



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:30 pm BST

PDB ID : 5A8W
Title : METHYL-COENZYME M REDUCTASE II FROM METHANOTHERMOBACTER WOLFEII AT 1.8 Å RESOLUTION
Authors : Wagner, T.; Ermler, U.
Deposited on : 2015-07-17
Resolution : 1.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

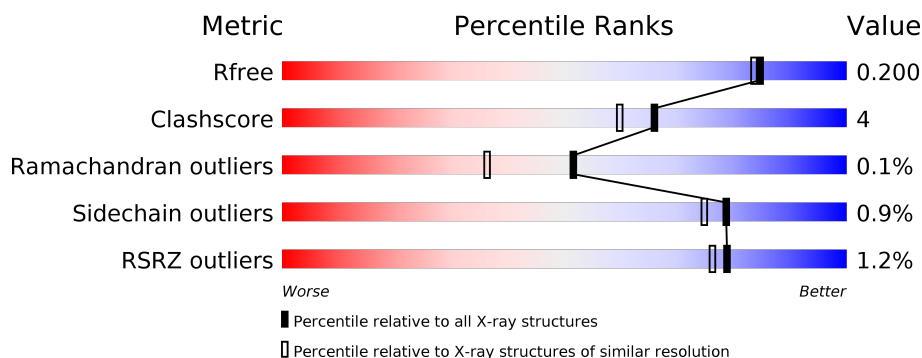
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	554	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>..</div> </div> </div>
1	D	554	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
1	G	554	<div> <div></div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	J	554	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
2	B	443	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
2	E	443	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	443	
2	K	443	
3	C	265	
3	F	265	
3	I	265	
3	L	265	

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
4	COM	J	1555	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 42336 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 II REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	8	0
			4273	2703	720	827	23			
1	D	549	Total	C	N	O	S	0	7	0
			4276	2705	718	830	23			
1	G	548	Total	C	N	O	S	0	8	0
			4271	2701	717	830	23			
1	J	548	Total	C	N	O	S	0	8	0
			4273	2704	716	831	22			

- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE II.

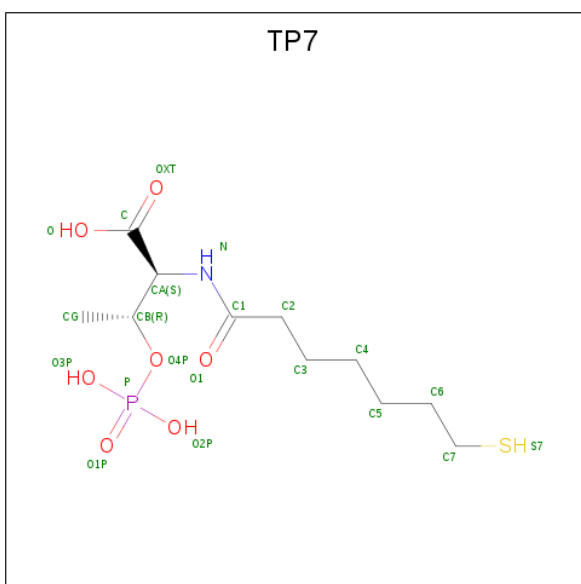
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	3	0
			3315	2101	558	642	14			
2	E	442	Total	C	N	O	S	0	4	0
			3319	2103	558	644	14			
2	H	442	Total	C	N	O	S	0	5	0
			3325	2108	560	643	14			
2	K	442	Total	C	N	O	S	0	8	0
			3348	2126	563	645	14			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	263	Total	C	N	O	S	0	4	0
			2155	1340	382	423	10			
3	F	263	Total	C	N	O	S	0	2	0
			2147	1334	383	420	10			
3	I	263	Total	C	N	O	S	0	2	0
			2147	1335	383	419	10			
3	L	263	Total	C	N	O	S	0	5	0
			2167	1348	388	421	10			

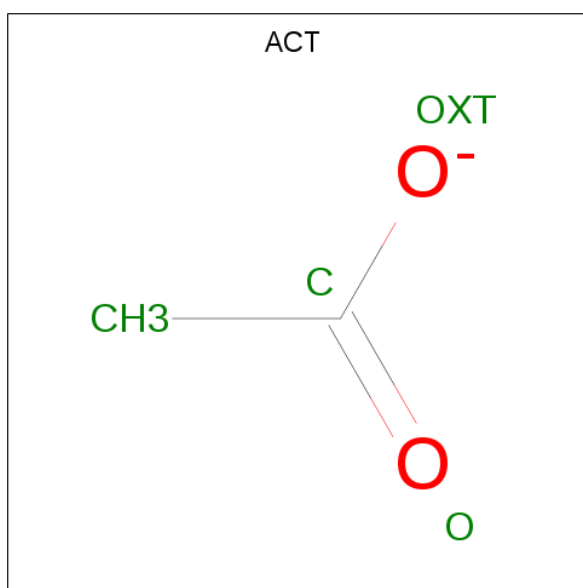
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- The diagram shows a chemical structure with a central sulfur atom (S) bonded to four oxygen atoms (O). The top-left oxygen is labeled O1S (green), the top-right is OH (red), the bottom-right is O2S (green), and the bottom-left is S2 (yellow). A yellow HS group (labeled S1 in green) is connected via a grey chain to two carbon atoms, C1 and C2 (both green). The label COM is at the top center.

- 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	C	N	O	P	S	
			21	11	1	7	1	1	0
5	D	1	Total	C	N	O	P	S	
			21	11	1	7	1	1	0
5	J	1	Total	C	N	O	P	S	
			21	11	1	7	1	1	0
5	J	1	Total	C	N	O	P	S	
			21	11	1	7	1	1	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



