



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2020 – 06:50 am BST

PDB ID : 5A0Y  
Title : METHYL-COENZYME M REDUCTASE FROM METHANOTHERMOBACTER MARBURGENSIS AT 1.1 Å RESOLUTION  
Authors : Wagner, T.; Ermiler, U.  
Deposited on : 2015-04-24  
Resolution : 1.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

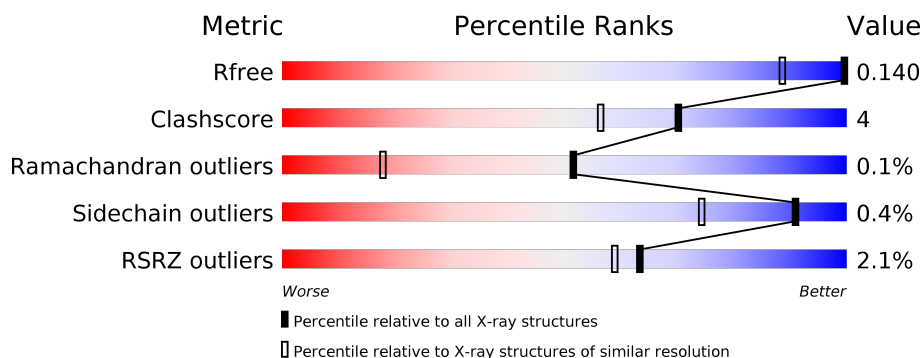
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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  $\geq 3$ , 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	550	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 94%, yellow 94%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>94%</span> <span>5%</span> </div> </div>
1	D	550	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 95%, yellow 95%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>95%</span> <span>5% •</span> </div> </div>
2	B	443	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 93%, yellow 93%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>93%</span> <span>6%</span> </div> </div>
2	E	443	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 94%, yellow 94%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>94%</span> <span>6%</span> </div> </div>
3	C	249	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, orange 6%, orange 90%, yellow 90%, yellow 98%, green 98%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>90%</span> <span>8% •</span> </div> </div>
3	F	249	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 7%, orange 7%, orange 94%, yellow 94%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>94%</span> <span>6%</span> </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
10	CL	A	565	-	-	X	-
10	CL	D	559	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 22747 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHYL-COENZYME M REDUCTASE I SUBUNIT ALPHA.

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

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

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

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

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

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

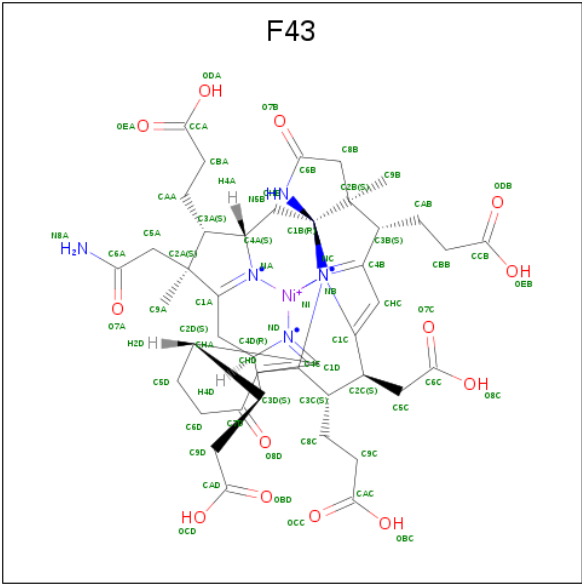
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	Mg	0	0
			3	3		
4	E	3	Total	Mg	0	0
			3	3		
4	B	2	Total	Mg	0	0
			2	2		

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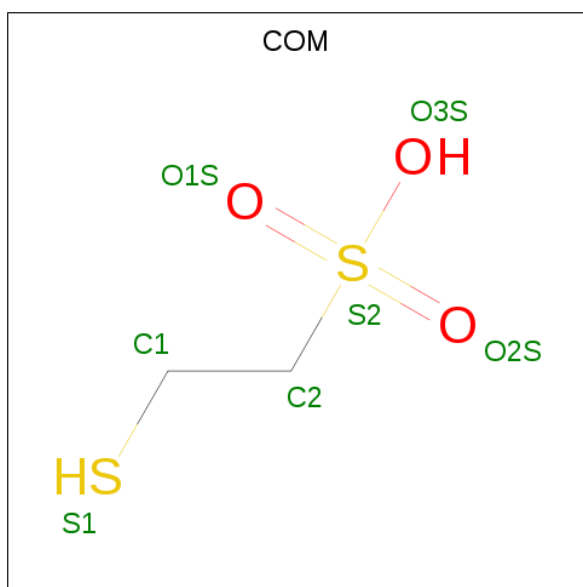
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Mg	0	0
			2	2		
4	A	4	Total	Mg	0	0
			4	4		
4	F	2	Total	Mg	0	0
			2	2		

- Molecule 5 is FACTOR 430 (three-letter code: F43) (formula: C<sub>42</sub>H<sub>51</sub>N<sub>6</sub>NiO<sub>13</sub>).



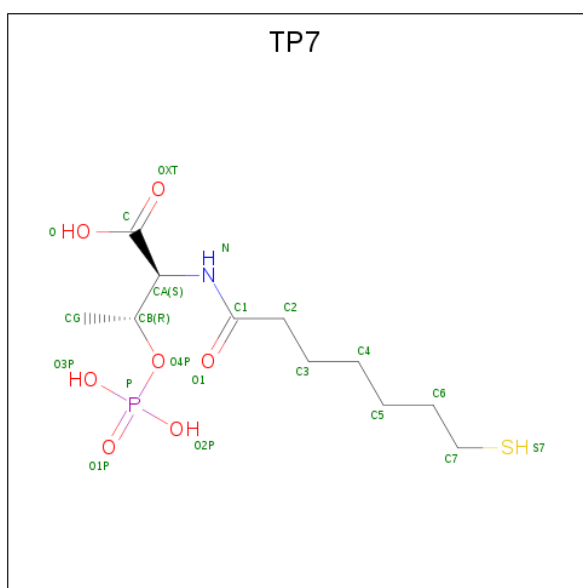
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
5	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>3</sub>S<sub>2</sub>).



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

- Molecule 7 is Coenzyme B (three-letter code: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).



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

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

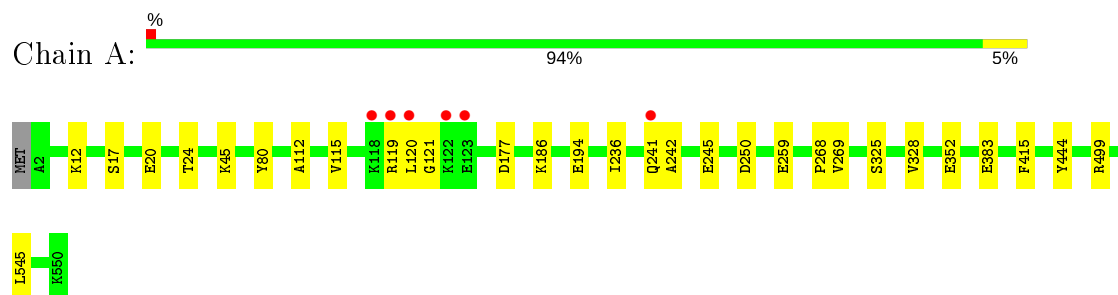
- Molecule 11 is water.

