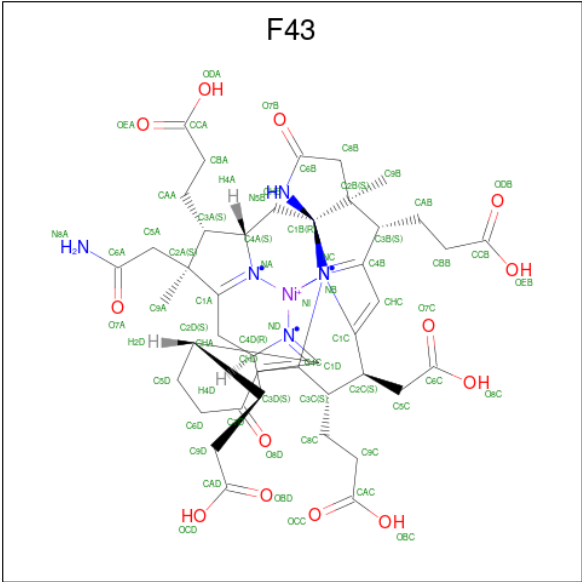
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

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



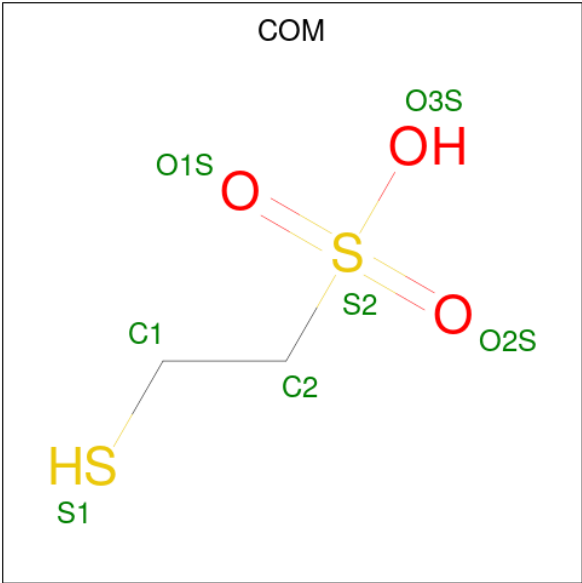
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	1
5	D	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	1

- Molecule 6 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



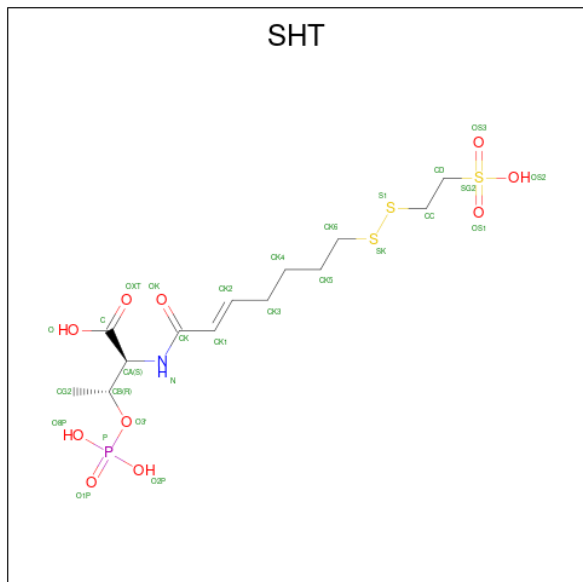
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
6	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 7 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: C₂H₆O₃S₂).



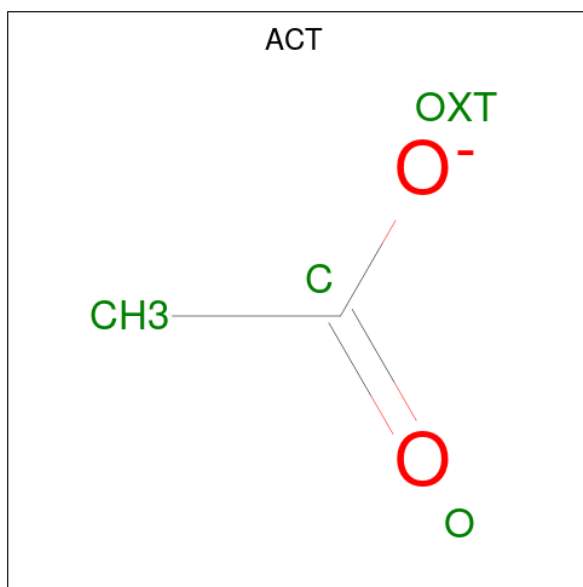
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	1
			7	2	3	2		
7	D	1	Total	C	O	S	0	1
			7	2	3	2		

- Molecule 8 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (three-letter code: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$).



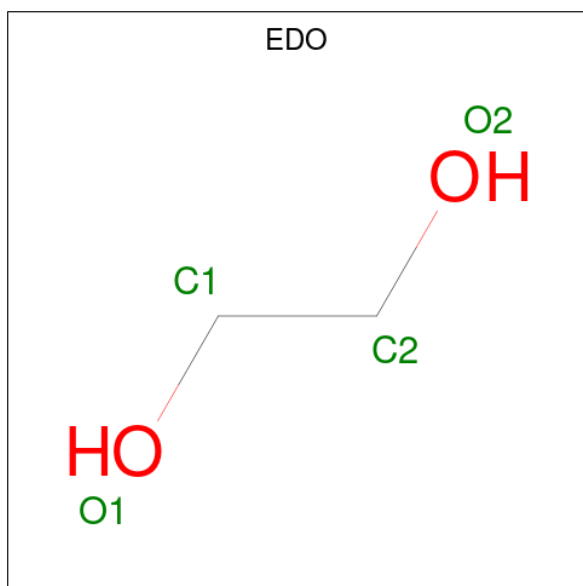
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			28	13	1	10	1	3		
8	D	1	Total	C	N	O	P	S	0	1
			28	13	1	10	1	3		

- 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		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

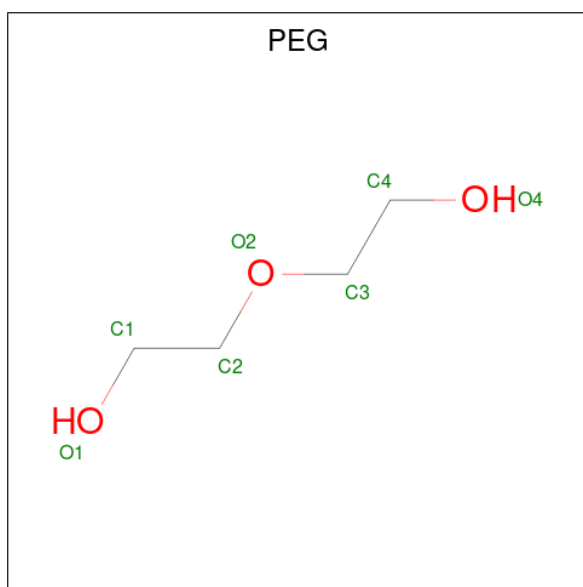


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

- 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	28
			522	522		
13	B	462	Total	O	0	24
			477	477		
13	C	254	Total	O	0	12
			262	262		
13	D	529	Total	O	0	20
			539	539		
13	E	414	Total	O	0	16
			421	421		
13	F	250	Total	O	0	8
			254	254		