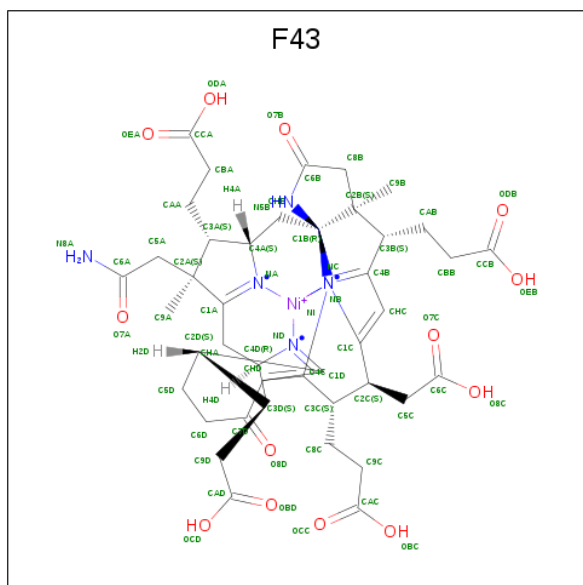
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			4	2 2		
6	D	1	Total	C O	0	0
			4	2 2		
6	E	1	Total	C O	0	0
			4	2 2		
6	E	1	Total	C O	0	0
			4	2 2		
6	F	1	Total	C O	0	0
			4	2 2		
6	G	1	Total	C O	0	0
			4	2 2		
6	H	1	Total	C O	0	0
			4	2 2		
6	I	1	Total	C O	0	0
			4	2 2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total	C	O	0	0
			4	2	2		
6	K	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	1	Total	Na	0	0
			1	1		

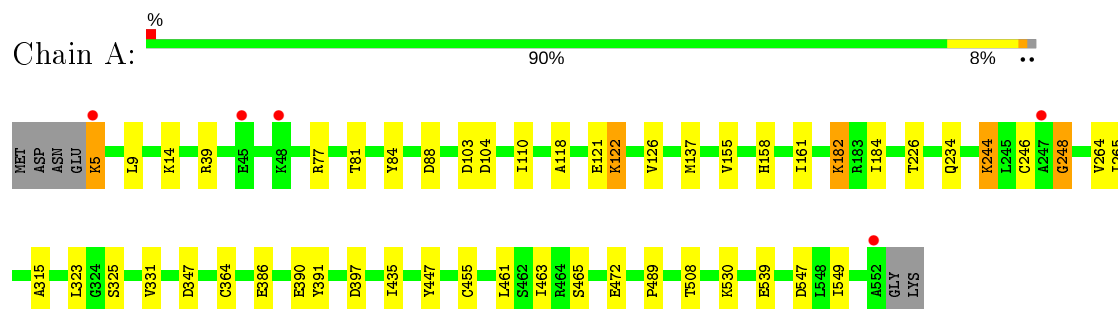
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	381	Total 381	O 381	0	0
9	B	281	Total 281	O 281	0	0
9	C	152	Total 152	O 152	0	0
9	D	284	Total 284	O 284	0	0
9	E	223	Total 223	O 223	0	0
9	F	145	Total 145	O 145	0	0
9	G	385	Total 385	O 385	0	0
9	H	269	Total 269	O 269	0	0
9	I	147	Total 147	O 147	0	0
9	J	291	Total 291	O 291	0	0
9	K	224	Total 224	O 224	0	0
9	L	133	Total 133	O 133	0	0

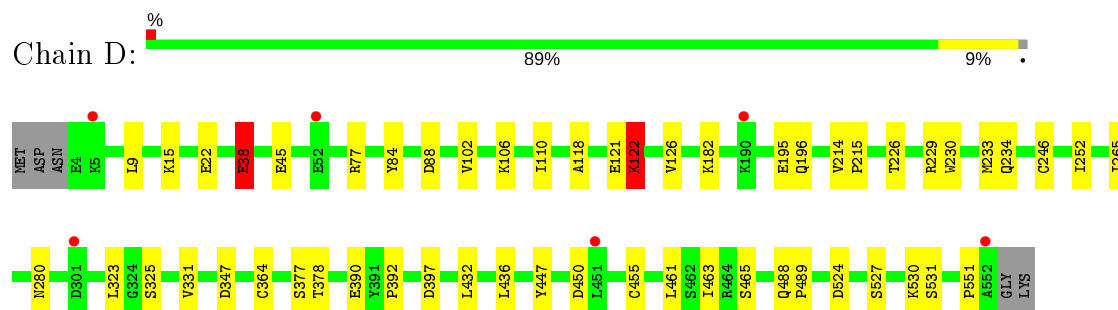
3 Residue-property plots [i](#)

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.

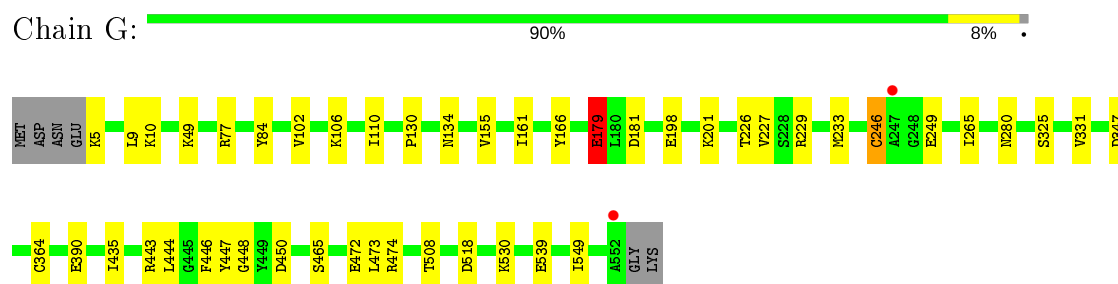
• Molecule 1: METHYL-COENZYME M II REDUCTASE



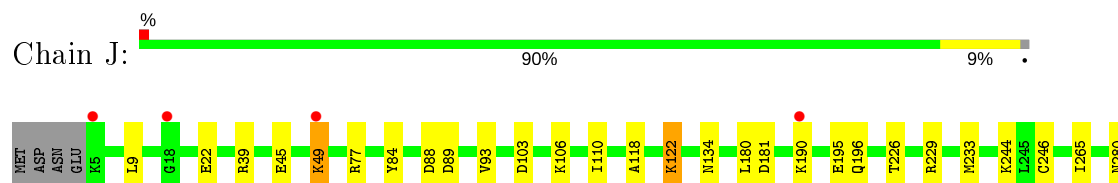
• Molecule 1: METHYL-COENZYME M II REDUCTASE