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

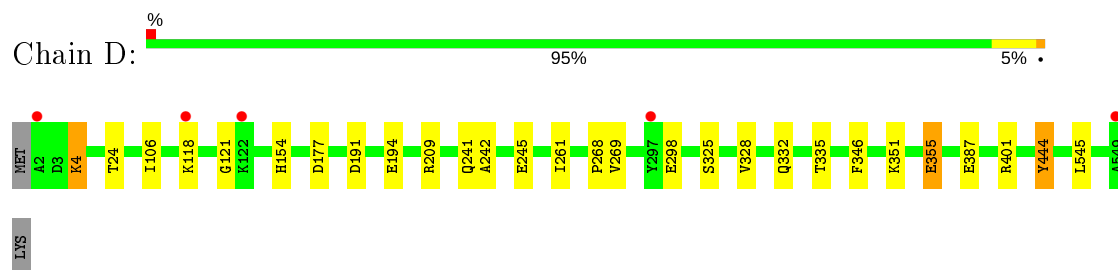
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

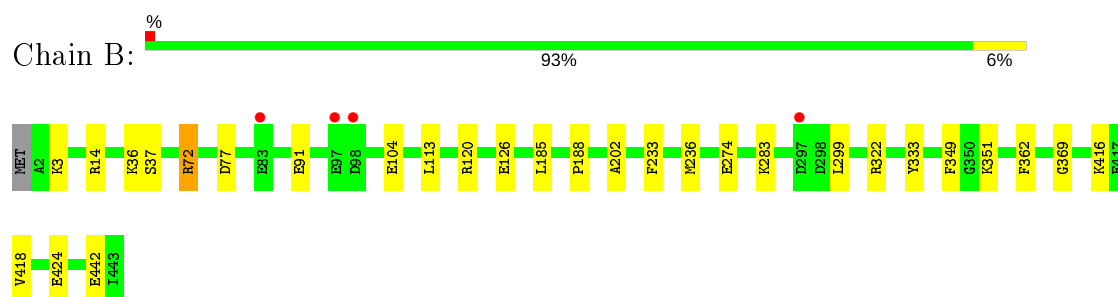
- Molecule 1: METHYL-COENZYME M REDUCTASE I SUBUNIT ALPHA



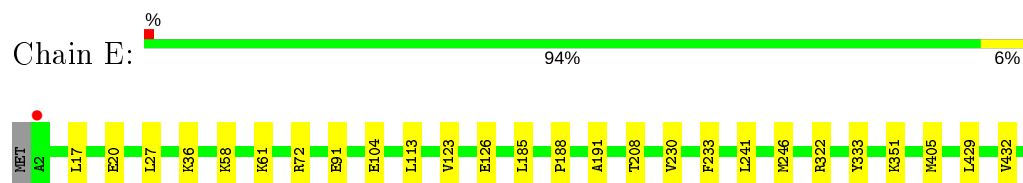
- Molecule 1: METHYL-COENZYME M REDUCTASE I SUBUNIT ALPHA



