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wwPDB X-ray Structure Validation Summary Report (i)

Oct 1, 2023 – 12:40 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

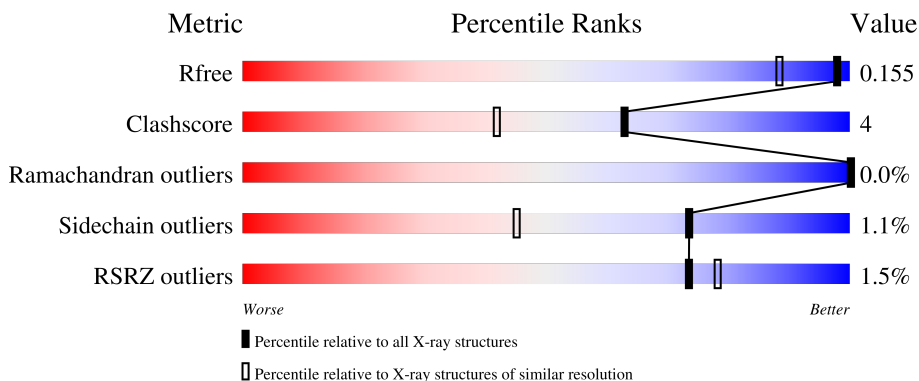|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	Percentile Ranks	Value
Rfree		0.155
Clashscore		4
Ramachandran outliers		0.0%
Sidechain outliers		1.1%
RSRZ outliers		1.5%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	549	83% 15% •
1	D	549	.% 83% 16% •
2	B	442	82% 16% •
2	E	442	.% 84% 15% •
3	C	248	5% 80% 18% •

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Mol	Chain	Length	Quality of chain
3	F	248	

2 Entry composition ⓘ

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 4431	C 2801	N 735	O 874	S 21	0	28	0
1	D	548	Total 4380	C 2779	N 727	O 853	S 21	0	22	0

- Molecule 2 is a protein called Methyl-coenzyme M reductase I subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total 3462	C 2211	N 560	O 668	S 23	0	24	0
2	E	442	Total 3471	C 2216	N 564	O 668	S 23	0	25	0

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

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

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

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

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

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

TP7
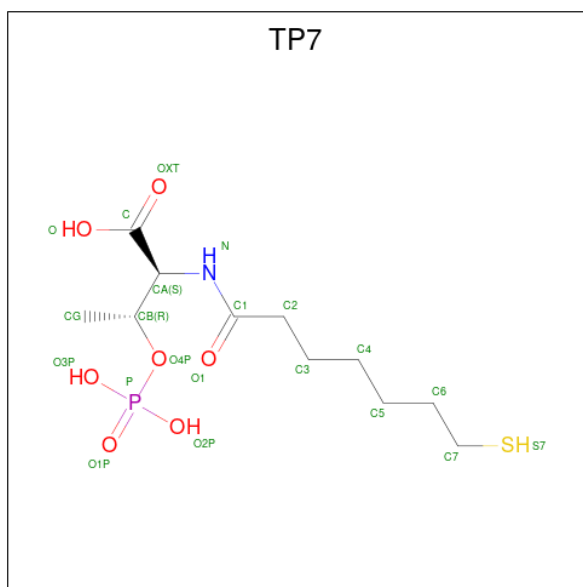
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	1
5	D	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	1

- 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: $C_2H_6O_3S_2$).

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: $C_{13}H_{24}NO_{10}PS_3$).
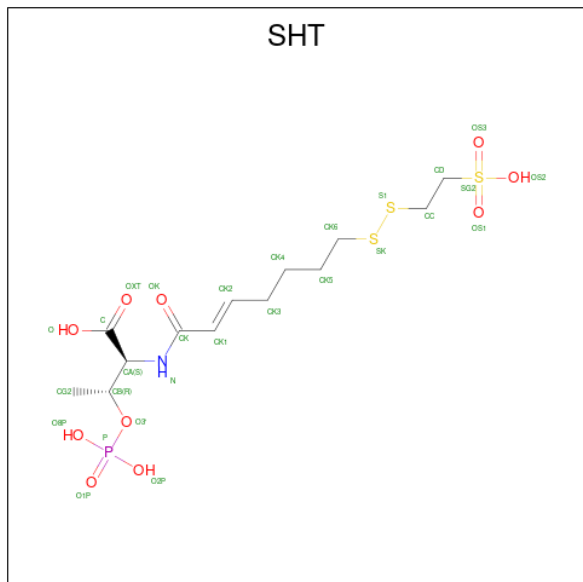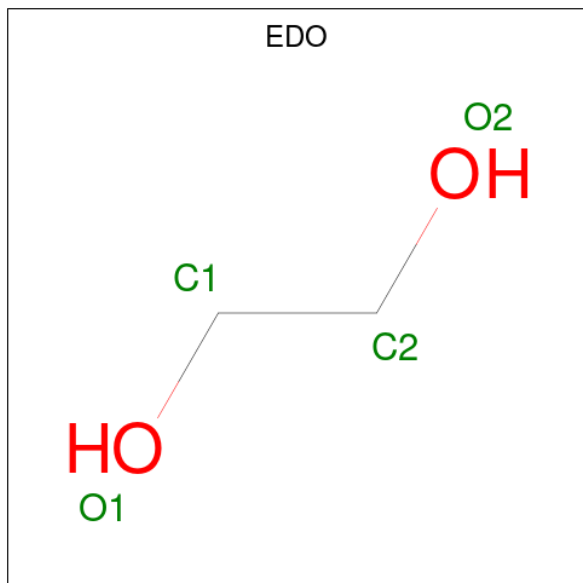

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			28	13	1	10	1	3		
8	D	1	Total	C	N	O	P	S	0	1
			28	13	1	10	1	3		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
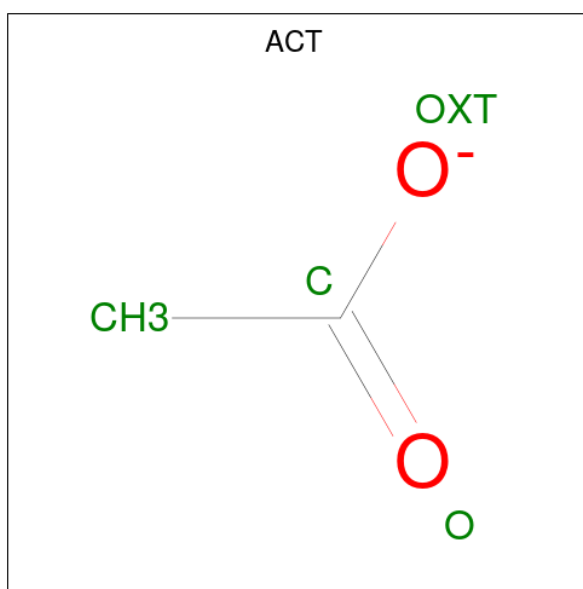
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 4	C 2	O 2	0	1

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

EDO

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

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

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

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

PEG

C4
OH O4
O2
O
C3
C1
HO
C2
O1

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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	507	Total 522	O 522	0	28
13	B	462	Total 477	O 477	0	24
13	C	254	Total 262	O 262	0	12
13	D	529	Total 539	O 539	0	20
13	E	414	Total 421	O 421	0	16
13	F	250	Total 254	O 254	0	8