• Molecule 1: METHYL-COENZYME M II REDUCTASE

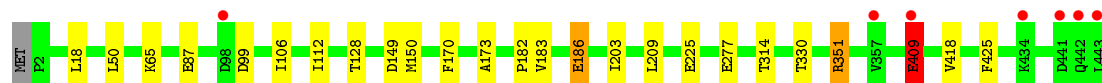


• Molecule 1: METHYL-COENZYME M II REDUCTASE

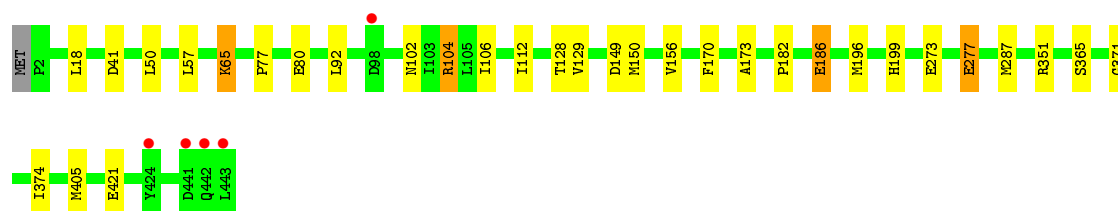




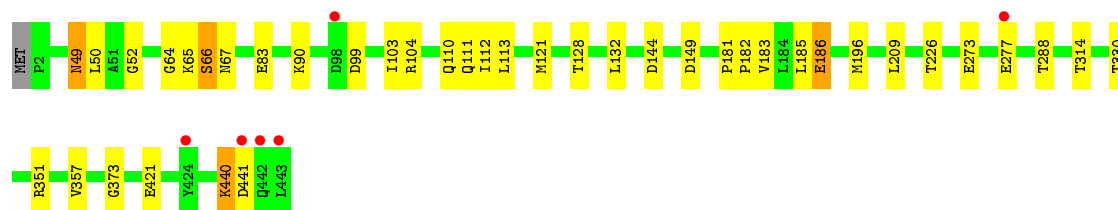
• Molecule 2: METHYL-COENZYME M REDUCTASE II



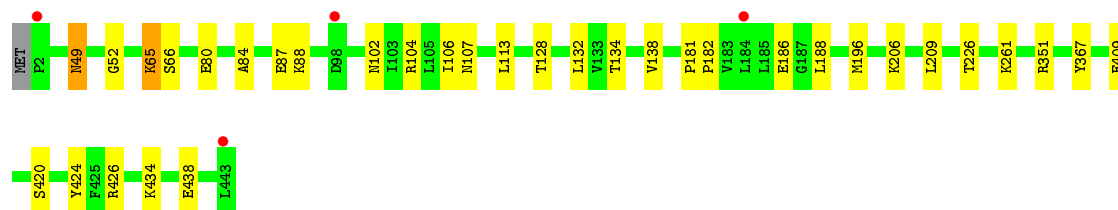
• Molecule 2: METHYL-COENZYME M REDUCTASE II



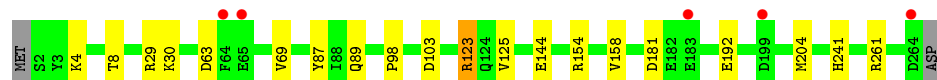
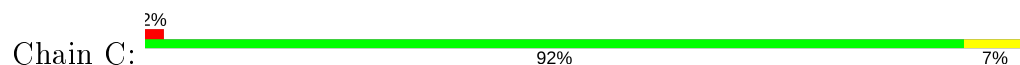
• Molecule 2: METHYL-COENZYME M REDUCTASE II



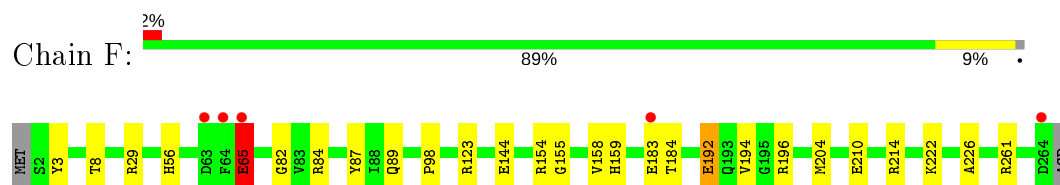
• Molecule 2: METHYL-COENZYME M REDUCTASE II



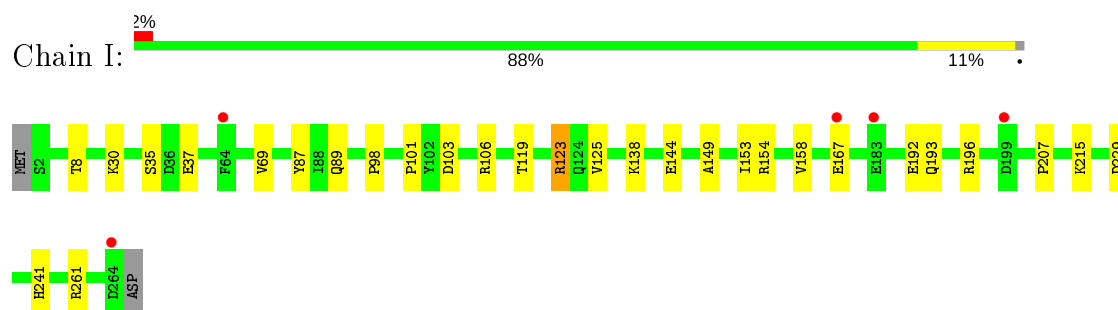
• Molecule 3: METHYL-COENZYME M REDUCTASE II



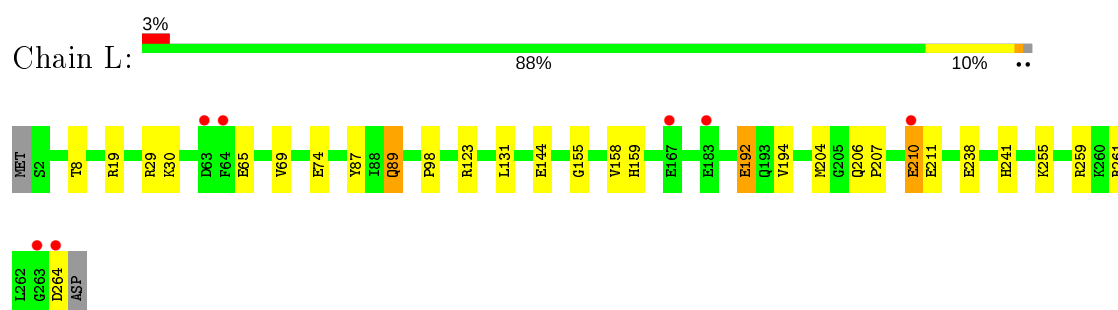
- Molecule 3: METHYL-COENZYME M REDUCTASE II