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

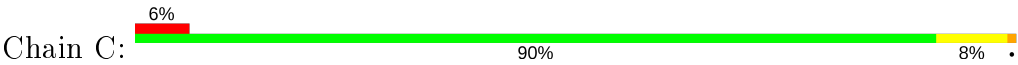


- Molecule 2: METHYL-COENZYME M REDUCTASE I SUBUNIT BETA



- 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, $\alpha$ , $\beta$ , $\gamma$	82.23Å 118.30Å 122.56Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	48.35 – 1.10 48.35 – 1.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.35-1.10) 92.3 (48.35-1.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 1.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.111 , 0.129 0.124 , 0.140	Depositor DCC
$R_{free}$ test set	46960 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k 0.012 for -h,-l,-k 0.018 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	22747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, AGM, F43, MGN, TP7, SMC, DYA, 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	0.62	0/4498	0.79	3/6106 (0.0%)
1	D	0.62	2/4473 (0.0%)	0.82	8/6070 (0.1%)
2	B	0.58	0/3532	0.75	5/4777 (0.1%)
2	E	0.56	0/3550	0.74	0/4801
3	C	0.63	1/2121 (0.0%)	0.86	8/2855 (0.3%)
3	F	0.60	0/2107	0.86	4/2835 (0.1%)
All	All	0.60	3/20281 (0.0%)	0.80	28/27444 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	E	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	19	CYS	CB-SG	-6.92	1.70	1.82
1	D	355	GLU	CB-CG	-6.48	1.39	1.52
1	D	269	VAL	CA-CB	5.32	1.66	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	LYS	CD-CE-NZ	-8.87	91.31	111.70
3	F	120	ARG	NE-CZ-NH1	8.68	124.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	120	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	D	4[A]	LYS	CD-CE-NZ	8.00	130.11	111.70
1	D	4[B]	LYS	CD-CE-NZ	8.00	130.11	111.70
3	C	81	ARG	NE-CZ-NH2	7.95	124.27	120.30
1	D	241	GLN	CA-CB-CG	6.99	128.77	113.40
1	A	177	ASP	CB-CG-OD1	6.87	124.48	118.30
3	C	147	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	B	322	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	D	444	TYR	CB-CG-CD2	-6.17	117.30	121.00
3	F	110	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	415	PHE	CB-CG-CD1	5.69	124.78	120.80
1	A	499	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	C	83	ARG	NE-CZ-NH1	5.64	123.12	120.30
3	C	59	MET	CG-SD-CE	-5.56	91.31	100.20
1	D	209	ARG	NE-CZ-NH2	-5.53	117.53	120.30
3	F	59	MET	CG-SD-CE	-5.52	91.37	100.20
3	C	63	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	D	346	PHE	CB-CG-CD1	5.26	124.48	120.80
2	B	72	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	401	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	177	ASP	CB-CG-OD1	5.13	122.92	118.30
3	C	183	ARG	NE-CZ-NH1	5.11	122.86	120.30
3	C	110	ARG	NE-CZ-NH2	-5.10	117.75	120.30
3	C	43	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	B	185	LEU	CB-CG-CD1	5.04	119.57	111.00
2	B	120	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	333	TYR	Sidechain
2	B	72	ARG	Sidechain
2	E	333	TYR	Sidechain
2	E	72	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4394	0	4233	30	0
1	D	4376	0	4225	24	0
2	B	3433	0	3472	28	0
2	E	3436	0	3503	27	0
3	C	2060	0	2000	25	0
3	F	2053	0	2002	18	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
5	A	62	0	43	1	0
5	D	62	0	43	2	0
6	A	7	0	4	0	0
6	D	7	0	5	0	0
7	A	21	0	19	0	0
7	D	21	0	19	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	3	0
10	D	1	0	0	2	0
11	A	685	0	0	23	1
11	B	553	0	0	14	0
11	C	287	0	0	13	1
11	D	571	0	0	13	2
11	E	444	0	0	14	0
11	F	254	0	0	3	2
All	All	22747	0	19568	144	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLN:OE1	11:A:2408:HOH:O	1.58	1.20
11:D:2504:HOH:O	2:E:351[B]:LYS:NZ	1.74	1.17
11:E:2386:HOH:O	3:F:67[A]:ARG:NH2	1.77	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2585:HOH:O	2:B:351[A]:LYS:NZ	1.76	1.16
1:A:259[B]:GLU:OE2	11:A:2227:HOH:O	1.61	1.16
2:B:442[A]:GLU:OE1	11:B:2549:HOH:O	1.68	1.09
11:E:2298:HOH:O	3:F:67[A]:ARG:NH1	1.84	1.08
2:E:230:VAL:O	11:E:2309:HOH:O	1.74	1.05
10:A:565:CL:CL	11:A:2403:HOH:O	2.18	0.98
10:D:559:CL:CL	11:D:2393:HOH:O	2.21	0.93
1:D:4[A]:LYS:NZ	11:D:2017:HOH:O	2.02	0.92
11:E:2030:HOH:O	3:F:63:GLU:OE1	1.91	0.89
2:E:91[A]:GLU:OE1	11:E:2178:HOH:O	1.99	0.78
1:A:120:LEU:N	1:A:120:LEU:HD22	1.97	0.78
11:B:2477:HOH:O	3:C:67[B]:ARG:NE	2.11	0.75
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.27	0.75
2:E:104[B]:GLU:OE2	11:E:2207:HOH:O	2.06	0.73
3:F:67[B]:ARG:HH11	3:F:67[B]:ARG:HG2	1.52	0.73
2:B:14[A]:ARG:CZ	3:C:63:GLU:OE2	2.37	0.72
3:F:10:LYS:NZ	11:F:2018:HOH:O	2.22	0.72
2:B:299[A]:LEU:HD21	2:B:349[A]:PHE:CE1	2.23	0.72
11:D:2503:HOH:O	2:E:351[A]:LYS:NZ	1.70	0.72
1:A:268:PRO:HG3	11:A:2600:HOH:O	1.89	0.71
1:D:387[A]:GLU:OE1	11:D:2017:HOH:O	2.09	0.70
2:E:322[B]:ARG:NH2	3:F:67[B]:ARG:HG3	2.06	0.70
3:C:243[A]:GLN:OE1	11:C:2276:HOH:O	2.08	0.69
3:C:248:LEU:HD13	3:C:248:LEU:O	1.91	0.69
1:A:121:GLY:HA3	11:A:2250:HOH:O	1.94	0.68
3:C:86:GLN:NE2	3:C:120[A]:ARG:HD2	2.08	0.68
2:E:208:THR:OG1	11:E:2298:HOH:O	2.13	0.66
3:C:248:LEU:CD1	3:C:248:LEU:O	2.44	0.66
2:E:246[B]:MET:HE2	2:E:432:VAL:HG11	1.76	0.65
11:C:2150:HOH:O	1:D:245[B]:GLU:OE2	2.15	0.65
1:A:115:VAL:HG22	2:E:405:MET:SD	2.37	0.65
2:E:17:LEU:HD21	2:E:20:GLU:HG3	1.77	0.65
2:E:246[B]:MET:CE	2:E:432:VAL:HG11	2.28	0.63
10:A:565:CL:CL	3:F:153[A]:LYS:NZ	2.68	0.63
2:B:104[B]:GLU:OE2	11:B:2248:HOH:O	2.15	0.62
2:E:322[B]:ARG:CZ	3:F:67[B]:ARG:HG3	2.30	0.62
1:A:120:LEU:N	1:A:120:LEU:CD2	2.63	0.61
1:A:269[B]:VAL:HG12	11:A:2444:HOH:O	2.01	0.61
2:E:233[A]:PHE:HD2	11:E:2309:HOH:O	1.82	0.60
1:A:119:ARG:HB3	1:A:120:LEU:HD22	1.83	0.60
11:B:2319:HOH:O	2:E:188:PRO:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:LYS:HD2	11:C:2178:HOH:O	2.02	0.59
3:C:155:VAL:HG21	11:C:2172:HOH:O	2.01	0.58
11:A:2250:HOH:O	3:F:81:ARG:HD3	2.03	0.58
2:B:14[A]:ARG:NH1	3:C:63:GLU:OE2	2.37	0.57
3:F:181:THR:HB	3:F:183[A]:ARG:HG3	1.86	0.57
1:A:112:ALA:HB2	11:A:2227:HOH:O	2.04	0.57
1:D:24[B]:THR:HG23	11:D:2099:HOH:O	2.05	0.57
11:A:2124:HOH:O	1:D:545[A]:LEU:HD11	2.05	0.56
1:A:194[A]:GLU:HG2	11:A:2366:HOH:O	2.03	0.56
3:C:120[B]:ARG:HG2	11:C:2172:HOH:O	2.05	0.56
2:B:299[A]:LEU:HD21	2:B:349[A]:PHE:CZ	2.41	0.55
3:C:52:VAL:O	1:D:118:LYS:NZ	2.34	0.55
1:A:545[B]:LEU:CD1	11:A:2301:HOH:O	2.55	0.54
11:C:2172:HOH:O	5:D:552:F43:H2C	2.06	0.54
2:E:241:LEU:HD11	2:E:246[B]:MET:HE3	1.90	0.54
1:D:194[A]:GLU:HG2	11:D:2327:HOH:O	2.07	0.53
1:A:24[B]:THR:HG23	11:A:2087:HOH:O	2.08	0.53
1:D:545[B]:LEU:CD1	11:D:2273:HOH:O	2.57	0.53
2:B:188:PRO:HD3	11:E:2253:HOH:O	2.09	0.52
2:B:14[A]:ARG:NH1	3:C:63:GLU:CG	2.73	0.52
11:B:2477:HOH:O	3:C:67[B]:ARG:CD	2.56	0.52
1:A:119:ARG:HB3	1:A:120:LEU:CD2	2.39	0.52
3:C:120[B]:ARG:CD	11:C:2172:HOH:O	2.59	0.51
3:C:120[B]:ARG:NH2	11:C:2154:HOH:O	2.43	0.51
11:A:2584:HOH:O	2:B:351[B]:LYS:NZ	1.70	0.51
2:E:246[A]:MET:CE	2:E:429:LEU:HD12	2.41	0.50
3:F:132:LYS:HD2	11:F:2152:HOH:O	2.12	0.50
1:A:17[A]:SER:OG	1:A:20:GLU:HG3	2.12	0.50
2:B:283:LYS:HE2	11:B:2440:HOH:O	2.12	0.50
2:B:113[B]:LEU:HD23	2:B:418:VAL:HG13	1.92	0.49
3:F:193:ASP:OD2	11:F:2192:HOH:O	2.19	0.49
3:C:248:LEU:HD12	11:C:2284:HOH:O	2.11	0.49
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.47	0.49
2:E:233[A]:PHE:HB2	11:E:2309:HOH:O	2.11	0.49
5:A:554:F43:H9A1	1:D:328:VAL:HB	1.95	0.49
1:D:4[A]:LYS:NZ	11:D:2018:HOH:O	2.32	0.48
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.48	0.48
11:A:2087:HOH:O	3:C:164:GLU:OE2	2.20	0.48
2:B:299[A]:LEU:CD1	11:B:2469:HOH:O	2.60	0.48
1:A:245[A]:GLU:OE2	11:A:2409:HOH:O	2.19	0.48
1:A:119:ARG:NH1	1:A:250:ASP:OD2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:67[B]:ARG:HH11	3:F:67[B]:ARG:CG	2.24	0.48
1:A:119:ARG:C	1:A:120:LEU:HD22	2.33	0.48
2:B:299[A]:LEU:CD2	2:B:349[A]:PHE:CZ	2.97	0.48
11:A:2383:HOH:O	2:E:61[B]:LYS:CE	2.61	0.48
2:B:299[A]:LEU:HD21	2:B:349[A]:PHE:HE1	1.76	0.48
11:C:2145:HOH:O	1:D:121:GLY:HA3	2.14	0.48
1:A:545[A]:LEU:HD12	11:A:2657:HOH:O	2.14	0.47
2:B:274[A]:GLU:OE2	11:B:2430:HOH:O	2.21	0.47
1:D:268:PRO:HB3	11:E:2285:HOH:O	2.13	0.47
1:D:191:ASP:HB2	11:D:2328:HOH:O	2.14	0.47
1:D:351:LYS:NZ	1:D:355:GLU:OE2	2.39	0.47
1:A:545[A]:LEU:CD1	11:A:2657:HOH:O	2.62	0.47
1:A:115:VAL:CG2	2:E:405:MET:SD	3.03	0.46
1:A:383[A]:GLU:HG3	11:A:2540:HOH:O	2.14	0.46
3:C:86:GLN:CD	3:C:120[A]:ARG:HD2	2.36	0.46
1:A:328:VAL:HB	5:D:552:F43:H9A1	1.97	0.46
1:D:545[B]:LEU:HD12	11:D:2273:HOH:O	2.14	0.46
1:A:45:LYS:NZ	11:A:2137:HOH:O	2.37	0.45
3:C:124:GLU:HG3	11:C:2170:HOH:O	2.16	0.45
2:B:299[A]:LEU:HD12	11:B:2469:HOH:O	2.17	0.45
2:B:91:GLU:OE1	11:B:2219:HOH:O	2.21	0.45
1:A:545[B]:LEU:HD12	11:A:2301:HOH:O	2.15	0.45
2:E:36:LYS:NZ	11:E:2073:HOH:O	2.40	0.45
2:B:36[B]:LYS:HA	2:E:123[B]:VAL:HG12	1.99	0.44
2:B:233[B]:PHE:HD1	2:B:236[B]:MET:HE3	1.81	0.44
2:E:185[B]:LEU:HD21	2:E:191:ALA:HA	1.99	0.44
1:A:236:ILE:HA	1:A:241:GLN:HB2	2.00	0.43
2:B:349[B]:PHE:HE1	11:B:2469:HOH:O	2.02	0.43
3:C:57:GLU:HG3	11:C:2116:HOH:O	2.17	0.43
2:B:202:ALA:HB1	2:B:416:LYS:HB2	2.00	0.43
2:E:91[A]:GLU:CD	11:E:2178:HOH:O	2.52	0.43
1:D:298:GLU:HB2	10:D:559:CL:CL	2.55	0.43
2:E:104[B]:GLU:HG2	11:E:2207:HOH:O	2.18	0.43
2:E:58:LYS:HB2	2:E:58:LYS:HE2	1.86	0.43
11:B:2467:HOH:O	3:C:248:LEU:HD11	2.19	0.42
1:A:186:LYS:HE3	1:A:186:LYS:HB2	1.84	0.42
2:B:77:ASP:OD1	11:B:2131:HOH:O	2.22	0.42
3:F:67[B]:ARG:HG2	3:F:67[B]:ARG:NH1	2.28	0.42
1:A:269[B]:VAL:CG1	11:A:2444:HOH:O	2.61	0.42
1:D:154:HIS:NE2	1:D:545[A]:LEU:HD21	2.35	0.42
2:B:104[B]:GLU:HG2	11:B:2248:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:GLN:HA	1:D:335:THR:OG1	2.20	0.42
1:D:545[A]:LEU:HD12	11:D:2567:HOH:O	2.19	0.41
3:F:181:THR:CB	3:F:183[A]:ARG:HG3	2.50	0.41
3:C:86:GLN:OE1	3:C:120[A]:ARG:NE	2.52	0.41
1:D:545[A]:LEU:CD1	11:D:2567:HOH:O	2.67	0.41
1:A:12:LYS:HG2	1:A:80:TYR:CD2	2.56	0.41
3:F:67[B]:ARG:NH1	3:F:67[B]:ARG:CG	2.83	0.41
2:B:362:PHE:O	2:B:369:GLY:HA3	2.20	0.41
2:B:37[B]:SER:HB3	2:B:424:GLU:OE1	2.20	0.41
1:D:242:ALA:HB3	1:D:245[A]:GLU:HG2	2.02	0.41
3:C:44:ALA:HB1	3:C:45:PRO:HD2	2.03	0.41
1:D:106:ILE:HB	1:D:261[A]:ILE:HB	2.02	0.41
10:A:565:CL:CL	3:F:153[B]:LYS:NZ	2.91	0.41
3:C:248:LEU:CD1	11:C:2284:HOH:O	2.68	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:2220:HOH:O	11:F:2027:HOH:O[1_556]	2.13	0.07
11:D:2167:HOH:O	11:F:2252:HOH:O[2_644]	2.13	0.07
11:A:2273:HOH:O	11:D:2238:HOH:O[2_644]	2.15	0.05