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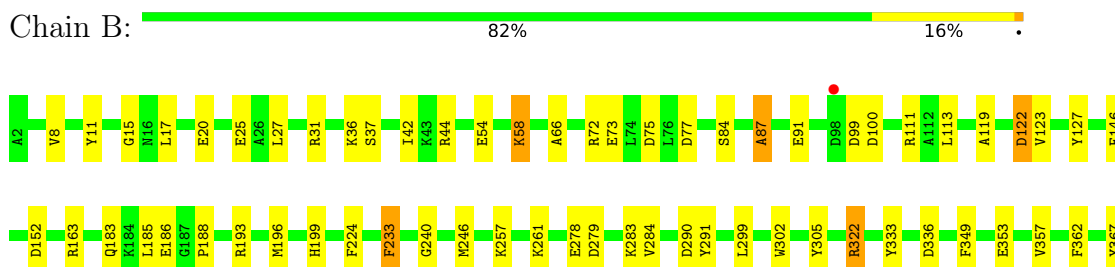
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha
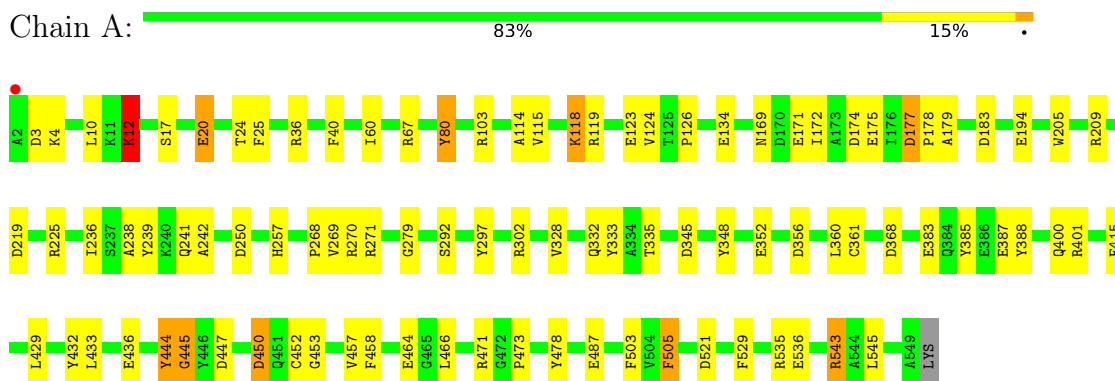
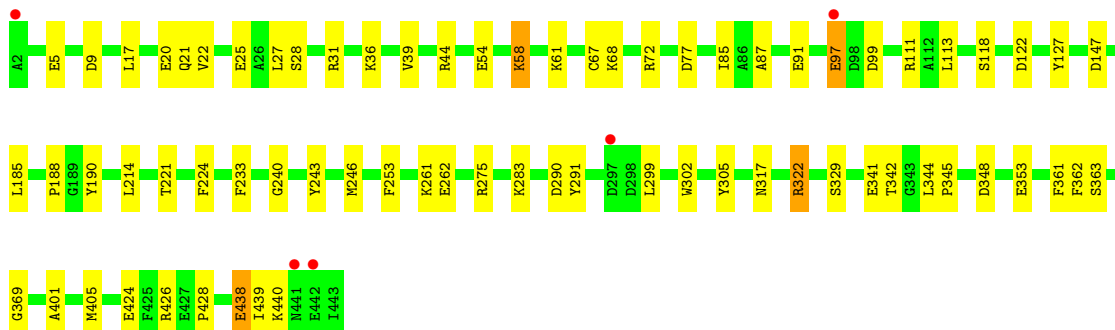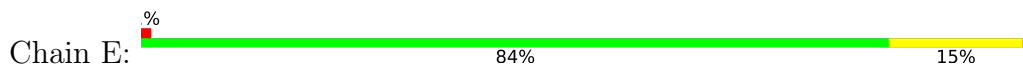- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

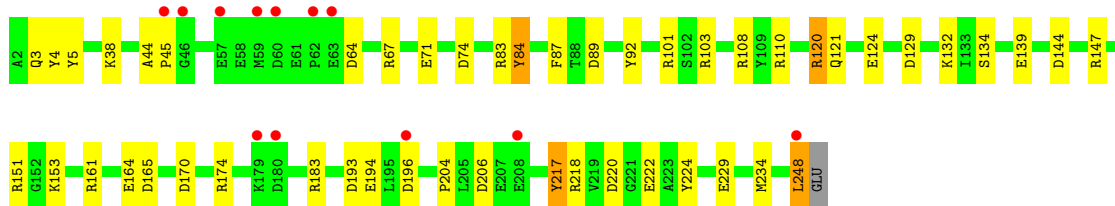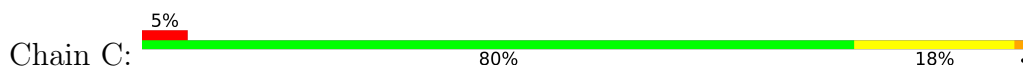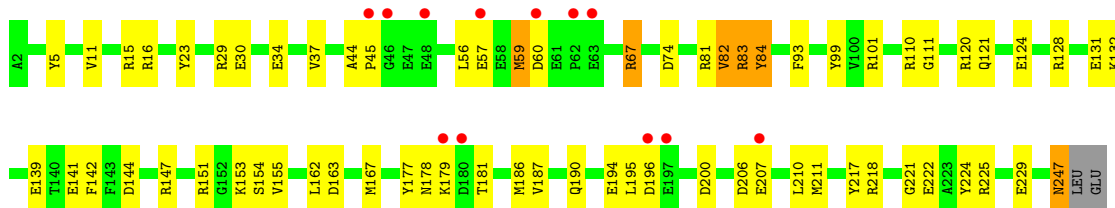- Molecule 2: Methyl-coenzyme M reductase I subunit beta

G368 G369 D400 M405 I415 K416 E417 V418 D423 E424 F425 R426 E427 P428 L429 V433 K440 I443

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

Chain E:

84% 15%

A2 E5 D9 L17 E20 Q21 V22 E25 A26 L27 S28 R31 K36 V39 R44 E54 K58 K61 C67 K68 R72 D77 I85 A86 A87 E91 E97 D98 D99 R111 A112 L113 S118 D122 Y127 D147

L185 P188 G189 Y190 L214 T221 F224 F233 G240 Y243 M246 F253 K261 E262 R275 K283 D290 Y291 D297 D298 L299 W302 Y305 N317 R322 S329 E341 T342 G343 L344 P345 D348 E353 F361 F362 S363

G369 A401 M405 E424 F425 R426 E427 P428 E438 I439 K440 N441 E442 I443

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

Chain C:

5% 80% 18%

A2 Q3 Y4 Y5 K38 A44 P45 G46 E57 E58 M59 D60 E61 P62 E63 D64 R67 E71 D74 R83 Y84 F87 T88 D89 Y92 R101 S102 R103 R108 Y109 R110 R120 Q121 E124 D129 K132 I133 S134 E139 D144 R147

R151 G152 K153 R161 E164 D165 D170 R174 K179 D180 R183 D193 E194 L195 D196 P204 L205 D206 E207 E208 Y217 R218 V219 D220 G221 E222 A223 Y224 E229 M234 L248 GLU

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

Chain F:

5% 72% 25%

A2 Y5 V11 R15 R16 Y23 R29 E30 E34 V37 A44 P45 G46 E47 E48 L56 E57 E58 M59 D60 E61 P62 E63 R67 D74 R81 V82 R83 Y84 F93 Y99 V100 R101 R110 G111 R120 Q121 E124 R128 E131 K132