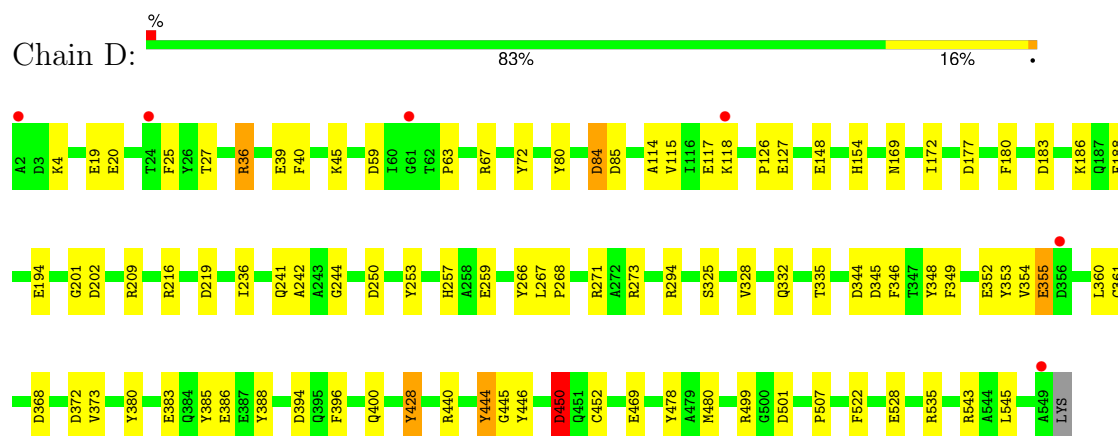
3 Residue-property plots

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.

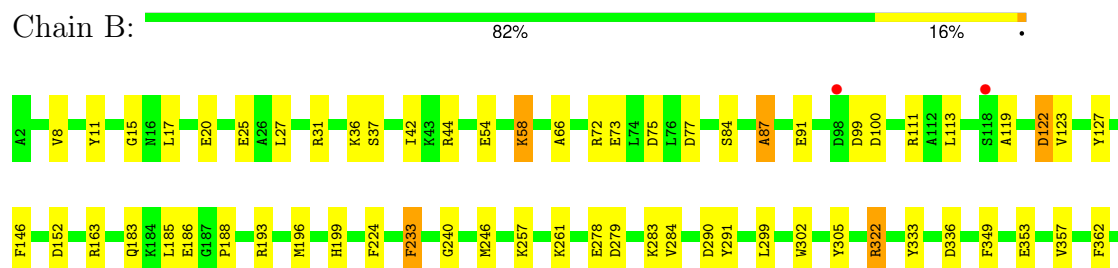
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



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

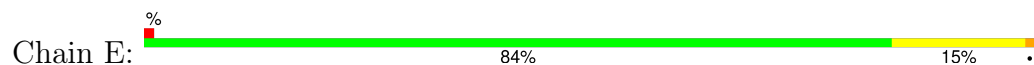


- Molecule 2: Methyl-coenzyme M reductase I subunit beta

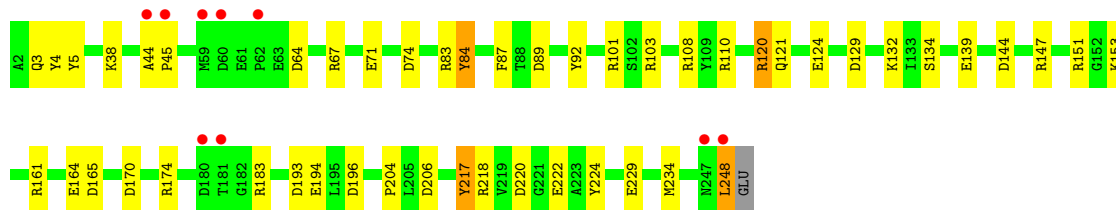
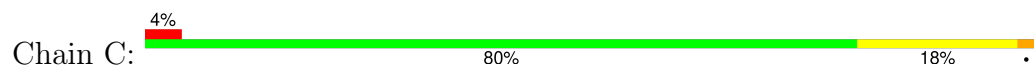




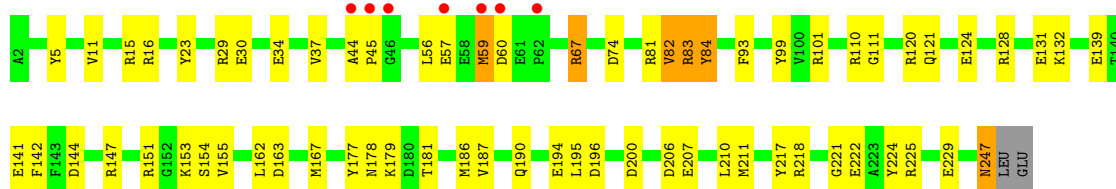
- Molecule 2: Methyl-coenzyme M reductase I subunit beta



- 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)	20.28 – 1.35 20.28 – 1.35	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.28-1.35) 93.1 (20.28-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 1.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.140 , 0.157 0.139 , 0.155	Depositor DCC
R_{free} test set	23829 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k 0.006 for -h,-l,-k 0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22665	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	1.58	28/4528 (0.6%)	1.45	44/6146 (0.7%)
1	D	1.62	29/4483 (0.6%)	1.52	55/6084 (0.9%)
2	B	1.58	27/3578 (0.8%)	1.49	37/4839 (0.8%)
2	E	1.65	28/3590 (0.8%)	1.41	25/4852 (0.5%)
3	C	1.80	20/2117 (0.9%)	1.63	29/2851 (1.0%)
3	F	1.84	31/2186 (1.4%)	1.68	40/2940 (1.4%)
All	All	1.65	163/20482 (0.8%)	1.51	230/27712 (0.8%)

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	0
1	D	1	0
3	C	0	2
All	All	2	2

The worst 5 of 163 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	124	GLU	CG-CD	9.37	1.66	1.51
1	A	352	GLU	CD-OE2	9.14	1.35	1.25
3	F	139	GLU	CD-OE2	8.46	1.34	1.25
2	E	341	GLU	CD-OE2	8.21	1.34	1.25
1	D	386	GLU	CD-OE1	7.83	1.34	1.25