## 5.3 Torsion angles ⓘ

### 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	566/550 (103%)	548 (97%)	17 (3%)	1 (0%)	47	17
1	D	562/550 (102%)	546 (97%)	15 (3%)	1 (0%)	47	17
2	B	460/443 (104%)	451 (98%)	9 (2%)	0	100	100
2	E	462/443 (104%)	455 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	255/249 (102%)	248 (97%)	7 (3%)	0	100	100
3	F	253/249 (102%)	245 (97%)	8 (3%)	0	100	100
All	All	2558/2484 (103%)	2493 (98%)	63 (2%)	2 (0%)	51	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
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	457/434 (105%)	454 (99%)	3 (1%)	84	57
1	D	454/434 (105%)	453 (100%)	1 (0%)	93	77
2	B	361/342 (106%)	360 (100%)	1 (0%)	92	76
2	E	363/342 (106%)	362 (100%)	1 (0%)	92	76
3	C	225/217 (104%)	224 (100%)	1 (0%)	91	74
3	F	223/217 (103%)	221 (99%)	2 (1%)	78	48
All	All	2083/1986 (105%)	2074 (100%)	9 (0%)	91	74

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352[A]	GLU
1	A	352[B]	GLU
1	A	444	TYR
2	B	126	GLU
3	C	248	LEU
1	D	444	TYR
2	E	126	GLU
3	F	148[A]	SER