- Molecule 3: METHYL-COENZYME M REDUCTASE II



- Molecule 3: METHYL-COENZYME M REDUCTASE II



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.39Å 102.19Å 118.74Å 89.20° 93.97° 90.98°	Depositor
Resolution (Å)	48.66 – 1.80 48.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.66-1.80) 96.9 (48.66-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.165 , 0.201 0.166 , 0.200	Depositor DCC
R_{free} test set	23256 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.247 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42336	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGM, NA, F43, MGN, TP7, SMC, ACT, 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	0.74	0/4336	0.83	8/5865 (0.1%)
1	D	0.76	0/4337	0.84	8/5870 (0.1%)
1	G	0.76	0/4335	0.80	5/5865 (0.1%)
1	J	0.77	0/4340	0.84	7/5874 (0.1%)
2	B	0.70	2/3378 (0.1%)	0.83	8/4589 (0.2%)
2	E	0.72	3/3385 (0.1%)	0.81	5/4598 (0.1%)
2	H	0.72	2/3394 (0.1%)	0.81	7/4610 (0.2%)
2	K	0.67	0/3427	0.77	1/4652 (0.0%)
3	C	0.73	0/2206	0.87	5/2974 (0.2%)
3	F	0.72	2/2192 (0.1%)	0.92	6/2955 (0.2%)
3	I	0.70	0/2192	0.83	3/2953 (0.1%)
3	L	0.73	0/2221	0.86	2/2993 (0.1%)
All	All	0.73	9/39743 (0.0%)	0.83	65/53798 (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
1	D	0	1
1	G	0	1
2	B	0	1
3	F	0	1
3	L	0	1
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	66	SER	CB-OG	-10.73	1.28	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	277	GLU	CG-CD	6.59	1.61	1.51
2	E	277	GLU	CB-CG	-6.28	1.40	1.52
2	B	409	GLU	CB-CG	-6.25	1.40	1.52
2	B	186	GLU	CB-CG	-5.18	1.42	1.52
3	F	210	GLU	CD-OE1	-5.12	1.20	1.25
2	H	186	GLU	CB-CG	-5.07	1.42	1.52
2	E	186	GLU	CB-CG	-5.05	1.42	1.52
3	F	65	GLU	CD-OE2	-5.00	1.20	1.25

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	122	LYS	CD-CE-NZ	-13.94	79.65	111.70
1	J	190	LYS	CB-CG-CD	12.94	145.24	111.60
1	A	244	LYS	CD-CE-NZ	12.33	140.05	111.70
3	C	4	LYS	CB-CG-CD	-10.62	83.99	111.60
1	A	244	LYS	CB-CG-CD	-9.75	86.24	111.60
3	C	4	LYS	CD-CE-NZ	9.37	133.24	111.70
1	J	122	LYS	CB-CG-CD	8.74	134.33	111.60
2	E	277	GLU	CA-CB-CG	8.48	132.05	113.40
1	G	179	GLU	N-CA-CB	-8.44	95.41	110.60
1	D	252	ILE	CA-CB-CG1	-8.28	95.27	111.00
3	C	4	LYS	CA-CB-CG	7.93	130.86	113.40
1	D	122	LYS	CB-CG-CD	7.93	132.21	111.60
1	D	38	GLU	OE1-CD-OE2	-7.82	113.92	123.30
2	B	183	VAL	CG1-CB-CG2	7.79	123.37	110.90
3	F	65	GLU	N-CA-CB	7.78	124.60	110.60
3	I	215	LYS	CA-CB-CG	7.64	130.20	113.40
3	I	215	LYS	CD-CE-NZ	7.50	128.96	111.70
3	F	214	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	J	190	LYS	CA-CB-CG	7.18	129.20	113.40
2	B	409	GLU	CB-CG-CD	-7.04	95.18	114.20
2	B	409	GLU	N-CA-CB	-6.96	98.08	110.60
3	F	204	MET	CG-SD-CE	6.85	111.17	100.20
2	H	66	SER	CB-CA-C	-6.66	97.44	110.10
2	E	104	ARG	NE-CZ-NH1	-6.66	116.97	120.30
2	K	351	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	D	450	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	182	LYS	CD-CE-NZ	6.59	126.85	111.70
2	B	409	GLU	OE1-CD-OE2	-6.46	115.54	123.30
3	L	210	GLU	N-CA-CB	-6.46	98.96	110.60
1	J	190	LYS	CG-CD-CE	-6.45	92.56	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	277	GLU	CG-CD-OE2	-6.38	105.53	118.30
2	H	440	LYS	CD-CE-NZ	-6.29	97.23	111.70
3	F	65	GLU	CA-CB-CG	6.21	127.07	113.40
1	A	397	ASP	CB-CG-OD1	6.12	123.81	118.30
2	H	99	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	104	ASP	CB-CG-OD2	-5.90	112.99	118.30
2	H	351	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	G	179	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	J	49	LYS	CD-CE-NZ	-5.74	98.50	111.70
3	I	123	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	J	122	LYS	CG-CD-CE	5.62	128.77	111.90
1	D	182	LYS	CD-CE-NZ	-5.60	98.83	111.70
2	B	99	ASP	CB-CG-OD1	5.57	123.32	118.30
2	H	99	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	D	122	LYS	CD-CE-NZ	-5.55	98.94	111.70
1	A	104	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	182	LYS	CA-CB-CG	5.52	125.53	113.40
1	G	443	ARG	NE-CZ-NH1	5.49	123.05	120.30
3	F	65	GLU	CB-CA-C	-5.46	99.47	110.40
2	B	351	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	B	99	ASP	CB-CG-OD2	-5.42	113.42	118.30
2	H	351	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	397	ASP	CB-CG-OD2	-5.38	113.45	118.30
2	H	121	MET	CG-SD-CE	-5.34	91.65	100.20
2	E	277	GLU	CG-CD-OE1	5.27	128.83	118.30
3	F	84	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	G	179	GLU	CG-CD-OE2	-5.25	107.80	118.30
3	L	19	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	351	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	122	LYS	CG-CD-CE	-5.12	96.53	111.90
2	E	104	ARG	NE-CZ-NH2	5.10	122.85	120.30
3	C	181	ASP	CB-CG-OD1	5.04	122.84	118.30
1	G	474	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	397	ASP	CB-CG-OD1	5.03	122.83	118.30
3	C	123	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	409	GLU	Sidechain
1	D	38	GLU	Sidechain