The worst 5 of 230 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	147	ARG	NE-CZ-NH1	16.68	128.64	120.30
2	B	44	ARG	NE-CZ-NH1	15.62	128.11	120.30
3	F	147	ARG	NE-CZ-NH1	14.07	127.33	120.30
1	D	499	ARG	NE-CZ-NH2	-13.57	113.52	120.30
2	B	44	ARG	NE-CZ-NH2	-12.99	113.80	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 (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	120	ARG	Sidechain
3	C	217	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	4431	0	4224	47	0
1	D	4380	0	4219	29	0
2	B	3462	0	3517	40	0
2	E	3471	0	3532	33	0
3	C	2056	0	2000	23	0
3	F	2113	0	2065	21	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	21	0	19	0	0
5	D	21	0	19	0	0
6	A	62	0	43	2	0
6	D	62	0	43	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	7	0	4	0	0
7	D	7	0	5	1	0
8	A	28	0	21	0	0
8	D	28	0	21	1	0
9	A	4	0	3	0	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
10	D	4	0	6	1	0
10	F	8	0	12	0	0
11	A	1	0	0	0	0
12	C	7	0	10	0	0
13	A	522	0	0	12	0
13	B	477	0	0	14	0
13	C	262	0	0	4	0
13	D	539	0	0	8	0
13	E	421	0	0	11	0
13	F	254	0	0	10	0
All	All	22665	0	19775	172	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 172 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:F:207[B]:GLU:HG3	13:F:3759:HOH:O	1.39	1.23
2:E:91[B]:GLU:HG2	13:E:3974:HOH:O	1.64	0.97
1:D:545[A]:LEU:HD12	13:D:2591:HOH:O	1.66	0.93
1:A:433:LEU:HD23	3:C:234[B]:MET:SD	2.08	0.93
1:A:433:LEU:CD2	3:C:234[B]:MET:SD	2.60	0.88

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	569/549 (104%)	555 (98%)	14 (2%)	0	100	100
1	D	563/549 (103%)	544 (97%)	18 (3%)	1 (0%)	44	19
2	B	465/442 (105%)	457 (98%)	8 (2%)	0	100	100
2	E	466/442 (105%)	457 (98%)	9 (2%)	0	100	100
3	C	255/248 (103%)	247 (97%)	8 (3%)	0	100	100
3	F	264/248 (106%)	258 (98%)	6 (2%)	0	100	100
All	All	2582/2478 (104%)	2518 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	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	461/434 (106%)	455 (99%)	6 (1%)	65	35
1	D	455/434 (105%)	450 (99%)	5 (1%)	70	42
2	B	366/341 (107%)	365 (100%)	1 (0%)	91	80
2	E	367/341 (108%)	361 (98%)	6 (2%)	58	27
3	C	225/216 (104%)	223 (99%)	2 (1%)	75	51
3	F	233/216 (108%)	226 (97%)	7 (3%)	36	8
All	All	2107/1982 (106%)	2080 (99%)	27 (1%)	70	35

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	58	LYS
2	E	438[A]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	179[B]	LYS
2	E	283	LYS
2	E	438[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	121	GLN
3	F	121	GLN
3	F	247	ASN

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	GL3	A	445	1	2,3,4	2.04	1 (50%)	1,2,4	0.28	0
1	GL3	D	445	1	2,3,4	2.22	1 (50%)	1,2,4	0.31	0
1	MGN	A	400	1	6,9,10	1.23	1 (16%)	7,12,14	1.00	1 (14%)
1	AGM	A	271	1	10,11,12	0.84	0	7,13,15	2.04	2 (28%)
1	MHS	A	257	1	7,11,12	1.64	2 (28%)	7,14,16	3.38	2 (28%)
1	SMC	A	452	1	5,6,7	1.21	0	3,6,8	1.91	1 (33%)
1	AGM	D	271	1	10,11,12	1.00	0	7,13,15	1.06	1 (14%)
1	MHS	D	257	1	7,11,12	1.37	1 (14%)	7,14,16	3.48	2 (28%)
1	SMC	D	452	1	5,6,7	1.20	0	3,6,8	1.58	1 (33%)
1	MGN	D	400	1	6,9,10	1.84	3 (50%)	7,12,14	1.01	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	GL3	A	445	1	-	1/1/1/2	-
1	GL3	D	445	1	-	1/1/1/2	-
1	MGN	A	400	1	-	0/7/9/12	-
1	AGM	A	271	1	-	2/10/11/13	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	SMC	A	452	1	-	1/3/5/7	-
1	AGM	D	271	1	-	1/10/11/13	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	SMC	D	452	1	-	1/3/5/7	-
1	MGN	D	400	1	-	0/7/9/12	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CE1-NE2	3.21	1.41	1.34
1	D	445	GL3	C-S	-3.14	1.67	1.80
1	D	400	MGN	CB1-CA	-3.09	1.51	1.55
1	A	445	GL3	C-S	-2.88	1.68	1.80
1	D	257	MHS	CE1-NE2	2.82	1.41	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	NE2-CE1-ND1	-7.82	100.64	112.26
1	A	257	MHS	NE2-CE1-ND1	-7.82	100.65	112.26
1	D	257	MHS	CD2-NE2-CE1	4.20	112.36	105.72
1	A	271	AGM	NH1-CZ-NE1	3.51	127.31	119.58
1	A	452	SMC	CA-CB-SG	-3.22	108.83	114.04

There are no chirality outliers.

5 of 7 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	A	271	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	GL3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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	$\# Z > 2$
9	ACT	A	556[B]	4	3,3,3	0.94	0	3,3,3	0.40	0
8	SHT	D	555[B]	6	26,27,27	2.66	3 (11%)	32,36,36	2.08	7 (21%)
7	COM	D	554[A]	6	6,6,6	1.56	1 (16%)	8,8,8	0.85	0
10	EDO	A	557	-	3,3,3	0.59	0	2,2,2	0.34	0
12	PEG	C	1	-	6,6,6	0.56	0	5,5,5	1.14	1 (20%)
5	TP7	D	553[A]	-	19,20,20	1.17	1 (5%)	24,26,26	1.26	3 (12%)
10	EDO	D	556	-	3,3,3	0.35	0	2,2,2	0.39	0
10	EDO	F	251	-	3,3,3	0.65	0	2,2,2	0.44	0
10	EDO	F	1	-	3,3,3	0.57	0	2,2,2	0.53	0
7	COM	A	554[A]	6	6,6,6	1.57	1 (16%)	8,8,8	2.14	2 (25%)
6	F43	A	1	7,1,8	63,71,71	2.62	16 (25%)	73,118,118	1.70	15 (20%)
10	EDO	B	445	-	3,3,3	0.73	0	2,2,2	0.24	0
6	F43	D	552	7,8,1	63,71,71	2.75	21 (33%)	73,118,118	2.02	25 (34%)
5	TP7	A	553[A]	-	19,20,20	1.04	1 (5%)	24,26,26	1.58	6 (25%)
8	SHT	A	555[B]	6	26,27,27	2.96	5 (19%)	32,36,36	1.93	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SHT	D	555[B]	6	-	3/31/31/31	-
7	COM	D	554[A]	6	-	0/4/4/4	-
10	EDO	A	557	-	-	1/1/1/1	-
12	PEG	C	1	-	-	0/4/4/4	-
5	TP7	D	553[A]	-	-	1/24/24/24	-
10	EDO	D	556	-	-	1/1/1/1	-
10	EDO	F	251	-	-	1/1/1/1	-
10	EDO	F	1	-	-	1/1/1/1	-
7	COM	A	554[A]	6	-	0/4/4/4	-
6	F43	A	1	7,1,8	-	10/28/185/185	-
10	EDO	B	445	-	-	1/1/1/1	-
6	F43	D	552	7,8,1	-	10/28/185/185	-
5	TP7	A	553[A]	-	-	2/24/24/24	-
8	SHT	A	555[B]	6	-	5/31/31/31	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	555[B]	SHT	CD-SG2	-11.99	1.60	1.77
6	D	552	F43	NI-NB	10.52	2.14	1.89
6	A	1	F43	CHB-C1B	-9.70	1.46	1.53
8	D	555[B]	SHT	CD-SG2	-9.34	1.64	1.77
6	D	552	F43	NI-NA	8.86	2.10	1.89