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Mol	Chain	Res	Type
3	F	148[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	AGM	A	271	1	10,11,12	0.67	0	6,13,15	0.99	0
1	DYA	D	450	1	4,7,8	1.79	1 (25%)	1,8,10	3.83	1 (100%)
1	GL3	A	445	1	2,3,4	3.47	1 (50%)	1,2,4	0.63	0
1	GL3	D	445	1	2,3,4	3.16	1 (50%)	1,2,4	0.55	0
1	MHS	D	257	1	7,11,12	1.07	0	6,14,16	1.14	0
1	DYA	A	450	1	4,7,8	2.01	1 (25%)	1,8,10	3.51	1 (100%)
1	SMC	D	452	1	5,6,7	1.15	1 (20%)	2,6,8	1.74	1 (50%)
1	MGN	D	400	1	6,9,10	0.58	0	5,12,14	0.53	0
1	AGM	D	271	1	10,11,12	0.86	0	6,13,15	0.59	0
1	SMC	A	452	1	5,6,7	0.63	0	2,6,8	1.94	1 (50%)
1	MGN	A	400	1	6,9,10	1.02	0	5,12,14	0.85	0
1	MHS	A	257	1	7,11,12	1.06	0	6,14,16	1.24	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	AGM	A	271	1	-	2/10/11/13	-
1	DYA	D	450	1	-	1/2/6/8	-
1	GL3	A	445	1	-	0/1/1/2	-
1	GL3	D	445	1	-	0/1/1/2	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	DYA	A	450	1	-	1/2/6/8	-
1	SMC	D	452	1	-	1/3/5/7	-
1	MGN	D	400	1	-	0/7/9/12	-
1	AGM	D	271	1	-	2/10/11/13	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MGN	A	400	1	-	0/7/9/12	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GL3	C-S	-4.89	1.63	1.80
1	D	445	GL3	C-S	-4.46	1.65	1.80
1	D	450	DYA	CA-N	2.94	1.42	1.35
1	A	450	DYA	CA-N	2.77	1.42	1.35
1	D	452	SMC	CB-SG	2.10	1.83	1.80

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	450	DYA	O-C-CA	-3.83	120.53	125.39
1	A	450	DYA	O-C-CA	-3.51	120.92	125.39
1	A	452	SMC	CA-CB-SG	-2.56	109.90	114.04
1	D	452	SMC	CA-CB-SG	-2.35	110.25	114.04

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	450	DYA	O-C-CA-CB
1	A	450	DYA	O-C-CA-CB
1	D	452	SMC	CA-CB-SG-CS
1	A	452	SMC	CA-CB-SG-CS
1	D	271	AGM	CE2-CD-NE1-CZ
1	A	271	AGM	CE2-CD-NE1-CZ
1	A	271	AGM	NE1-CD-CG-CB
1	D	271	AGM	NE1-CD-CG-CB

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	F43	D	552	1,6	46,71,71	2.47	6 (13%)	48,118,118	1.19	5 (10%)
5	F43	A	554	1,6	46,71,71	2.47	5 (10%)	48,118,118	1.13	3 (6%)
6	COM	A	555	5	6,6,6	1.19	1 (16%)	7,8,8	1.08	0
7	TP7	A	557	-	16,20,20	0.64	0	18,26,26	0.76	0
6	COM	D	555	5	6,6,6	0.70	0	7,8,8	0.65	0
7	TP7	D	556	-	16,20,20	0.61	0	18,26,26	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	F43	D	552	1,6	-	1/18/185/185	-
5	F43	A	554	1,6	-	1/18/185/185	-
6	COM	A	555	5	-	0/4/4/4	-
7	TP7	A	557	-	-	1/20/24/24	-
6	COM	D	555	5	-	0/4/4/4	-
7	TP7	D	556	-	-	0/20/24/24	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	554	F43	NI-NA	10.27	2.11	1.89
5	D	552	F43	NI-NA	9.85	2.10	1.89
5	A	554	F43	NI-NB	9.51	2.10	1.89
5	D	552	F43	NI-NB	9.17	2.09	1.89
5	A	554	F43	NI-ND	7.69	2.06	1.89
5	D	552	F43	NI-ND	7.30	2.05	1.89
5	D	552	F43	CHC-C4B	3.16	1.48	1.39
5	A	554	F43	CHC-C4B	2.67	1.46	1.39
5	D	552	F43	CHD-C1D	-2.52	1.40	1.43
5	D	552	F43	C4C-NC	2.36	1.38	1.35
6	A	555	COM	O2S-S2	2.32	1.51	1.45
5	A	554	F43	CHD-C1D	-2.26	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	552	F43	O8D-C7D-C6D	-3.00	115.95	120.86
5	A	554	F43	O8D-C7D-C6D	-2.84	116.21	120.86
5	D	552	F43	C3D-C4D-ND	2.54	106.29	102.34
5	A	554	F43	C2B-C1B-NB	2.37	105.39	101.84
5	A	554	F43	C3D-C4D-ND	2.32	105.94	102.34
5	D	552	F43	C1B-C2B-C3B	2.22	104.80	101.51
5	D	552	F43	C2B-C1B-NB	2.19	105.12	101.84
5	D	552	F43	CAB-C3B-C2B	-2.00	114.85	119.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	554	F43	C3A-CAA-CBA-CCA
5	D	552	F43	C3A-CAA-CBA-CCA
7	A	557	TP7	CB-O4P-P-O3P

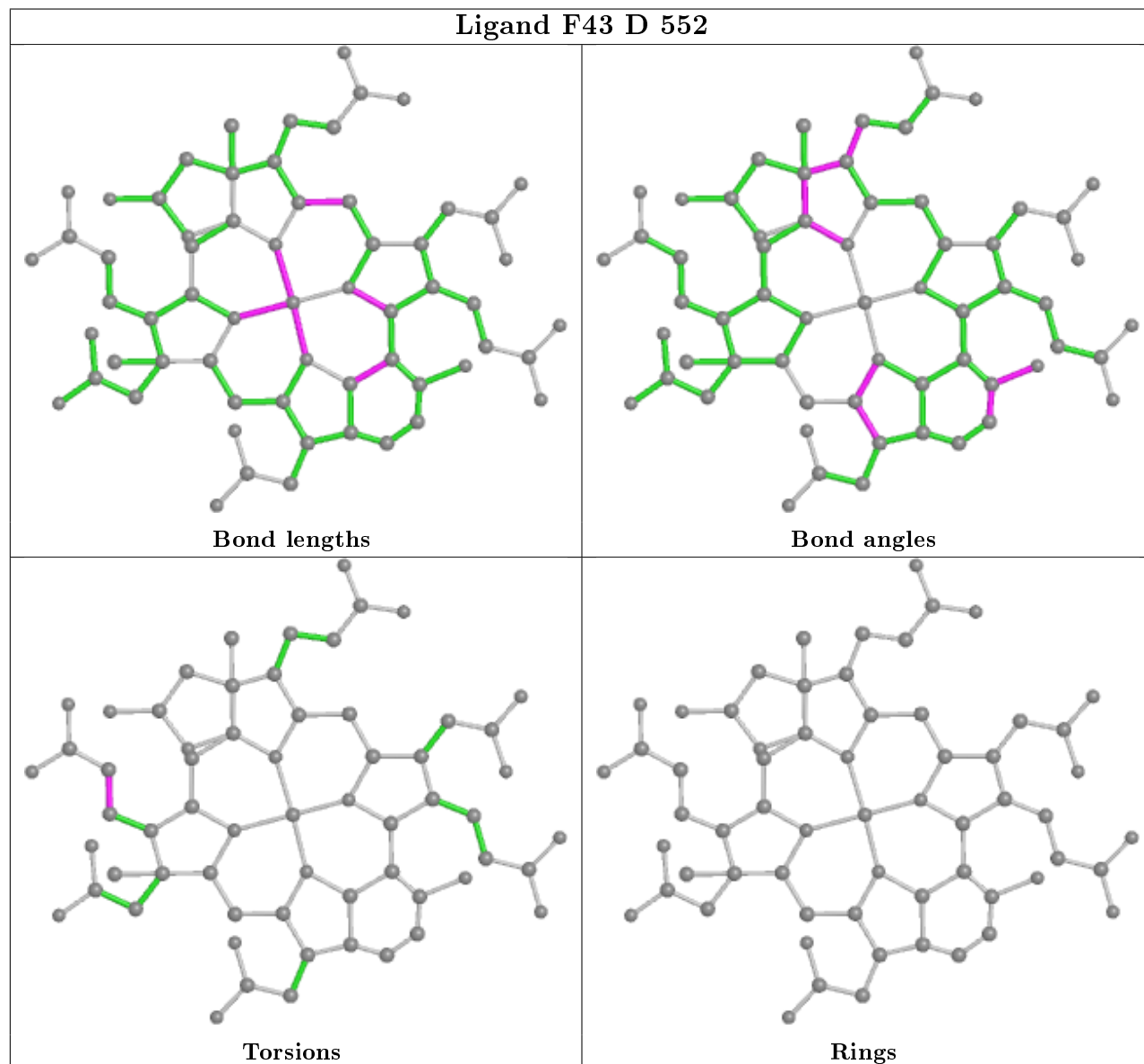
There are no ring outliers.