E139 T140 E141 F142 F143 D144 R147 R151 G152 K153 S154 V155 L162 D163 M167 Y177 N178 K179 D180 T181 M186 V187 Q190 E194 L195 D196 E197 D200 D206 E207 L210 M211 Y217 R218 G221 E222 A223 Y224 R225 E229 N247 LEU GLU

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 19.89 – 1.35	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.28-1.35) 92.4 (19.89-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	23861 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)	0.40 , 51.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	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.*

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[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: AGM, GL3, TP7, ACT, COM, ZN, SHT, PEG, SMC, MG, EDO, MGN, MHS, 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	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(^{o})	Ideal(^{o})
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 ⓘ

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

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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 ⓘ

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	569/549 (104%)	555 (98%)	14 (2%)	0	100	100
1	D	563/549 (103%)	544 (97%)	18 (3%)	1 (0%)	47	21
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%)	69	37
1	D	455/434 (105%)	450 (99%)	5 (1%)	73	45
2	B	366/341 (107%)	365 (100%)	1 (0%)	92	83
2	E	367/341 (108%)	361 (98%)	6 (2%)	62	30
3	C	225/216 (104%)	223 (99%)	2 (1%)	78	53
3	F	233/216 (108%)	226 (97%)	7 (3%)	41	9
All	All	2107/1982 (106%)	2080 (99%)	27 (1%)	73	37

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

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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	D	445	1	2,3,4	2.66	1 (50%)	1,2,4	0.26	0
1	MHS	A	257	1	7,11,12	1.63	2 (28%)	6,14,16	3.87	3 (50%)
1	SMC	A	452	1	5,6,7	1.21	1 (20%)	2,6,8	2.28	1 (50%)
1	AGM	D	271	1	10,11,12	0.96	0	6,13,15	1.11	0
1	GL3	A	445	1	2,3,4	2.45	1 (50%)	1,2,4	0.24	0
1	SMC	D	452	1	5,6,7	1.25	0	2,6,8	1.90	1 (50%)
1	MGN	D	400	1	6,9,10	1.80	2 (33%)	5,12,14	0.79	0
1	AGM	A	271	1	10,11,12	0.81	0	6,13,15	1.97	1 (16%)
1	MGN	A	400	1	6,9,10	1.23	1 (16%)	5,12,14	0.39	0
1	MHS	D	257	1	7,11,12	1.36	1 (14%)	6,14,16	3.84	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	GL3	D	445	1	-	0/1/1/2	-
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	GL3	A	445	1	-	1/1/1/2	-
1	SMC	D	452	1	-	1/3/5/7	-
1	MGN	D	400	1	-	0/7/9/12	-
1	AGM	A	271	1	-	<mark>3/10/11/13</mark>	-
1	MGN	A	400	1	-	0/7/9/12	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-3.76	1.67	1.80
1	A	445	GL3	C-S	-3.46	1.68	1.80
1	A	257	MHS	CE1-NE2	3.17	1.41	1.34
1	D	400	MGN	CB1-CA	-3.00	1.51	1.55
1	D	257	MHS	CE1-NE2	2.79	1.41	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	4.22	112.36	105.78
1	A	257	MHS	CB-CA-C	-3.79	104.37	111.47
1	A	271	AGM	NH1-CZ-NE1	3.47	127.31	119.55

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	A	271	AGM	CE2-CD-NE1-CZ
1	D	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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).

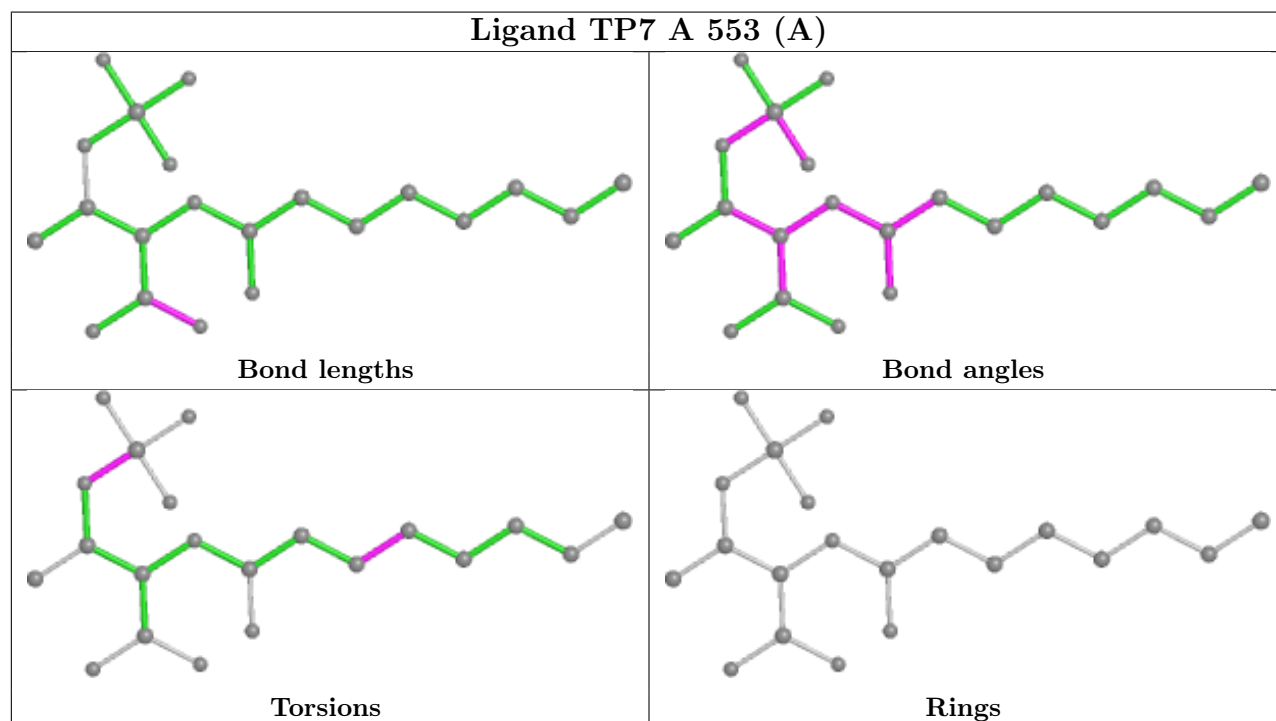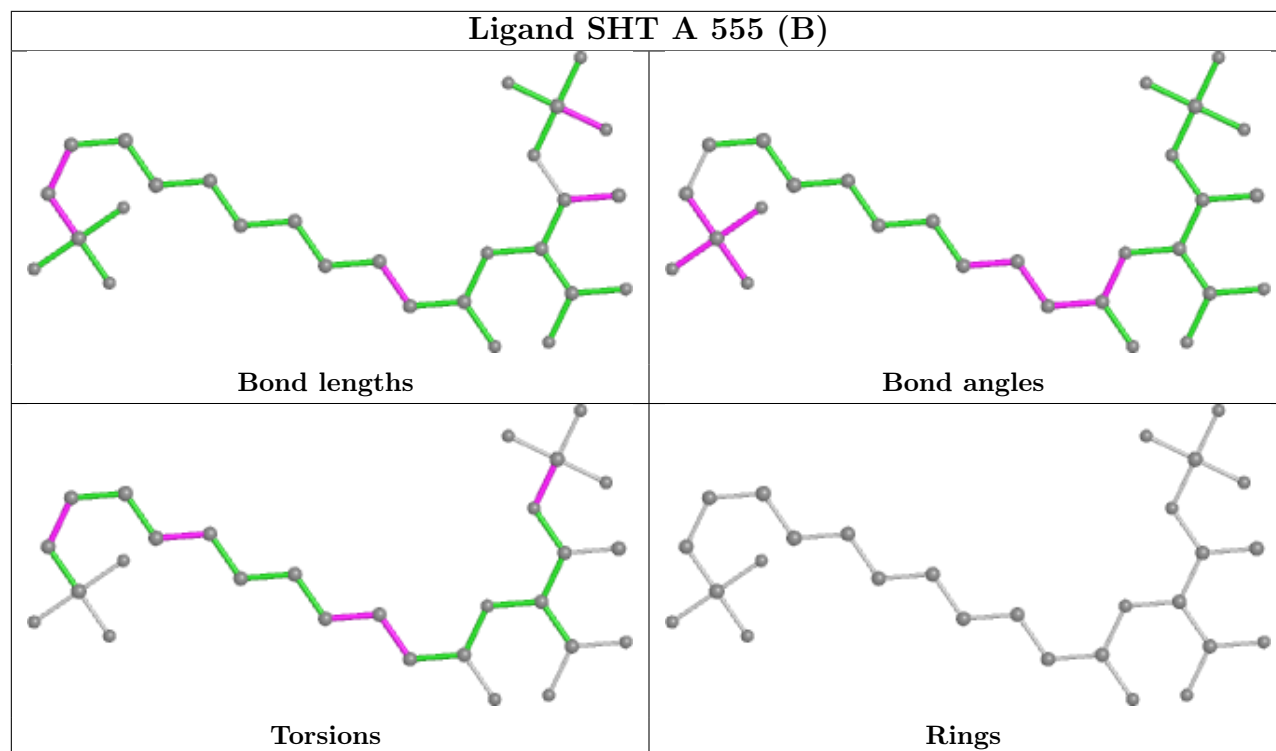| Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
6	F43	A	1	8,1,7	61,71,71	2.73	15 (24%)	64,118,118	1.73	14 (21%)
12	PEG	C	1	-	6,6,6	0.55	0	5,5,5	1.14	1 (20%)
10	EDO	A	557	-	3,3,3	0.59	0	2,2,2	0.33	0
7	COM	A	554[A]	6	6,6,6	1.52	1 (16%)	7,8,8	1.66	1 (14%)
10	EDO	D	556	-	3,3,3	0.36	0	2,2,2	0.38	0
9	ACT	A	556[B]	4	3,3,3	0.88	0	3,3,3	0.38	0
10	EDO	B	445	-	3,3,3	0.75	0	2,2,2	0.29	0
8	SHT	A	555[B]	6	26,27,27	2.97	5 (19%)	30,36,36	1.95	5 (16%)
5	TP7	A	553[A]	-	19,20,20	1.01	1 (5%)	24,26,26	1.56	6 (25%)
8	SHT	D	555[B]	6	26,27,27	2.68	3 (11%)	30,36,36	1.92	5 (16%)
5	TP7	D	553[A]	-	19,20,20	1.16	2 (10%)	24,26,26	1.22	2 (8%)
6	F43	D	552	8,1,7	61,71,71	3.00	20 (32%)	64,118,118	2.06	22 (34%)
7	COM	D	554[A]	6	6,6,6	1.51	1 (16%)	7,8,8	0.83	0
10	EDO	F	1	-	3,3,3	0.58	0	2,2,2	0.53	0
10	EDO	F	251	-	3,3,3	0.68	0	2,2,2	0.47	0