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	555[B]	SHT	CK3-CK2-CK1	-7.19	110.95	125.92
6	D	552	F43	C5D-C2D-C1D	6.38	118.75	110.43
6	D	552	F43	C2D-C1D-CHD	-5.80	114.66	121.85
8	A	555[B]	SHT	CK3-CK2-CK1	-5.02	115.46	125.92
8	D	555[B]	SHT	CK2-CK1-CK	-4.99	110.26	122.94

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	555[B]	SHT	S1-CC-CD-SG2
8	A	555[B]	SHT	CK-CK1-CK2-CK3

Continued on next page...

Continued from previous page...

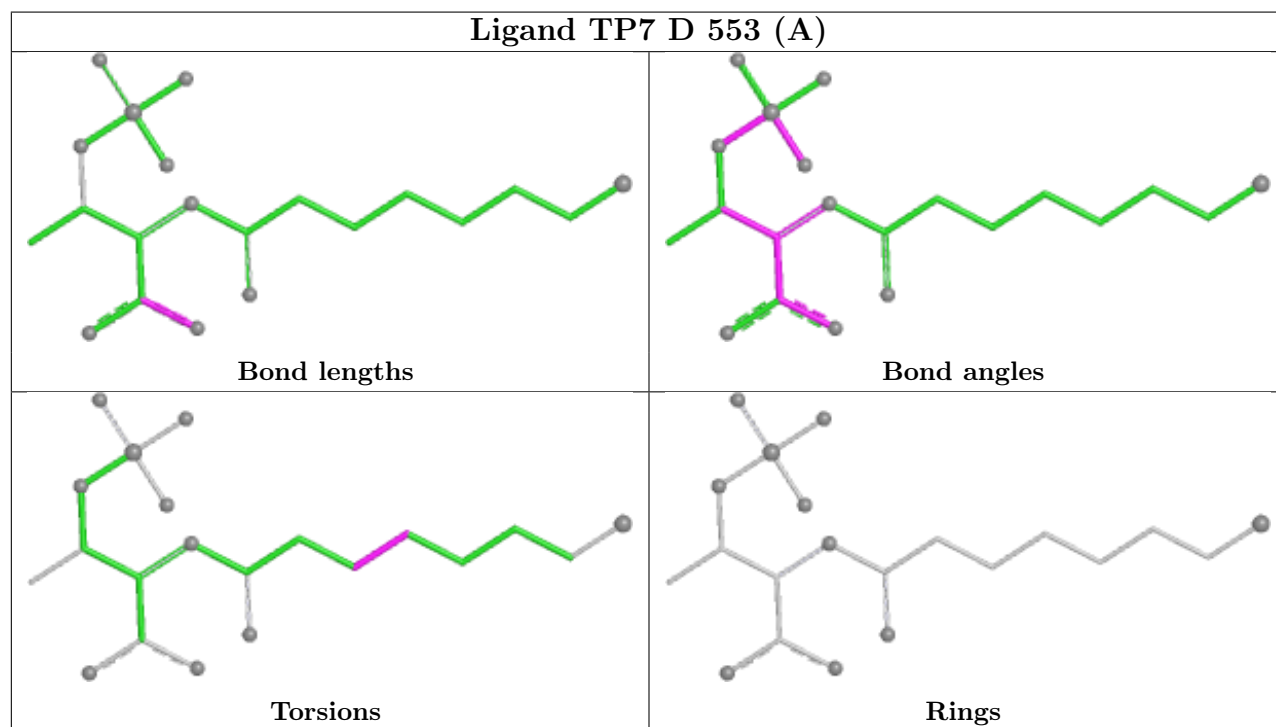
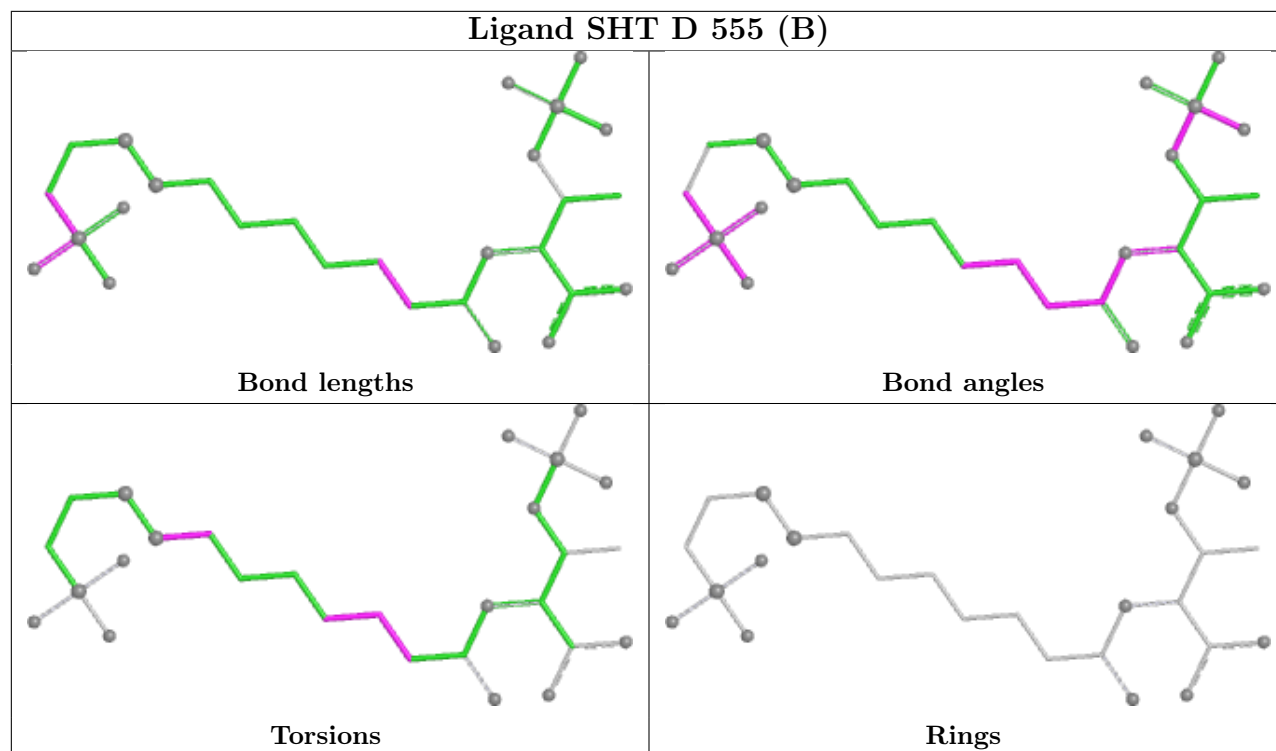
Mol	Chain	Res	Type	Atoms
8	D	555[B]	SHT	CK-CK1-CK2-CK3
6	A	1	F43	C3A-CAA-CBA-CCA
6	D	552	F43	C3A-CAA-CBA-CCA