2 monomers are involved in 3 short contacts:

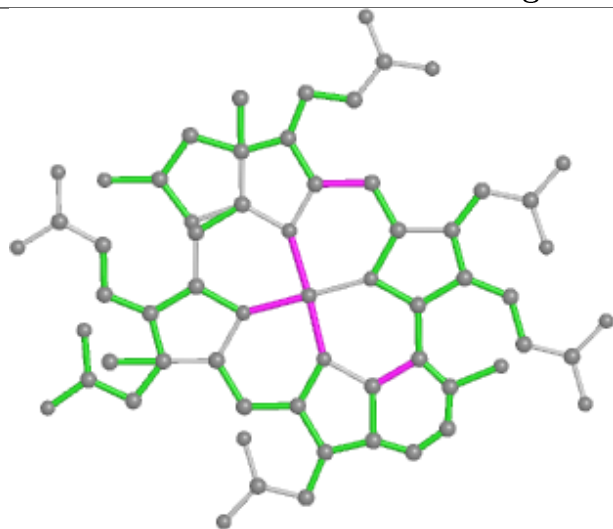
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	552	F43	2	0
5	A	554	F43	1	0

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

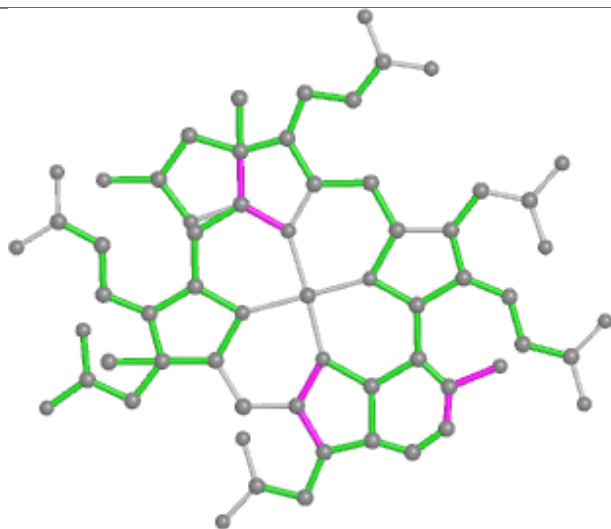
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