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

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

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

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	555[B]	SHT	CD-SG2	-11.77	1.60	1.77
6	D	552	F43	NI-NB	11.71	2.14	1.89
6	D	552	F43	NI-NA	9.87	2.10	1.89
6	A	1	F43	NI-NB	9.64	2.10	1.89
6	A	1	F43	CHB-C1B	-9.55	1.46	1.53

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	555[B]	SHT	CK3-CK2-CK1	-6.95	110.95	125.85
6	D	552	F43	C5D-C2D-C1D	6.17	118.75	110.45
6	D	552	F43	C2D-C1D-CHD	-5.62	114.66	121.85
8	A	555[B]	SHT	OS2-SG2-CD	4.93	113.74	105.77
8	A	555[B]	SHT	CK3-CK2-CK1	-4.84	115.46	125.85

There are no chirality outliers.

5 of 35 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

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PROTEIN DATA BANK

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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

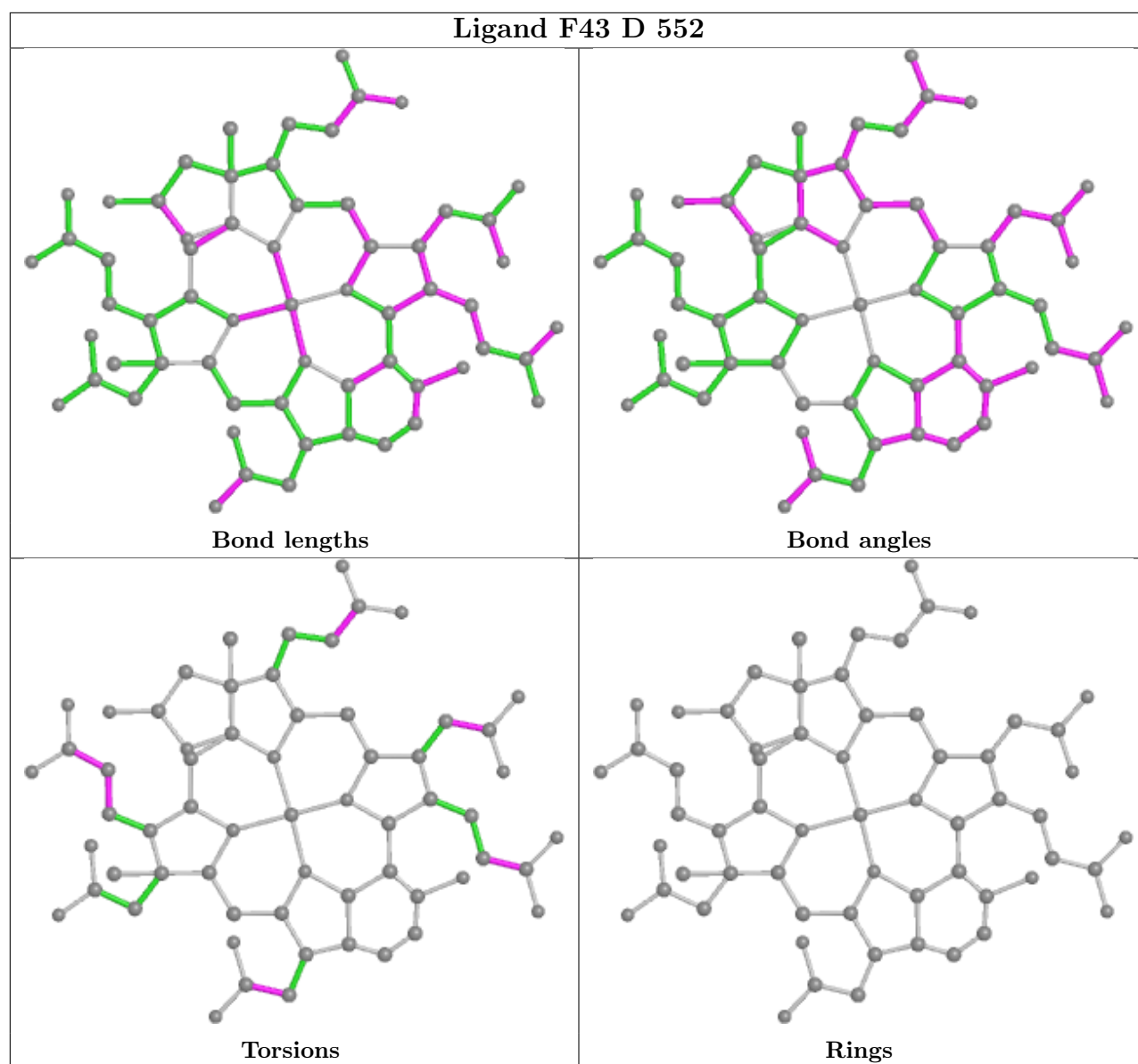There are no ring outliers.