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Mol	Chain	Res	Type	Group
3	F	65	GLU	Sidechain
1	G	179	GLU	Sidechain
3	L	210	GLU	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	4273	0	4138	42	0
1	D	4276	0	4132	39	0
1	G	4271	0	4129	41	0
1	J	4273	0	4136	40	0
2	B	3315	0	3332	18	0
2	E	3319	0	3334	28	1
2	H	3325	0	3351	34	1
2	K	3348	0	3382	35	0
3	C	2155	0	2098	17	0
3	F	2147	0	2090	17	1
3	I	2147	0	2096	23	0
3	L	2167	0	2123	28	1
4	A	7	0	5	1	0
4	D	7	0	5	0	0
4	G	7	0	4	1	0
4	J	7	0	5	1	0
5	A	21	0	19	0	0
5	D	21	0	19	0	0
5	J	42	0	38	0	0
6	A	4	0	3	0	0
6	D	4	0	3	0	0
6	E	8	0	6	1	0
6	F	4	0	3	0	0
6	G	4	0	3	0	0
6	H	4	0	3	0	0
6	I	4	0	3	0	0
6	J	4	0	3	0	0
6	K	4	0	3	0	0
6	L	4	0	3	0	0
7	D	124	0	86	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	62	0	43	2	0
7	J	62	0	43	1	0
8	F	1	0	0	0	0
9	A	381	0	0	12	0
9	B	281	0	0	6	0
9	C	152	0	0	4	1
9	D	284	0	0	7	0
9	E	223	0	0	5	0
9	F	145	0	0	2	0
9	G	385	0	0	7	0
9	H	269	0	0	8	0
9	I	147	0	0	5	0
9	J	291	0	0	6	0
9	K	224	0	0	8	0
9	L	133	0	0	4	1
All	All	42336	0	38641	310	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 (310) 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)
2:K:80:GLU:OE1	9:K:2043:HOH:O	1.63	1.16
3:I:89[B]:GLN:NE2	1:J:246:CYS:SG	2.19	1.13
3:C:89[B]:GLN:NE2	1:D:246[B]:CYS:SG	2.30	1.05
9:C:2070:HOH:O	1:D:246[B]:CYS:SG	2.19	0.99
2:H:83:GLU:OE1	9:H:2063:HOH:O	1.81	0.99
1:A:246[B]:CYS:SG	3:F:89[B]:GLN:NE2	2.36	0.98
3:C:30:LYS:NZ	9:C:2024:HOH:O	1.97	0.98
2:K:409:GLU:OE1	9:K:2126:HOH:O	1.86	0.94
1:G:246[A]:CYS:SG	9:G:2210:HOH:O	2.25	0.94
1:A:386:GLU:O	1:A:390:GLU:HG3	1.74	0.87
3:L:259:ARG:NH2	3:L:264:ASP:OD2	2.08	0.87
9:D:2050:HOH:O	1:G:10:LYS:NZ	1.77	0.85
2:B:128[B]:THR:OG1	9:B:2108:HOH:O	1.96	0.84
1:G:198:GLU:OE2	9:G:2174:HOH:O	1.97	0.82
9:C:2070:HOH:O	1:D:246[A]:CYS:SG	2.35	0.82
1:A:234:GLN:HE22	7:D:1554:F43:HN82	1.21	0.82
2:B:409:GLU:OE2	9:B:2263:HOH:O	2.00	0.78
9:D:2045:HOH:O	1:G:10:LYS:HE3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:84:ALA:O	2:K:87:GLU:HG3	1.83	0.78
9:H:2111:HOH:O	3:L:259:ARG:NH1	1.84	0.78
2:K:104:ARG:HH12	2:K:113:LEU:HD23	1.48	0.78
1:D:234:GLN:HE22	7:D:1556:F43:HN82	1.31	0.77
1:J:195:GLU:OE2	1:J:196:GLN:HG3	1.84	0.77
2:H:277:GLU:OE2	9:H:2199:HOH:O	2.03	0.76
1:J:118:ALA:O	1:J:122:LYS:HG3	1.85	0.76
1:J:195:GLU:OE1	9:J:2123:HOH:O	2.01	0.76
2:H:144:ASP:OD1	9:H:2111:HOH:O	2.03	0.76
3:L:206:GLN:OE1	9:L:2112:HOH:O	2.03	0.76
2:H:128[B]:THR:OG1	9:H:2101:HOH:O	2.02	0.75
2:E:405:MET:HE2	9:E:2207:HOH:O	1.86	0.75
9:B:2184:HOH:O	2:E:128[B]:THR:OG1	2.04	0.75
2:B:87:GLU:OE1	9:B:2067:HOH:O	2.03	0.74
3:C:89[A]:GLN:OE1	3:C:123:ARG:NE	2.17	0.73
3:L:65:GLU:HB2	9:L:2060:HOH:O	1.87	0.73
1:G:130:PRO:HG2	1:G:179:GLU:OE1	1.88	0.72
2:K:434:LYS:NZ	2:K:438:GLU:OE1	2.21	0.72
2:K:104:ARG:NH1	2:K:113:LEU:HD23	2.04	0.72
1:A:246[A]:CYS:HB2	3:F:87:TYR:CZ	2.24	0.72
3:I:229:ASP:OD2	9:I:2129:HOH:O	2.07	0.71
3:I:87:TYR:CZ	1:J:246:CYS:HB2	2.25	0.71
1:G:246[B]:CYS:HB3	3:L:87:TYR:CZ	2.25	0.71
2:E:277:GLU:OE2	9:E:2163:HOH:O	2.08	0.71
9:A:2242:HOH:O	6:E:1445:ACT:O	2.09	0.71
3:C:87:TYR:CZ	1:D:246[A]:CYS:HB2	2.26	0.71
2:H:104:ARG:NH2	2:H:421:GLU:OE2	2.23	0.71
1:A:81:THR:HB	9:A:2363:HOH:O	1.90	0.70
2:H:209:LEU:HD22	3:I:69:VAL:HG21	1.74	0.70
9:I:2079:HOH:O	1:J:246:CYS:SG	2.25	0.69
1:A:81:THR:HG22	1:A:530:LYS:HD2	1.73	0.69