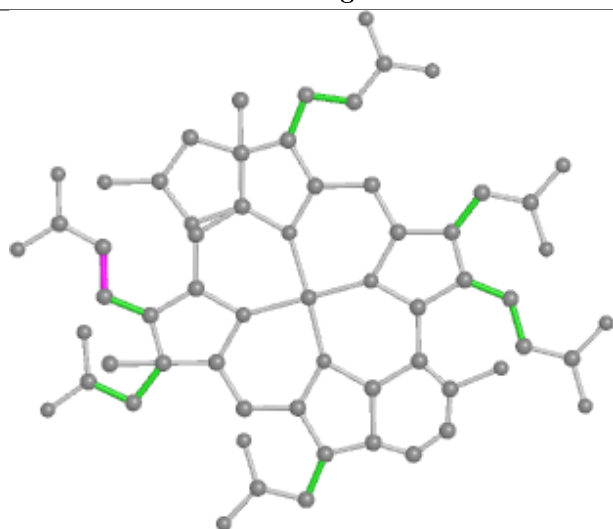
## Ligand F43 A 554



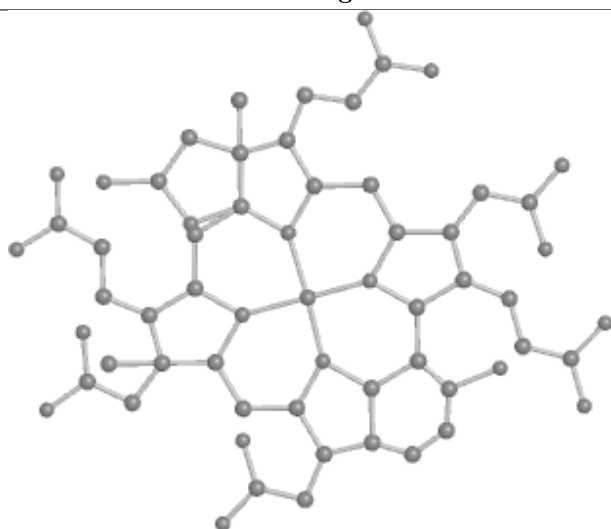
Bond lengths



Bond angles

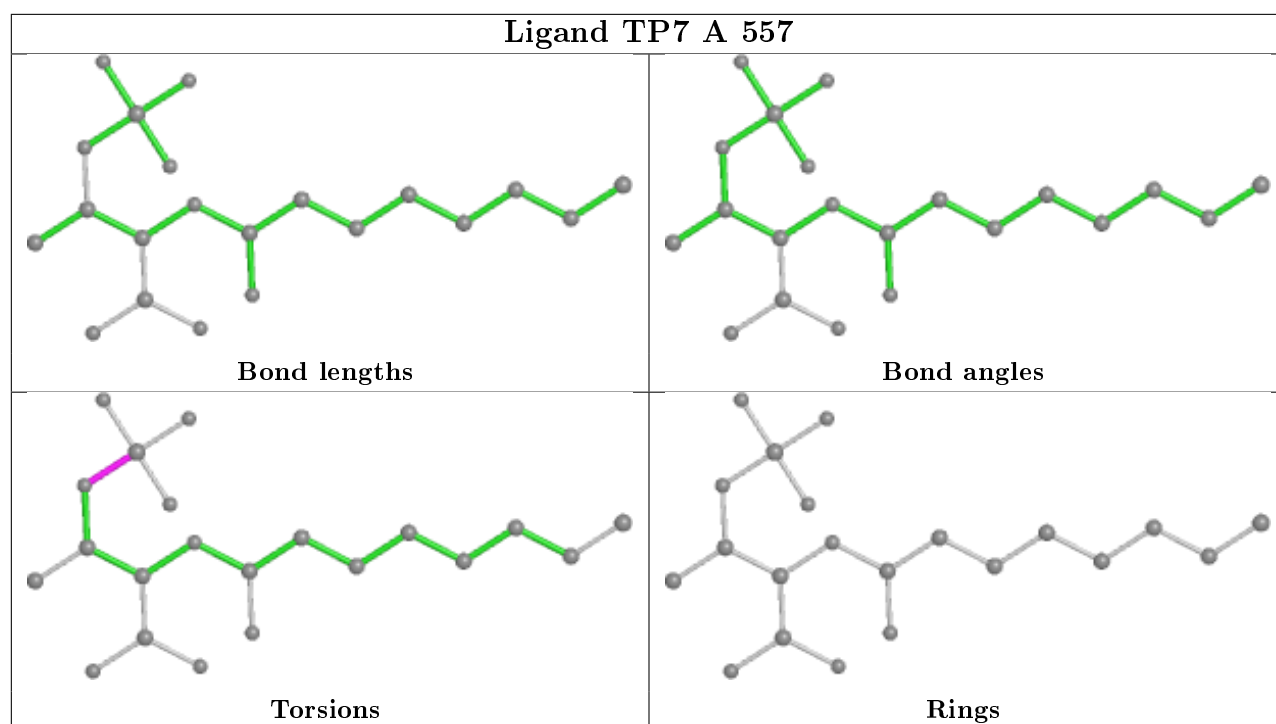


Torsions



Rings





## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	543/550 (98%)	0.02	6 (1%)	80 77	5, 9, 22, 53	2 (0%)
1	D	542/550 (98%)	-0.04	5 (0%)	84 82	5, 9, 20, 73	0
2	B	442/443 (99%)	-0.10	4 (0%)	84 82	6, 12, 21, 48	0
2	E	442/443 (99%)	-0.09	4 (0%)	84 82	6, 12, 24, 52	0
3	C	248/249 (99%)	0.18	15 (6%)	21 21	9, 15, 38, 61	0
3	F	248/249 (99%)	0.17	17 (6%)	16 17	8, 15, 40, 83	0
All	All	2465/2484 (99%)	-0.00	51 (2%)	63 59	5, 11, 25, 83	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	248	LEU	9.0
3	F	248	LEU	6.3
3	C	45	PRO	5.8
1	A	118	LYS	5.8
3	F	60	ASP	5.6
1	A	123	GLU	5.5
3	F	180	ASP	5.4
1	A	122	LYS	5.0
3	F	181	THR	4.9
3	C	179	LYS	4.8
1	D	549	ALA	4.8
3	F	249	GLU	4.6
3	C	180	ASP	4.5
3	F	45	PRO	4.5
3	F	63	GLU	4.4
2	E	441	ASN	4.2
1	A	120	LEU	4.1
3	C	60	ASP	4.1
1	D	2	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
3	F	196	ASP	3.8
3	F	194	GLU	3.6
3	C	181	THR	3.4
2	E	2	ALA	3.3
1	A	119	ARG	3.3
1	A	241	GLN	3.3
2	E	443	ILE	3.2
3	F	57	GLU	3.2
1	D	118	LYS	3.0
3	C	62	PRO	3.0
3	C	63	GLU	3.0
3	C	249	GLU	3.0
3	F	178	ASN	2.9
3	C	196	ASP	2.9
3	F	179	LYS	2.9
3	C	178	ASN	2.8
3	C	46	GLY	2.8
2	B	98	ASP	2.7
2	E	442	GLU	2.7
2	B	297	ASP	2.6
1	D	122	LYS	2.5
2	B	83	GLU	2.3
3	F	62	PRO	2.3
3	C	247	ASN	2.3
3	F	48	GLU	2.2
3	C	57	GLU	2.2
3	C	59	MET	2.2
2	B	97	GLU	2.2
1	D	297	TYR	2.1
3	F	58	GLU	2.1
3	F	46	GLY	2.1
3	F	51	SER	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	MHS	A	257	11/12	0.97	0.06	10,11,15,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MGN	A	400	10/11	0.98	0.09	7,8,8,8	0
1	MHS	D	257	11/12	0.98	0.06	9,11,13,16	0
1	DYA	A	450	8/9	0.99	0.08	7,8,9,9	0
1	SMC	D	452	7/8	0.99	0.08	7,7,9,10	0
1	MGN	D	400	10/11	0.99	0.07	6,6,7,8	0
1	AGM	D	271	12/13	0.99	0.11	5,6,6,7	0
1	SMC	A	452	7/8	0.99	0.08	7,8,9,9	0
1	DYA	D	450	8/9	0.99	0.07	7,7,9,10	0
1	AGM	A	271	12/13	0.99	0.10	5,6,7,7	0
1	GL3	A	445	4/5	1.00	0.09	7,7,7,8	0
1	GL3	D	445	4/5	1.00	0.07	6,6,6,6	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	MG	B	445	1/1	0.93	0.35	20,20,20,20	1
4	MG	D	560	1/1	0.94	0.12	22,22,22,22	1
10	CL	A	565	1/1	0.94	0.12	24,24,24,24	1
4	MG	E	446	1/1	0.95	0.30	34,34,34,34	0
10	CL	D	559	1/1	0.95	0.11	25,25,25,25	1
4	MG	F	251	1/1	0.96	0.13	15,15,15,15	1
4	MG	E	445	1/1	0.97	0.29	16,16,16,16	1
4	MG	D	557	1/1	0.98	0.15	21,21,21,21	0
7	TP7	A	557	21/21	0.98	0.07	7,8,8,9	0
7	TP7	D	556	21/21	0.98	0.07	6,8,8,8	0
4	MG	A	551	1/1	0.99	0.19	18,18,18,18	0
4	MG	C	251	1/1	0.99	0.07	12,12,12,12	1
6	COM	A	555	7/7	0.99	0.06	9,10,11,12	0
4	MG	E	444	1/1	0.99	0.28	24,24,24,24	0
5	F43	A	554	62/62	0.99	0.07	5,6,9,12	0
9	NA	A	564	1/1	0.99	0.07	15,15,15,15	0
4	MG	A	553	1/1	0.99	0.10	11,11,11,11	1