5 monomers are involved in 5 short contacts:

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

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

Ligand F43 A 1

Bond lengths

Bond angles

Torsions

Rings

Ligand SHT A 555 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand TP7 A 553 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand SHT D 555 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand TP7 D 553 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand F43 D 552

Bond lengths

Bond angles

Torsions

Rings
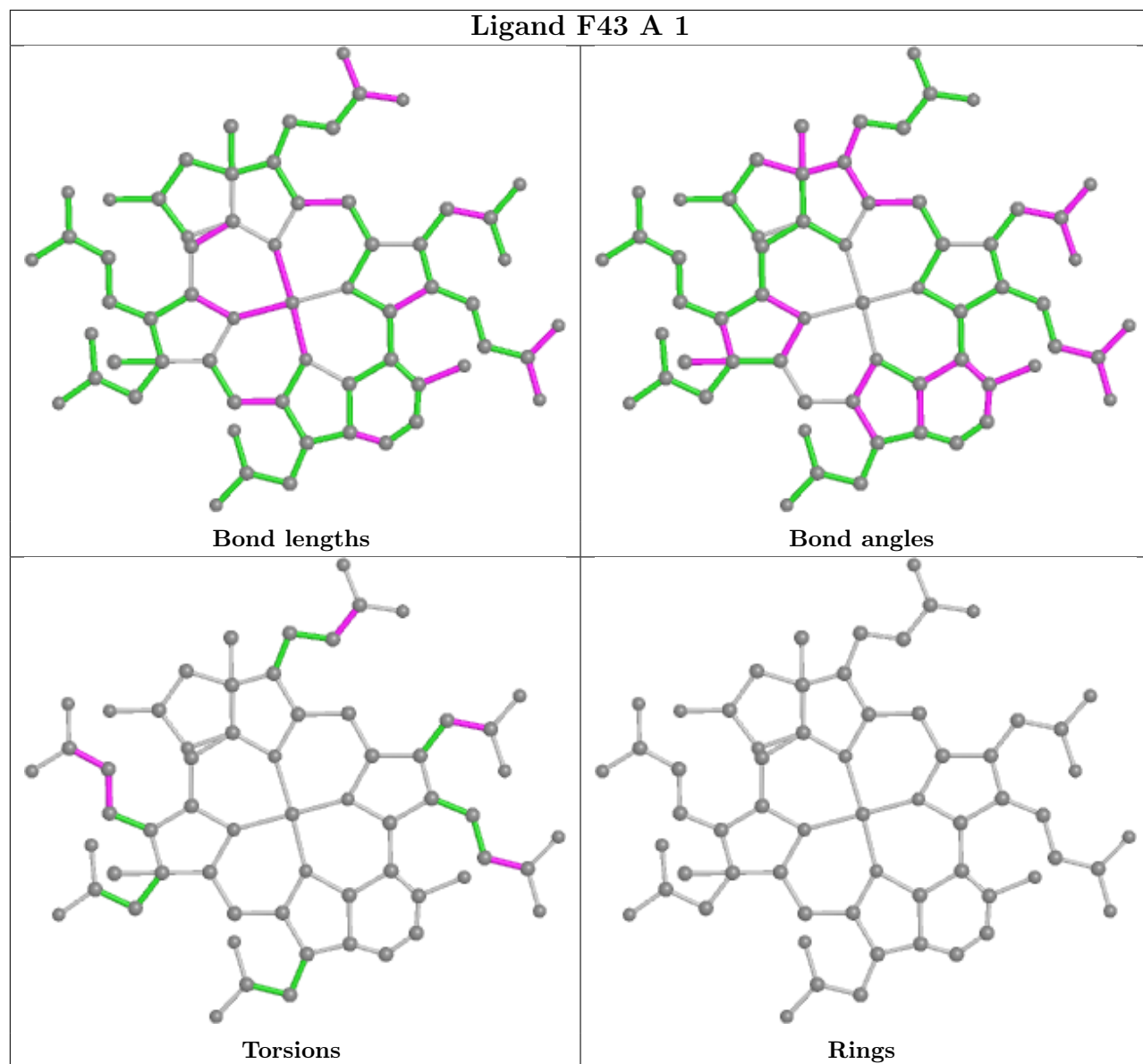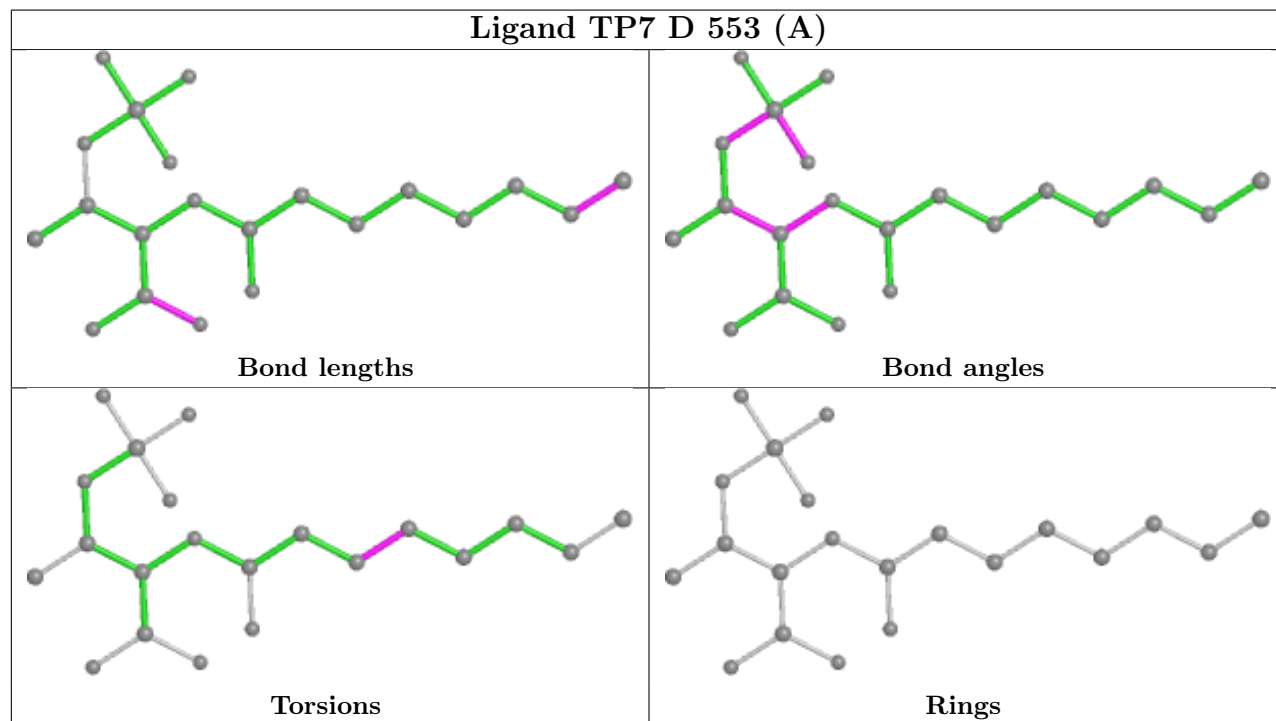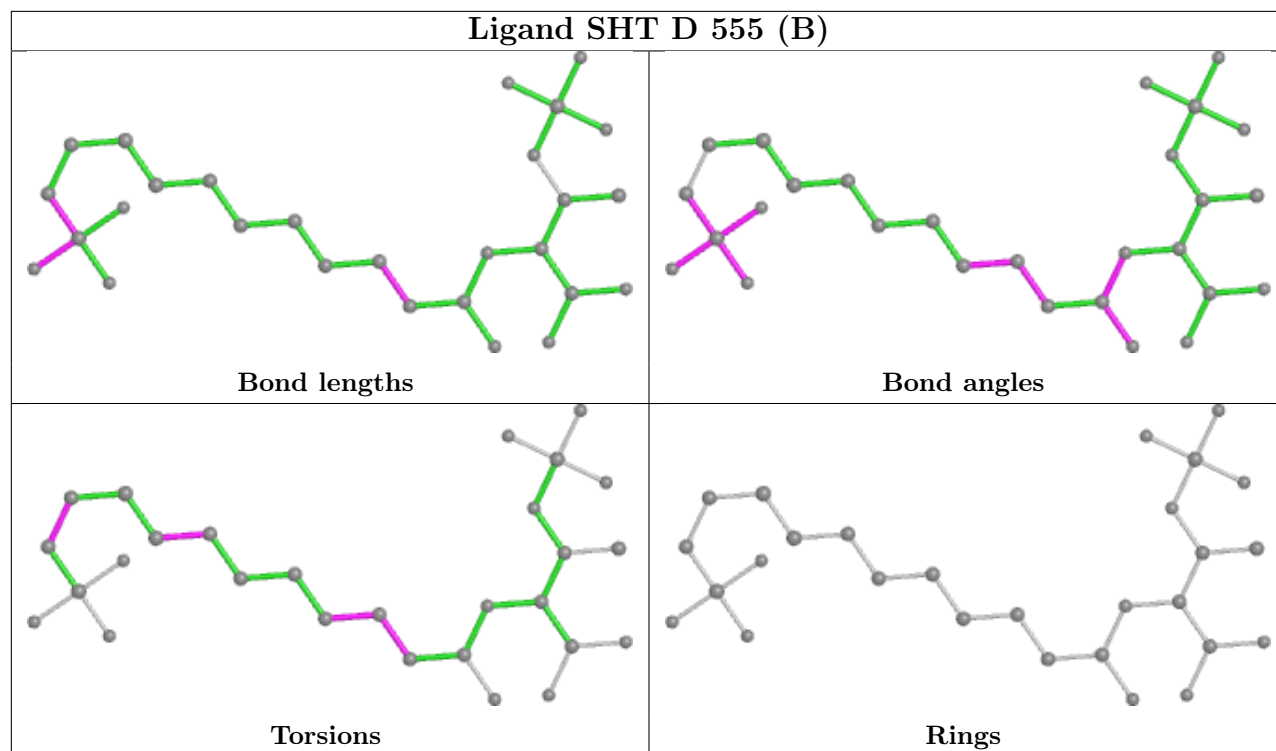
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	543/549 (98%)	-0.46	1 (0%)	95	95	6, 10, 21, 33	0
1	D	543/549 (98%)	-0.45	5 (0%)	84	87	6, 10, 20, 37	0
2	B	442/442 (100%)	-0.46	1 (0%)	95	95	7, 12, 21, 35	0
2	E	442/442 (100%)	-0.39	5 (1%)	80	84	7, 12, 23, 40	0
3	C	247/248 (99%)	-0.22	12 (4%)	29	33	9, 14, 32, 47	0
3	F	246/248 (99%)	-0.15	12 (4%)	29	33	8, 14, 30, 53	0
All	All	2463/2478 (99%)	-0.39	36 (1%)	73	78	6, 12, 23, 53	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	6.9
3	C	60	ASP	5.0
3	F	45	PRO	4.8
2	E	441	ASN	4.6
1	D	549	ALA	4.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.
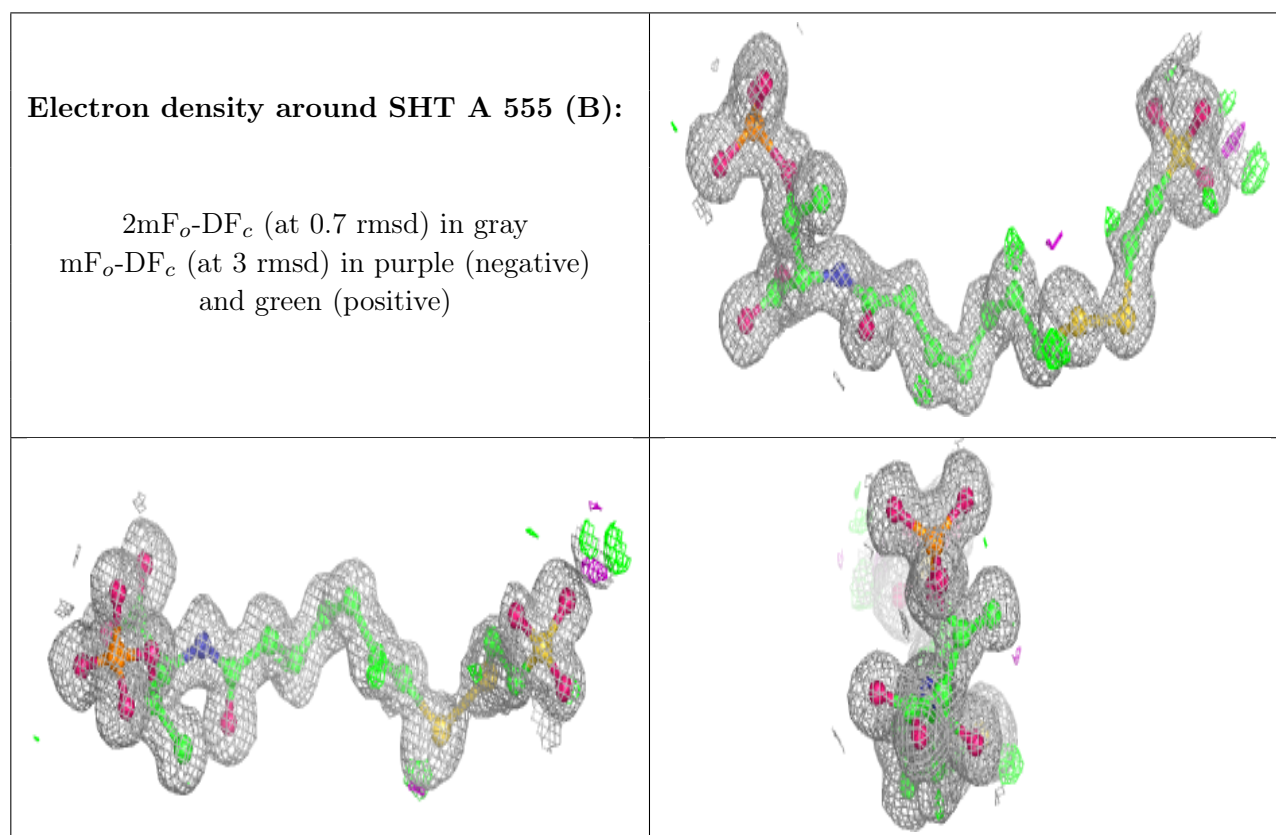
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	MHS	A	257	11/12	0.97	0.05	8,10,14,17	0
1	AGM	D	271	12/13	0.97	0.07	6,7,7,8	0
1	MGN	A	400	10/11	0.98	0.05	7,8,9,10	0