3:C:87:TYR:CZ	1:D:246[B]:CYS:HB2	2.28	0.67
3:C:29:ARG:NH2	3:C:144:GLU:OE1	2.28	0.66
2:B:277:GLU:OE1	9:B:2214:HOH:O	2.13	0.66
1:J:89:ASP:OD2	9:J:2038:HOH:O	2.14	0.65
2:K:209:LEU:HD22	3:L:69:VAL:HG21	1.77	0.65
2:B:409:GLU:CD	9:B:2263:HOH:O	2.35	0.65
2:E:102[A]:ASN:OD1	9:E:2068:HOH:O	2.14	0.65
1:D:364:CYS:SG	9:D:2204:HOH:O	2.40	0.64
1:G:364:CYS:SG	9:G:2284:HOH:O	2.50	0.64
1:A:234:GLN:NE2	7:D:1554:F43:HN82	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:104:ARG:NH1	2:E:421:GLU:OE2	2.32	0.63
3:C:89[A]:GLN:CD	3:C:123:ARG:HE	2.01	0.63
1:A:248[A]:GLY:HA2	9:A:2209:HOH:O	1.98	0.63
2:H:49:ASN:ND2	2:H:111:GLN:HE21	1.97	0.62
2:K:102[A]:ASN:ND2	9:K:2038:HOH:O	2.18	0.62
2:H:288[B]:THR:HG23	9:H:2207:HOH:O	2.00	0.62
3:F:192:GLU:OE2	3:F:194:VAL:HG12	2.00	0.61
1:A:264:VAL:O	2:E:65:LYS:HE2	2.01	0.61
1:G:265:ILE:HD11	2:K:65:LYS:HD2	1.83	0.61
1:G:246[A]:CYS:HB2	3:L:87:TYR:CZ	2.35	0.60
1:G:246[B]:CYS:SG	1:G:249:GLU:HB3	2.41	0.60
2:H:83:GLU:CD	2:H:83:GLU:H	2.04	0.60
1:D:234:GLN:NE2	7:D:1556:F43:HN82	1.99	0.59
1:A:246[B]:CYS:HB2	3:F:87:TYR:CZ	2.37	0.59
1:J:134:ASN:ND2	1:J:181:ASP:H	2.02	0.58
1:A:5:LYS:NZ	9:A:2003:HOH:O	2.21	0.58
3:I:89[A]:GLN:NE2	3:I:123:ARG:HD2	2.19	0.57
1:A:248[B]:GLY:HA2	9:A:2209:HOH:O	2.03	0.57
1:A:364:CYS:SG	9:A:2279:HOH:O	2.51	0.57
1:D:118:ALA:O	1:D:122:LYS:HB2	2.04	0.57
2:H:66:SER:HB2	1:J:509:ASN:HD21	1.68	0.57
1:G:134:ASN:HD21	1:G:181:ASP:H	1.52	0.56
1:A:14:LYS:HD3	1:A:84:TYR:CZ	2.41	0.56
2:B:50:LEU:HD11	2:B:112:ILE:HD11	1.88	0.56
3:I:30:LYS:HD2	9:I:2032:HOH:O	2.06	0.56
1:J:364:CYS:SG	9:J:2208:HOH:O	2.57	0.56
4:A:1553:COM:O2S	9:A:2379:HOH:O	2.18	0.56
2:K:196:MET:HG3	9:K:2115:HOH:O	2.05	0.56
1:G:390[A]:GLU:HG3	9:G:2017:HOH:O	2.05	0.55
3:I:106:ARG:NH1	9:I:2006:HOH:O	2.36	0.55
2:K:209:LEU:HD13	3:L:69:VAL:HG11	1.89	0.55
1:G:134:ASN:ND2	1:G:181:ASP:H	2.03	0.55
1:A:244:LYS:HE2	3:F:196:ARG:NE	2.22	0.55
9:G:2241:HOH:O	2:H:186:GLU:HG2	2.06	0.55
9:J:2164:HOH:O	2:K:186:GLU:HG2	2.06	0.54
2:H:209:LEU:HD13	3:I:69:VAL:HG11	1.90	0.54
1:D:378:THR:HG23	1:D:436[B]:LEU:HD11	1.90	0.54
2:H:440:LYS:HG3	2:H:441:ASP:N	2.21	0.54
9:A:2209:HOH:O	2:E:365:SER:HA	2.07	0.54
2:H:273:GLU:HG3	9:H:2199:HOH:O	2.07	0.53
3:L:29:ARG:NH1	3:L:144:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:2195:HOH:O	1:J:103:ASP:OD1	2.19	0.52
1:J:134:ASN:HD21	1:J:181:ASP:H	1.57	0.52
3:L:89[A]:GLN:OE1	3:L:123[A]:ARG:HD2	2.07	0.52
1:G:5:LYS:HE2	1:G:9:LEU:HB3	1.91	0.52
3:I:30:LYS:NZ	9:I:2024:HOH:O	2.42	0.52
1:D:214[A]:VAL:HG13	1:D:215:PRO:HD2	1.92	0.51
3:F:29:ARG:NH1	9:F:2029:HOH:O	2.42	0.51
2:K:88:LYS:HE2	9:K:2061:HOH:O	2.09	0.51
2:K:84:ALA:HB1	9:K:2061:HOH:O	2.10	0.51
1:D:195:GLU:HG2	1:D:196:GLN:N	2.25	0.51
1:A:226:THR:HG23	1:D:325:SER:O	2.10	0.51
2:H:196:MET:HG3	2:H:373:GLY:O	2.11	0.51
9:D:2162:HOH:O	2:E:186:GLU:HG2	2.10	0.51
2:E:104:ARG:NH1	2:E:421:GLU:CD	2.64	0.51
1:A:77:ARG:HB2	1:A:84:TYR:CE2	2.45	0.50
3:F:89[A]:GLN:CD	3:F:123:ARG:HE	2.12	0.50
1:D:102:VAL:HG12	1:D:106:LYS:HD3	1.93	0.50
1:A:118:ALA:O	1:A:122:LYS:HB2	2.11	0.50
2:K:49:ASN:ND2	2:K:52:GLY:H	2.09	0.50
3:L:192:GLU:OE2	3:L:194:VAL:HG12	2.10	0.50
2:E:104:ARG:NH1	2:E:106:ILE:CD1	2.74	0.50
1:G:539:GLU:HA	1:J:551:PRO:HG3	1.94	0.50
2:B:106:ILE:HD13	2:B:418:VAL:HG22	1.94	0.49
1:G:102:VAL:HG12	1:G:106:LYS:HD3	1.92	0.49
1:J:22:GLU:HA	1:J:392:PRO:HD2	1.93	0.49