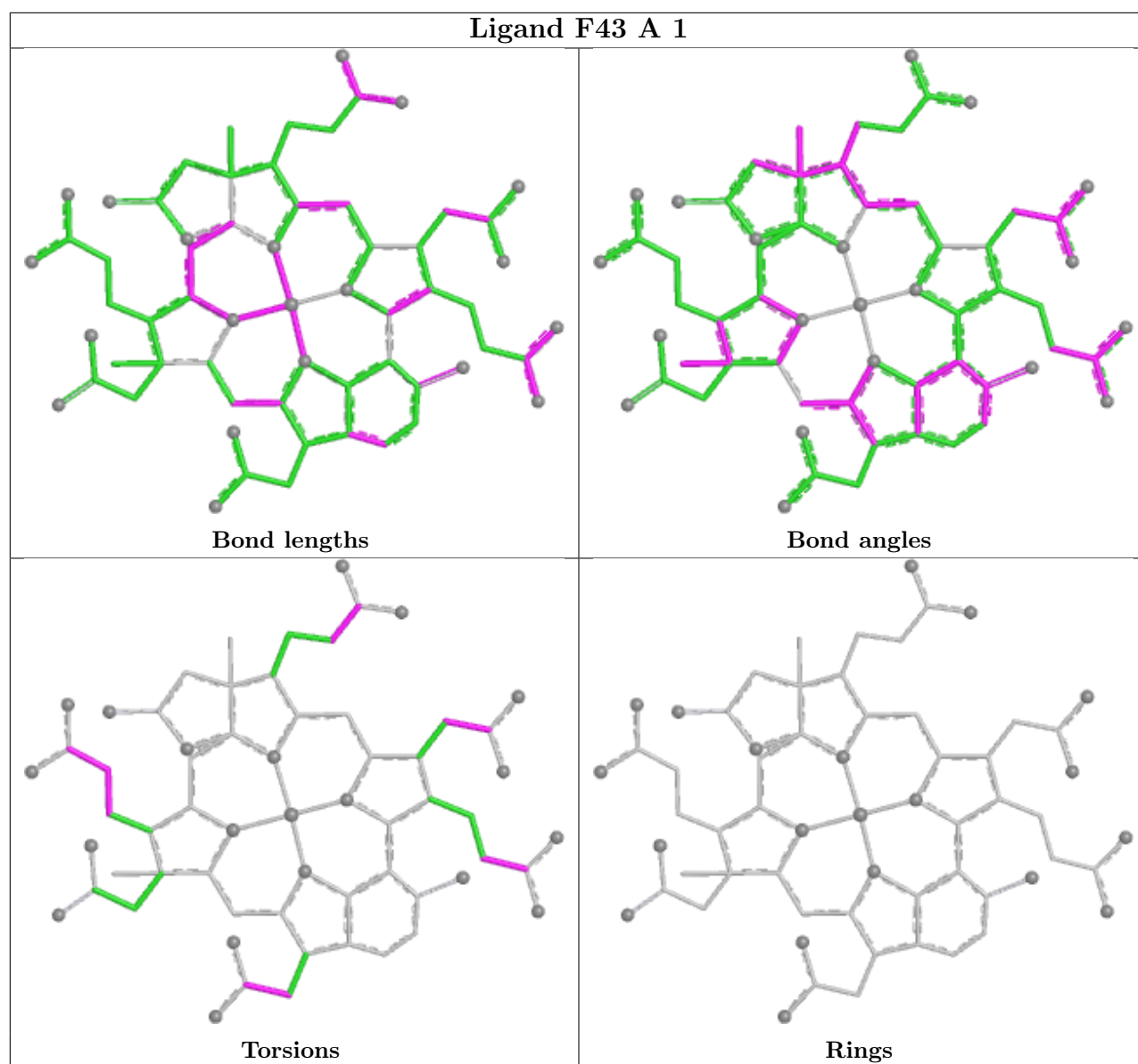
There are no ring outliers.

5 monomers are involved in 5 short contacts:

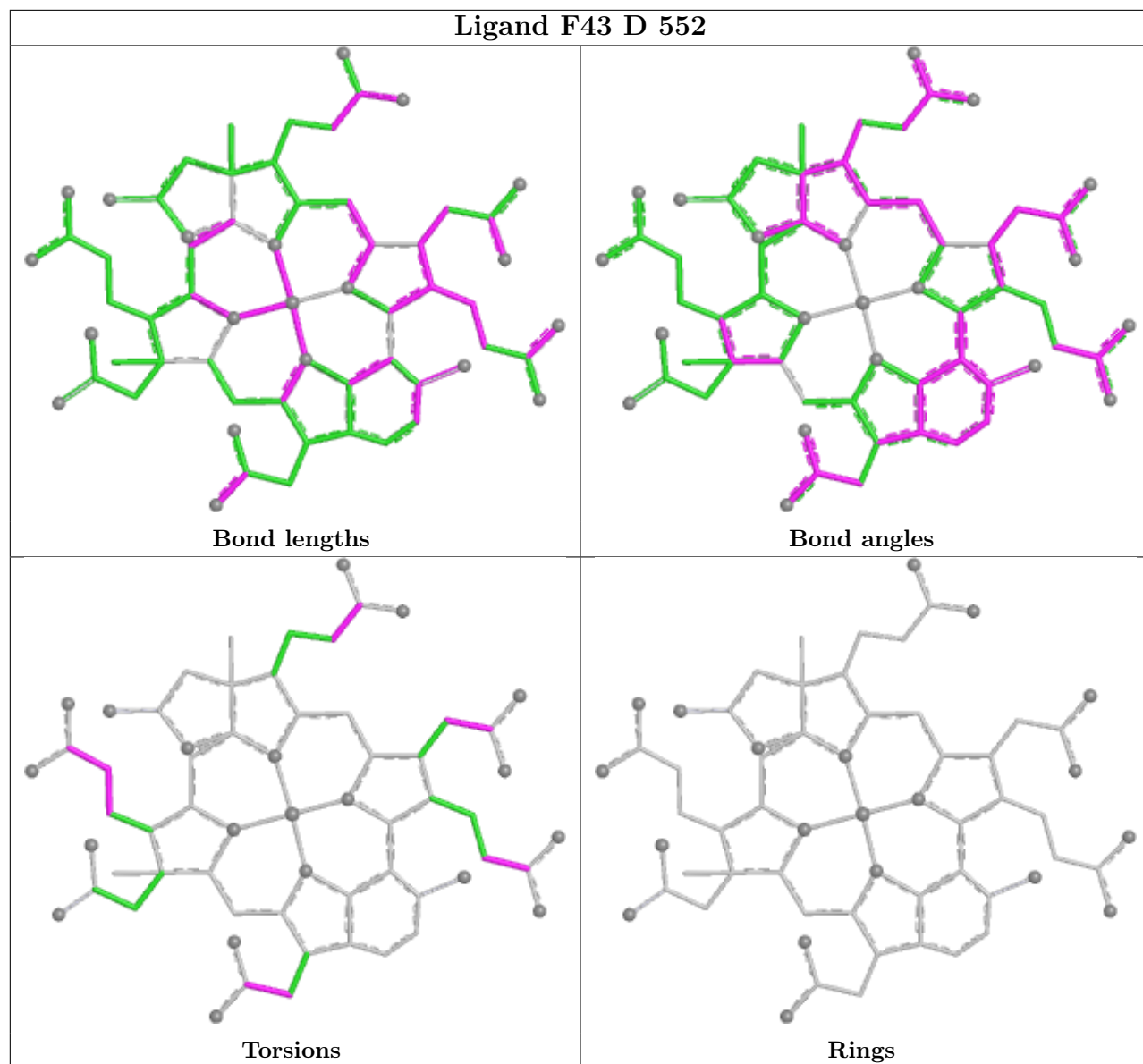
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	555[B]	SHT	1	0
7	D	554[A]	COM	1	0
10	D	556	EDO	1	0
6	A	1	F43	2	0
6	D	552	F43	1	0