1	MHS	D	257	11/12	0.98	0.05	9,10,12,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	AGM	A	271	12/13	0.98	0.05	6,6,7,8	0
1	MGN	D	400	10/11	0.98	0.05	6,8,8,8	0
1	SMC	A	452	7/8	0.99	0.05	7,7,9,10	0
1	GL3	A	445	4/5	0.99	0.06	6,7,7,8	0
1	GL3	D	445	4/5	0.99	0.06	6,6,7,7	0
1	SMC	D	452	7/8	0.99	0.05	7,8,9,11	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
10	EDO	F	251	4/4	0.81	0.16	39,42,43,48	0
10	EDO	B	445	4/4	0.82	0.08	42,42,43,46	0
10	EDO	A	557	4/4	0.85	0.08	30,35,39,42	0
12	PEG	C	1	7/7	0.86	0.13	34,38,42,42	0
10	EDO	F	1	4/4	0.87	0.11	38,39,39,39	0
10	EDO	D	556	4/4	0.89	0.10	32,38,40,44	0
4	MG	B	444	1/1	0.97	0.15	23,23,23,23	0
4	MG	B	1[B]	1/1	0.97	0.19	21,21,21,21	1
7	COM	D	554[A]	7/7	0.98	0.06	6,9,10,10	7
8	SHT	A	555[B]	28/28	0.98	0.06	6,7,12,14	28
9	ACT	A	556[B]	4/4	0.98	0.06	15,16,17,19	4
4	MG	A	551[A]	1/1	0.98	0.22	18,18,18,18	1
4	MG	C	250	1/1	0.98	0.10	17,17,17,17	0
4	MG	D	1	1/1	0.98	0.13	20,20,20,20	0
4	MG	E	444	1/1	0.98	0.20	22,22,22,22	0
4	MG	F	250	1/1	0.98	0.08	16,16,16,16	0
5	TP7	A	553[A]	21/21	0.98	0.06	5,7,7,8	21
5	TP7	D	553[A]	21/21	0.99	0.05	4,6,8,8	21
6	F43	A	1	62/62	0.99	0.05	6,8,11,13	0
6	F43	D	552	62/62	0.99	0.05	6,8,11,12	0
7	COM	A	554[A]	7/7	0.99	0.04	8,9,12,12	7
4	MG	A	552[B]	1/1	0.99	0.17	14,14,14,14	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	D	551	1/1	0.99	0.17	18,18,18,18	0
8	SHT	D	555[B]	28/28	0.99	0.05	6,7,11,13	28
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 SHT A 555 (B):