2:B:182:PRO:HB2	2:E:182:PRO:HB2	1.94	0.49
3:C:154:ARG:HD3	3:C:158:VAL:HA	1.94	0.49
2:H:182:PRO:HB2	2:K:182:PRO:HB2	1.94	0.49
3:L:123[B]:ARG:HD2	3:L:158:VAL:HG11	1.94	0.49
3:I:167:GLU:H	3:I:167:GLU:CD	2.15	0.49
1:D:524:ASP:HB3	1:D:531:SER:OG	2.13	0.49
2:K:209:LEU:HD13	3:L:69:VAL:HG21	1.95	0.49
1:J:524:ASP:HB3	1:J:531:SER:OG	2.12	0.49
3:L:89[A]:GLN:HE21	3:L:155:GLY:HA2	1.78	0.49
1:J:378:THR:OG1	3:L:238:GLU:OE2	2.27	0.49
1:D:38:GLU:HB2	1:G:10:LYS:HE2	1.94	0.48
1:J:77:ARG:HB2	1:J:84:TYR:CE2	2.48	0.48
3:L:255:LYS:O	3:L:259:ARG:HG2	2.12	0.48
2:H:50:LEU:HD11	2:H:112:ILE:HD11	1.94	0.48
2:E:170:PHE:HB3	2:E:173:ALA:HB2	1.95	0.48
1:G:530:LYS:HB3	1:G:530:LYS:HE2	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:LYS:HE2	1:G:9:LEU:CB	2.43	0.48
2:H:273:GLU:O	2:H:277:GLU:HG2	2.13	0.48
1:G:435:ILE:HD11	3:I:241:HIS:HB2	1.94	0.48
1:J:367:GLU:HG3	1:J:368:PRO:HD2	1.95	0.48
3:C:89[B]:GLN:HG2	3:C:125:VAL:HG23	1.96	0.48
3:F:56:HIS:CE1	3:F:82:GLY:HA2	2.49	0.48
1:G:331:VAL:HB	7:G:1554:F43:H9A1	1.96	0.48
3:I:89[B]:GLN:HG2	3:I:125:VAL:HG23	1.96	0.47
3:L:259:ARG:NH1	9:L:2129:HOH:O	2.32	0.47
2:K:420:SER:O	2:K:426:ARG:HD3	2.14	0.47
3:L:30:LYS:NZ	9:L:2025:HOH:O	2.21	0.47
2:K:209:LEU:CD1	3:L:69:VAL:HG11	2.44	0.47
1:A:121:GLU:HG2	1:A:126:VAL:O	2.15	0.47
3:F:154:ARG:HD3	3:F:158:VAL:HA	1.95	0.47
1:D:110:ILE:HB	1:D:265:ILE:HB	1.95	0.47
1:G:106:LYS:O	1:G:227:VAL:HG21	2.13	0.47
1:A:110:ILE:HB	1:A:265:ILE:HB	1.96	0.47
2:K:87:GLU:HG2	9:K:2062:HOH:O	2.15	0.47
1:G:10:LYS:HA	1:G:10:LYS:HD2	1.60	0.47
1:G:110:ILE:HB	1:G:265:ILE:HB	1.96	0.47
2:H:182:PRO:HA	2:H:185:LEU:HG	1.97	0.47
3:F:183:GLU:HG3	3:F:184:THR:HG23	1.96	0.47
2:H:66:SER:HB2	1:J:509:ASN:ND2	2.30	0.47
1:D:121:GLU:HG2	1:D:126:VAL:O	2.16	0.46
2:H:183:VAL:HG11	9:K:2110:HOH:O	2.14	0.46
2:K:104:ARG:NH1	2:K:104:ARG:HB3	2.31	0.46
1:A:455:SMC:SG	2:B:351:ARG:HA	2.55	0.46
1:A:461:LEU:HD13	2:E:150:MET:HG2	1.97	0.46
1:G:446:PHE:HB2	4:G:1553:COM:H11	1.97	0.46
7:G:1554:F43:H3C	7:G:1554:F43:O8D	2.16	0.46
3:I:37:GLU:H	3:I:37:GLU:CD	2.18	0.46
1:J:134:ASN:HD21	1:J:180:LEU:HA	1.81	0.46
2:B:209:LEU:HD22	3:C:69:VAL:HG21	1.97	0.46
1:G:444:LEU:HD23	1:G:450:ASP:HB3	1.98	0.46
1:G:166:TYR:OH	1:G:518:ASP:OD2	2.20	0.45
1:D:463:ILE:HG13	9:D:2253:HOH:O	2.17	0.45
1:D:77:ARG:HB2	1:D:84:TYR:CE2	2.51	0.45
3:I:196:ARG:HG3	1:J:244:LYS:NZ	2.31	0.45
1:J:463:ILE:HG13	9:J:2258:HOH:O	2.16	0.45
2:B:150:MET:HG2	1:D:461:LEU:HD13	1.99	0.45
3:L:98:PRO:HB2	3:L:144:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:GLU:CD	2:H:83:GLU:N	2.69	0.45
1:J:331:VAL:HB	7:J:1554:F43:H9A1	1.99	0.45
1:D:455:SMC:SG	2:E:351:ARG:HA	2.56	0.45
3:F:158:VAL:O	3:F:159:HIS:C	2.56	0.45
1:G:448:GL3:HA2	2:H:357:VAL:HG12	1.99	0.45
1:A:137:MET:HG3	1:A:184:ILE:HD13	1.98	0.44
3:F:155:GLY:HA3	9:F:2077:HOH:O	2.17	0.44
1:A:435:ILE:HD11	3:C:241:HIS:HB2	1.99	0.44
1:J:444:LEU:HD23	1:J:450:ASP:HB3	2.00	0.44
1:J:309:GLU:OE1	1:J:528:PRO:HD2	2.18	0.44
2:K:106:ILE:HG22	2:K:107:ASN:CG	2.37	0.44
1:D:331:VAL:HB	7:D:1554:F43:H9A1	1.98	0.44
2:H:128[A]:THR:HG21	2:K:188:LEU:HB3	2.00	0.44
1:D:9:LEU:HD23	1:D:9:LEU:HA	1.86	0.44
1:J:39:ARG:HG2	1:J:88:ASP:HB2	1.99	0.44
1:A:161[A]:ILE:HD11	1:A:549:ILE:CG2	2.47	0.44
1:D:45:GLU:HG2	9:D:2049:HOH:O	2.16	0.44
1:J:229:ARG:O	1:J:233:MET:HG2	2.16	0.44
2:K:206[B]:LYS:HE2	2:K:206[B]:LYS:HB3	1.80	0.44