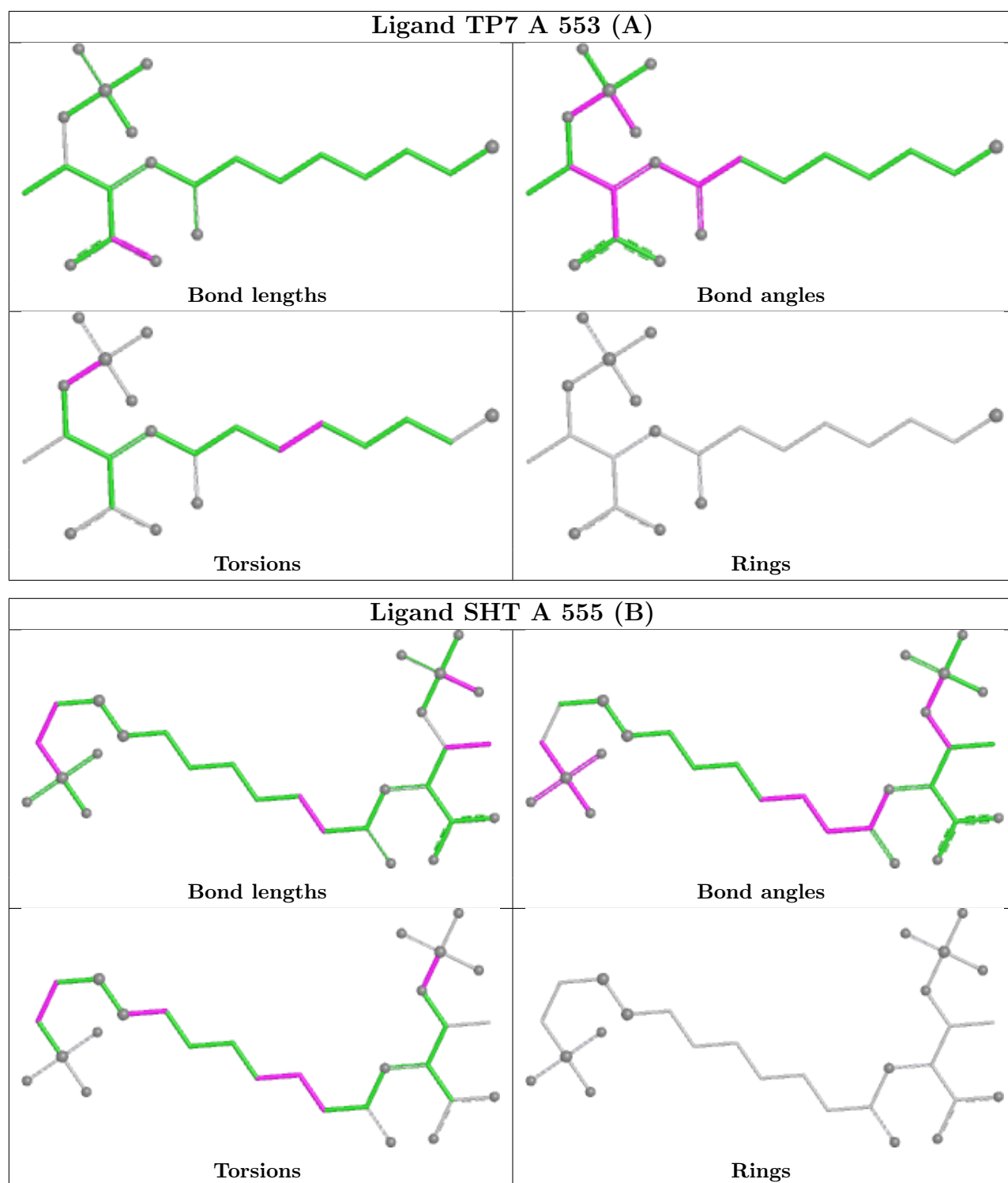
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.





Ligand F43 D 552





5.7 Other polymers [i](#)

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 [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%)	-0.46	2 (0%) 89 94	4, 9, 20, 33	27 (4%)
1	D	543/549 (98%)	-0.44	6 (1%) 77 88	4, 10, 20, 37	22 (4%)
2	B	442/442 (100%)	-0.34	2 (0%) 87 93	5, 12, 19, 35	24 (5%)
2	E	442/442 (100%)	-0.25	4 (0%) 81 90	5, 12, 23, 40	25 (5%)
3	C	247/248 (99%)	-0.03	9 (3%) 46 58	6, 14, 32, 47	10 (4%)
3	F	246/248 (99%)	0.01	7 (2%) 55 66	5, 14, 30, 53	20 (8%)
All	All	2463/2478 (99%)	-0.31	30 (1%) 76 86	4, 11, 23, 53	128 (5%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	3.8
1	D	2	ALA	3.7
3	F	45	PRO	3.6
3	C	248	LEU	3.2
3	C	45	PRO	3.1