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

Electron density around TP7 A 553 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
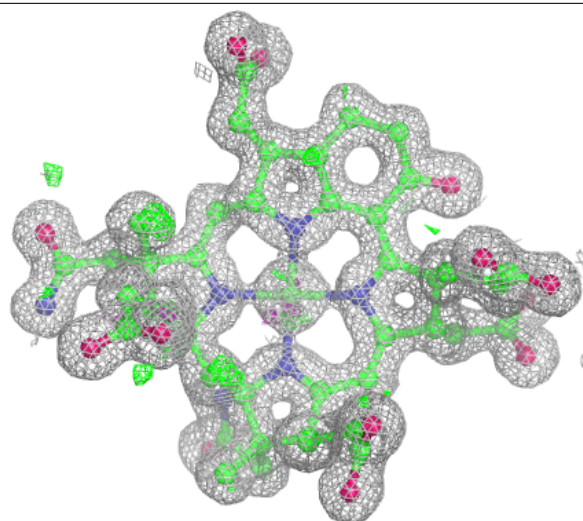and green (positive)
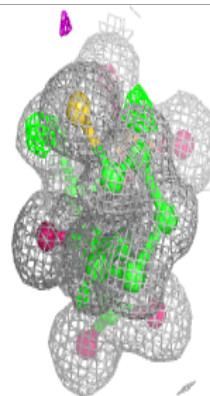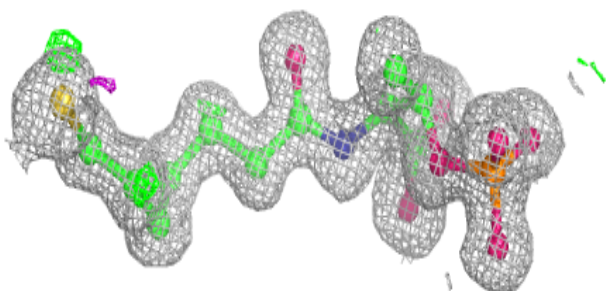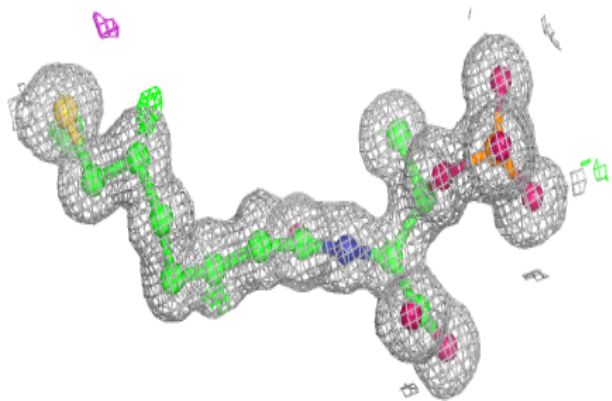
Electron density around TP7 D 553 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
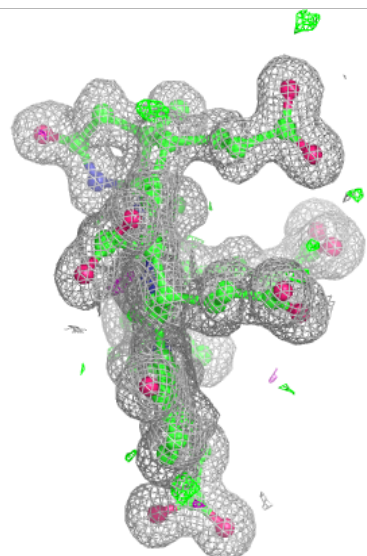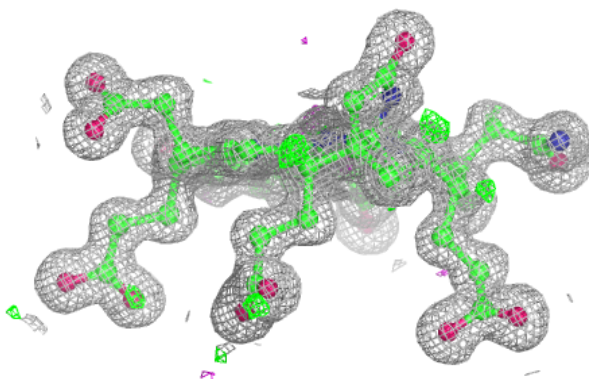$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