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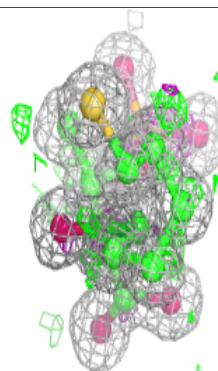
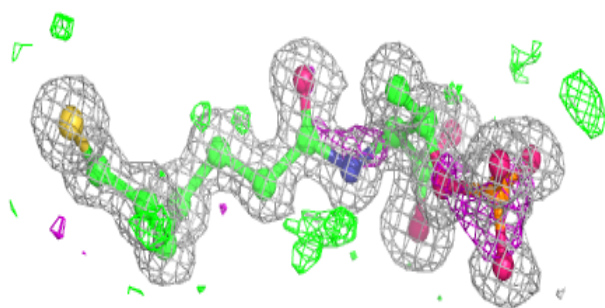
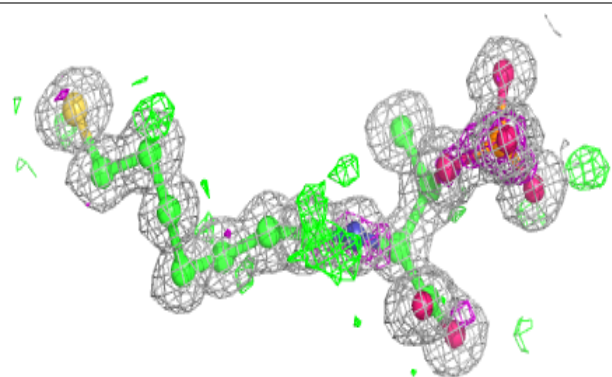
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	D	551	1/1	0.99	0.23	20,20,20,20	0
4	MG	A	563	1/1	0.99	0.21	23,23,23,23	0
9	NA	D	558	1/1	0.99	0.11	14,14,14,14	0
6	COM	D	555	7/7	0.99	0.06	8,10,10,10	0
4	MG	B	444	1/1	0.99	0.17	25,25,25,25	0
4	MG	A	562	1/1	0.99	0.20	18,18,18,18	0
5	F43	D	552	62/62	0.99	0.07	6,7,10,13	0
4	MG	F	250	1/1	1.00	0.07	16,16,16,16	0
8	K	A	561	1/1	1.00	0.04	9,9,9,9	0
4	MG	C	250	1/1	1.00	0.06	16,16,16,16	0

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

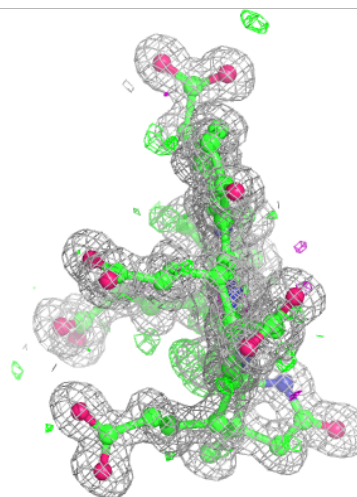
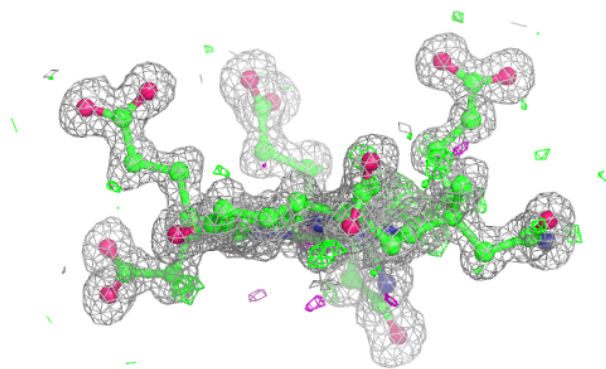
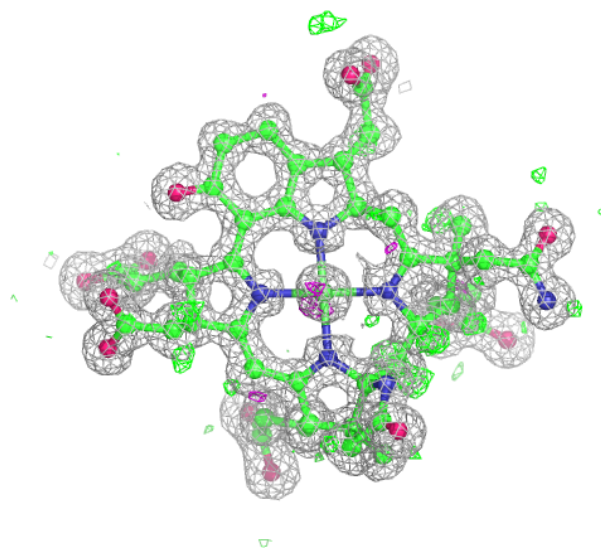
**Electron density around TP7 A 557:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



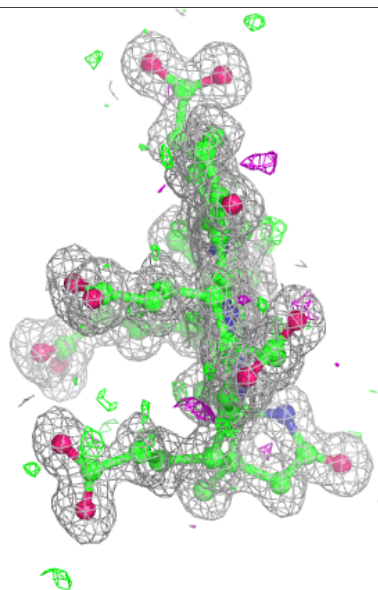
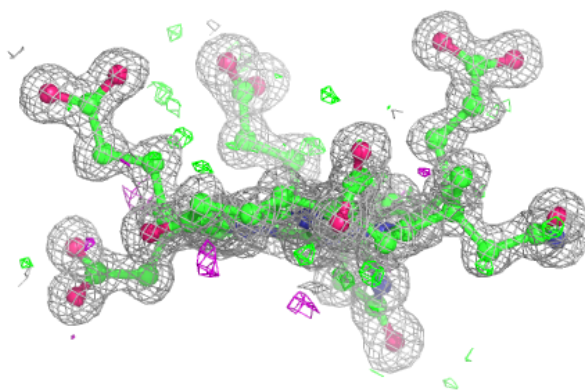
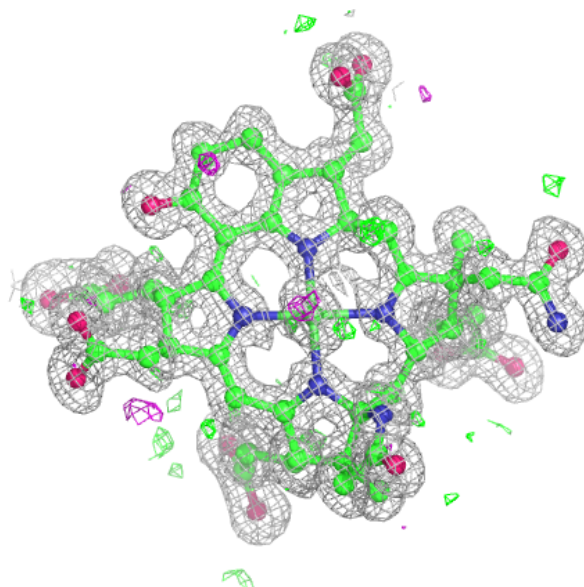
**Electron density around F43 A 554:**

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



**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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.