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	MHS	A	257	11/12	0.97	0.06	8,10,14,17	0
1	MHS	D	257	11/12	0.97	0.05	9,10,12,16	0
1	AGM	D	271	12/13	0.97	0.05	6,7,7,8	0
1	MGN	A	400	10/11	0.98	0.04	7,8,9,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	AGM	A	271	12/13	0.99	0.03	6,6,7,8	0
1	SMC	A	452	7/8	0.99	0.04	7,7,9,10	0
1	MGN	D	400	10/11	0.99	0.04	6,8,8,8	0
1	SMC	D	452	7/8	0.99	0.04	7,8,9,11	0
1	GL3	D	445	4/5	1.00	0.02	6,6,7,7	0
1	GL3	A	445	4/5	1.00	0.04	6,7,7,8	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, 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	D	556	4/4	0.89	0.10	32,38,40,44	0
12	PEG	C	1	7/7	0.90	0.14	34,38,42,42	0
10	EDO	F	1	4/4	0.91	0.09	38,39,39,39	0
10	EDO	A	557	4/4	0.91	0.11	30,35,39,42	0
10	EDO	B	445	4/4	0.92	0.10	42,42,43,46	0
10	EDO	F	251	4/4	0.92	0.11	39,42,43,48	0
4	MG	B	444	1/1	0.94	0.13	23,23,23,23	0
4	MG	D	1	1/1	0.96	0.15	20,20,20,20	0
9	ACT	A	556[B]	4/4	0.96	0.07	15,16,17,19	4
8	SHT	A	555[B]	28/28	0.98	0.05	6,7,12,14	28
4	MG	A	551[A]	1/1	0.98	0.10	18,18,18,18	1
4	MG	B	1[B]	1/1	0.98	0.06	21,21,21,21	1
4	MG	C	250	1/1	0.98	0.09	17,17,17,17	0
4	MG	A	552[B]	1/1	0.98	0.09	14,14,14,14	1
4	MG	E	444	1/1	0.98	0.14	22,22,22,22	0
4	MG	F	250	1/1	0.98	0.07	16,16,16,16	0
7	COM	D	554[A]	7/7	0.98	0.05	6,9,10,10	7
5	TP7	D	553[A]	21/21	0.99	0.03	4,6,8,8	21
6	F43	A	1	62/62	0.99	0.04	6,8,11,13	0
6	F43	D	552	62/62	0.99	0.03	6,8,11,12	0
7	COM	A	554[A]	7/7	0.99	0.06	8,9,12,12	7
4	MG	D	551	1/1	0.99	0.15	18,18,18,18	0

Continued on next page...

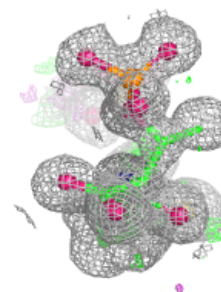
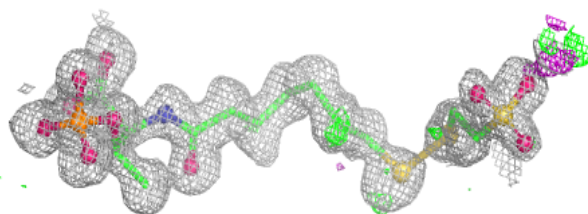
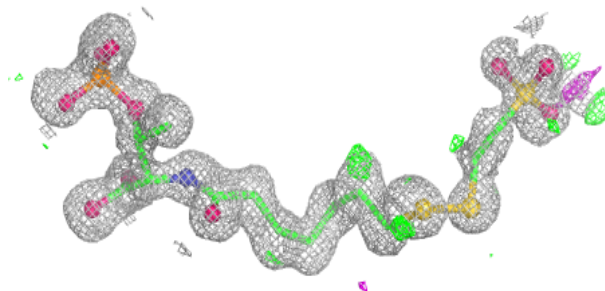
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	TP7	A	553[A]	21/21	0.99	0.04	5,7,7,8	21
11	ZN	A	558	1/1	0.99	0.04	10,10,10,10	1
8	SHT	D	555[B]	28/28	0.99	0.04	6,7,11,13	28

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.

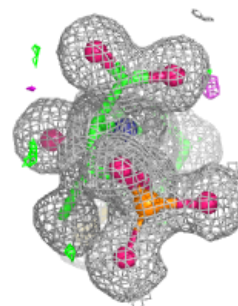
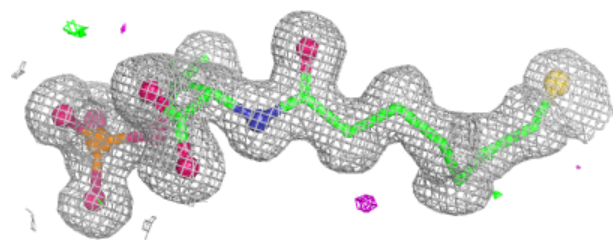
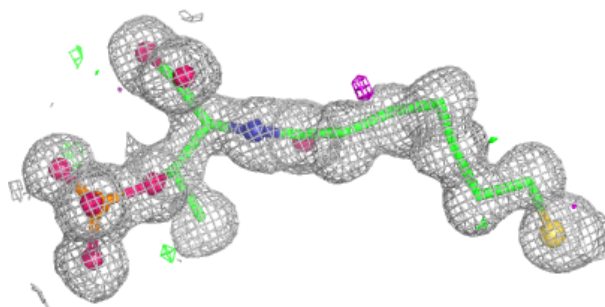
Electron density around SHT A 555 (B):

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



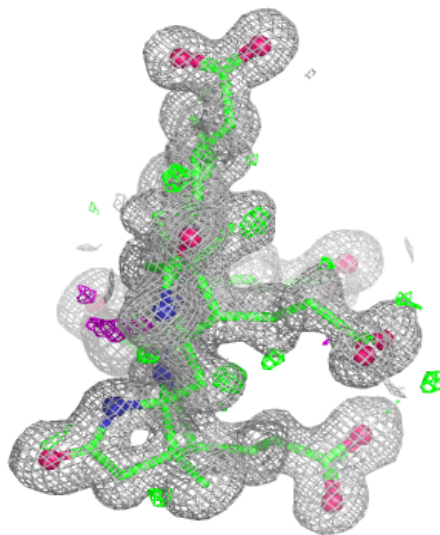
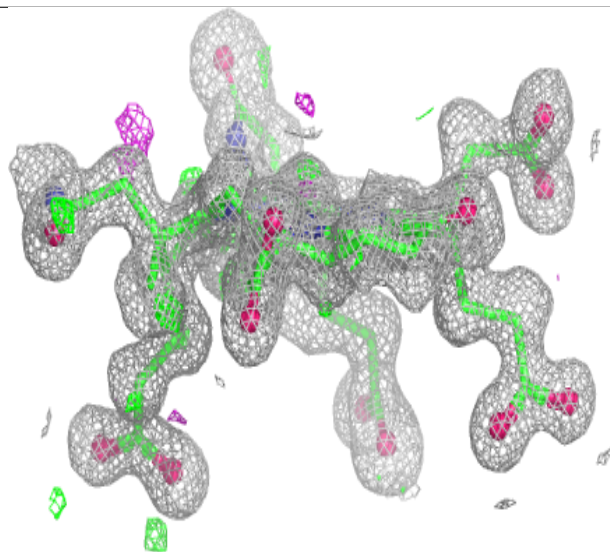
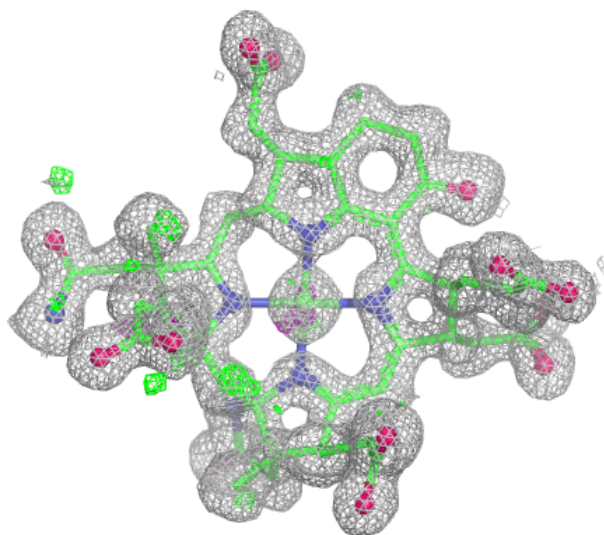
Electron density around TP7 D 553 (A):