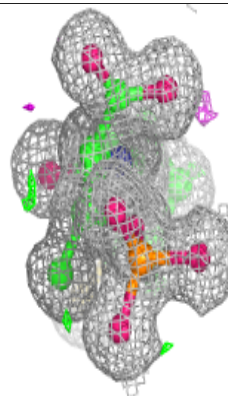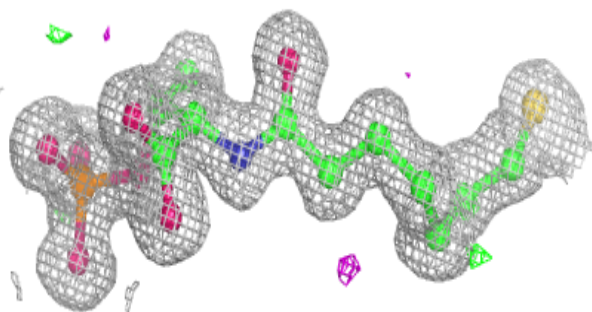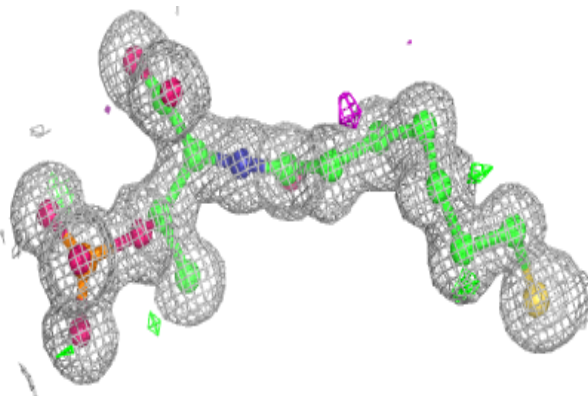
Electron density around F43 A 1:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
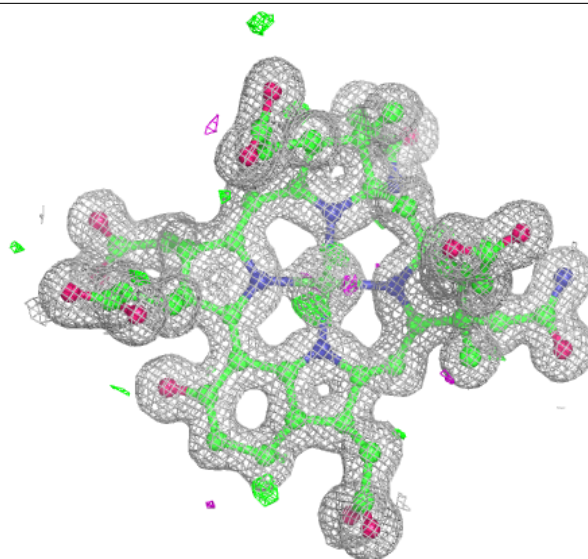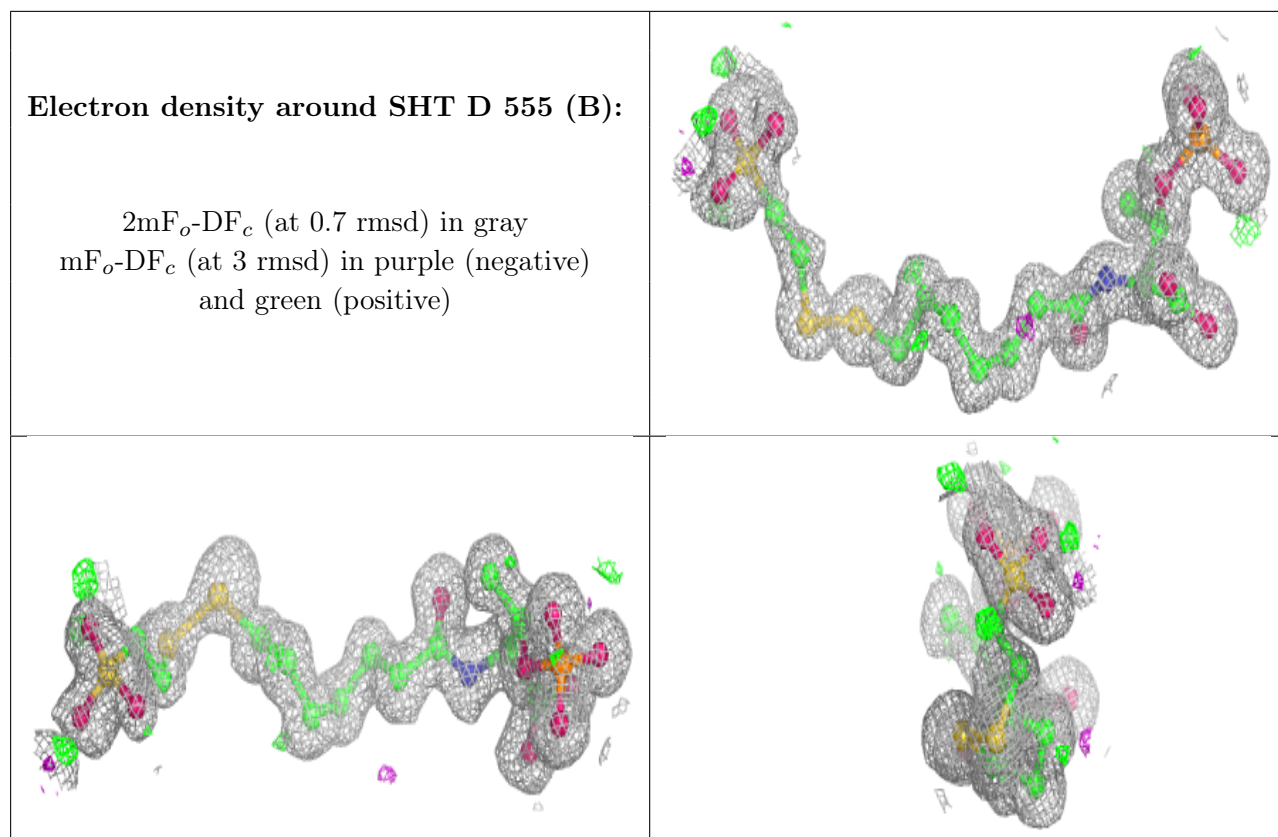and green (positive)
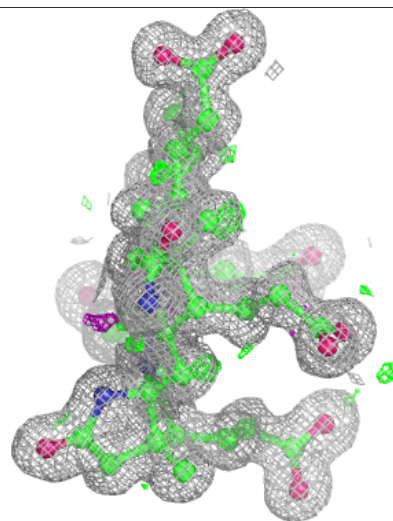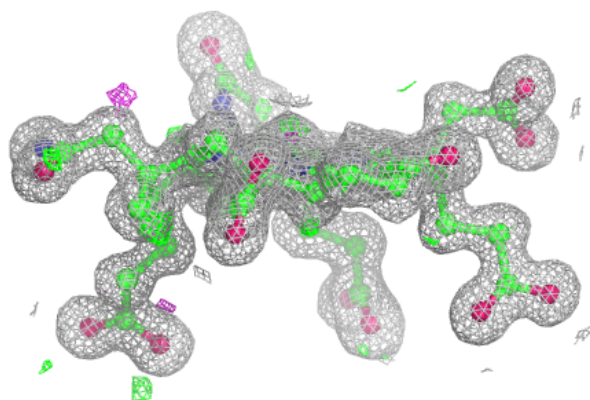
Electron density around F43 D 552:

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

Electron density around SHT D 555 (B):

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

6.5 Other polymers ⓘ

There are no such residues in this entry.