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



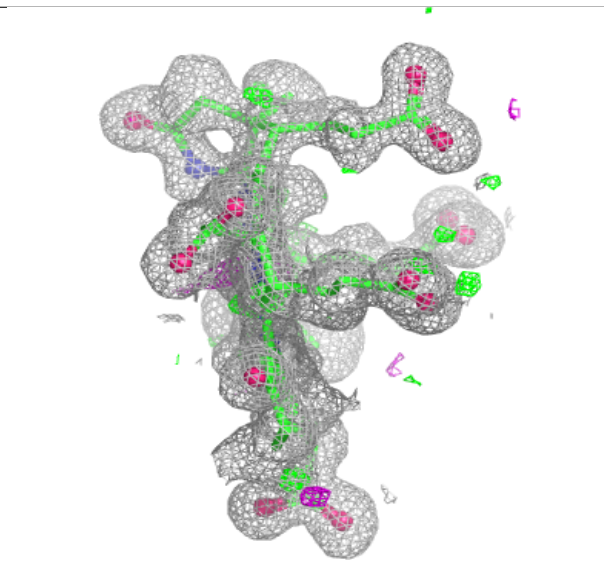
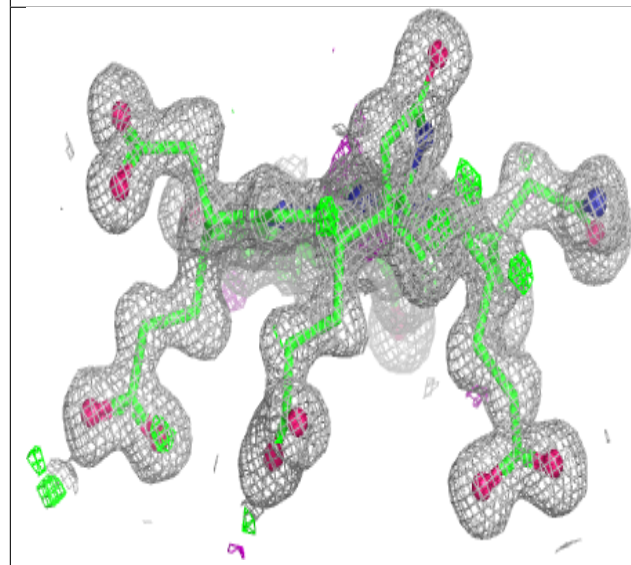
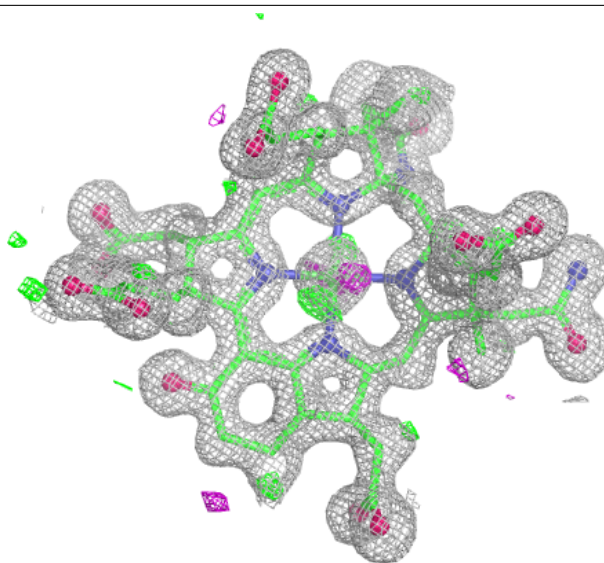
Electron density around F43 A 1:

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



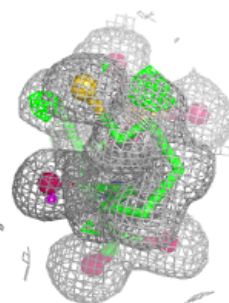
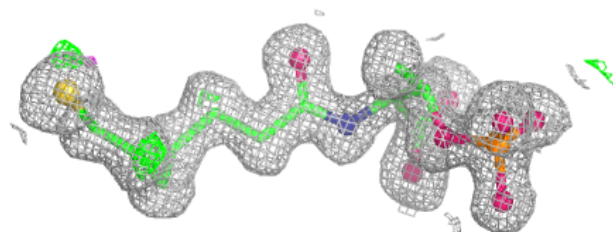
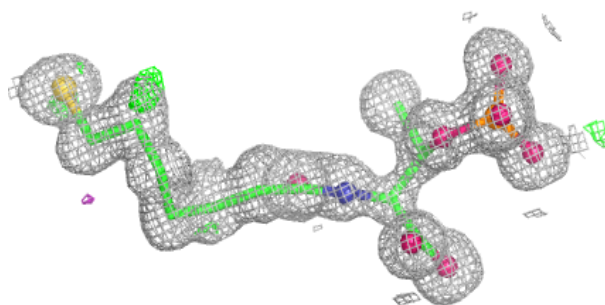
Electron density around F43 D 552:

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

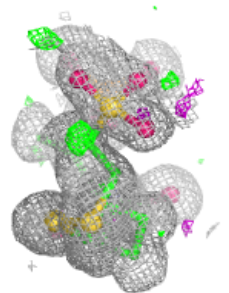
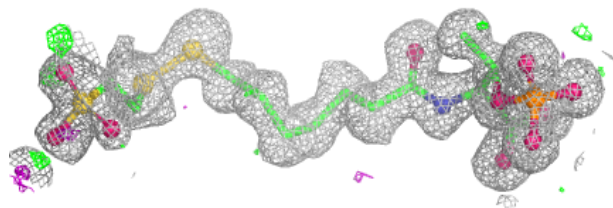
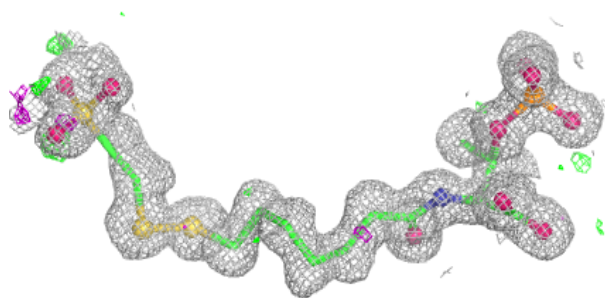


Electron density around TP7 A 553 (A):

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

**Electron density around SHT 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.