1:D:527:SER:CB	1:D:530:LYS:HG3	2.48	0.44
2:H:104:ARG:HH12	2:H:421:GLU:CD	2.21	0.44
2:E:104:ARG:NH1	2:E:106:ILE:HD11	2.33	0.44
4:J:1555:COM:H21	2:K:367:TYR:HE2	1.82	0.44
3:I:154:ARG:HD3	3:I:158:VAL:HA	2.00	0.44
2:E:371:GLY:O	2:E:374:ILE:HG13	2.19	0.43
1:D:229:ARG:O	1:D:233:MET:HG2	2.18	0.43
3:I:30:LYS:HB2	3:I:30:LYS:HE2	1.66	0.43
3:I:89[A]:GLN:CD	3:I:123:ARG:HE	2.21	0.43
1:D:488:GLN:HB2	1:D:489:PRO:HD3	1.99	0.43
1:G:49:LYS:HE2	1:G:49:LYS:HB2	1.82	0.43
1:J:110:ILE:HB	1:J:265:ILE:HB	1.99	0.43
1:A:39:ARG:HG2	1:A:88:ASP:HB2	2.00	0.43
1:G:77:ARG:HB2	1:G:84:TYR:CE2	2.53	0.43
3:L:204:MET:HE3	3:L:204:MET:HB3	1.65	0.43
2:K:104:ARG:HB3	2:K:104:ARG:HH11	1.83	0.43
2:K:134:THR:O	2:K:138:VAL:HG23	2.19	0.43
3:C:63:ASP:HB3	9:C:2058:HOH:O	2.19	0.43
1:G:155:VAL:HB	1:J:88:ASP:HA	1.99	0.43
1:J:9:LEU:HD23	1:J:9:LEU:HA	1.80	0.43
1:A:463:ILE:HG13	9:A:2337:HOH:O	2.17	0.43
1:D:377[B]:SER:HB2	1:D:432:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:287:MET:HB3	2:E:287:MET:HE3	1.87	0.43
1:D:22:GLU:HA	1:D:392:PRO:HD2	2.00	0.43
1:D:214[A]:VAL:HG22	1:D:230:TRP:CD1	2.54	0.43
2:E:273:GLU:HB2	3:F:3:TYR:HB2	2.00	0.43
1:G:106:LYS:HG2	1:G:280:ASN:O	2.19	0.43
2:K:65:LYS:O	2:K:66:SER:OG	2.31	0.43
1:A:9:LEU:HD21	1:A:391:TYR:CE1	2.53	0.43
2:E:106:ILE:HG23	2:E:106:ILE:HD12	1.83	0.43
3:C:123:ARG:HD2	3:C:158:VAL:HG11	2.00	0.42
1:A:315:ALA:HA	1:A:489:PRO:CG	2.48	0.42
1:A:530:LYS:HE3	1:A:530:LYS:HB3	1.57	0.42
2:B:170:PHE:HB3	2:B:173:ALA:HB2	2.00	0.42
3:C:98:PRO:HB2	3:C:144:GLU:O	2.19	0.42
2:E:41:ASP:OD2	9:E:2033:HOH:O	2.21	0.42
2:E:57:LEU:HD21	2:E:156:VAL:HA	2.01	0.42
1:A:161[A]:ILE:HD11	1:A:549:ILE:HG21	1.99	0.42
2:K:409:GLU:N	2:K:409:GLU:OE1	2.29	0.42
1:G:473:LEU:HA	1:G:473:LEU:HD23	1.89	0.42
2:H:104:ARG:NH2	2:H:113:LEU:HD23	2.34	0.42
2:H:181:PRO:HA	2:H:182:PRO:HD3	1.90	0.42
1:A:103:ASP:OD1	9:A:2094:HOH:O	2.22	0.42
1:G:325:SER:O	1:J:226:THR:HG23	2.20	0.42
3:L:29:ARG:CZ	3:L:144:GLU:OE1	2.67	0.42
1:A:331:VAL:HB	7:D:1556:F43:H9A1	2.01	0.42
2:B:314:THR:HA	2:B:330:THR:HG21	2.02	0.42
3:C:204:MET:HE3	3:C:204:MET:HB3	1.85	0.42
2:B:203:ILE:CG2	2:B:425:PHE:HB3	2.50	0.42
1:D:15:LYS:HB3	1:D:15:LYS:HE3	1.88	0.42
2:H:49:ASN:ND2	2:H:52:GLY:H	2.18	0.42
1:A:325:SER:O	1:D:226:THR:HG23	2.19	0.42
2:B:209:LEU:HD13	3:C:69:VAL:HG11	2.02	0.42
2:K:261:LYS:HE2	3:L:74[B]:GLU:OE1	2.19	0.42
1:G:130:PRO:CG	1:G:179:GLU:OE1	2.63	0.42
1:G:161[B]:ILE:HD11	1:J:93:VAL:HG12	2.02	0.42
2:E:196:MET:HG3	2:E:199:HIS:H	1.84	0.42
1:A:244:LYS:HD2	3:F:196:ARG:NH2	2.34	0.42
3:I:98:PRO:HB2	3:I:144:GLU:O	2.20	0.42
1:J:315:ALA:HA	1:J:489:PRO:CG	2.49	0.42
3:F:98:PRO:HB2	3:F:144:GLU:O	2.20	0.41
1:A:182:LYS:NZ	9:A:2158:HOH:O	2.35	0.41
2:E:77:PRO:HB2	2:E:80:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161[A]:ILE:HD11	1:G:549:ILE:CG2	2.50	0.41
2:H:90:LYS:HB2	2:H:103:ILE:HG13	2.01	0.41
2:H:132:LEU:HD13	2:K:226:THR:HA	2.02	0.41
1:J:244:LYS:HG2	9:J:2144:HOH:O	2.21	0.41
2:K:209:LEU:CD2	3:L:69:VAL:HG21	2.49	0.41
9:H:2170:HOH:O	2:K:128[B]:THR:OG1	2.20	0.41
2:B:18:LEU:HA	2:B:18:LEU:HD23	1.90	0.41
1:D:390[A]:GLU:HG3	9:D:2019:HOH:O	2.20	0.41
2:H:64:GLY:O	2:H:67:ASN:HB2	2.21	0.41
3:I:196:ARG:HG3	1:J:244:LYS:HZ3	1.84	0.41
1:J:45:GLU:O	1:J:49:LYS:HG3	2.21	0.41
1:D:106:LYS:HG2	1:D:280:ASN:O	2.20	0.41
2:E:80:GLU:CD	9:E:2043:HOH:O	2.58	0.41
3:I:101:PRO:HB3	3:I:119:THR:HG23	2.02	0.41
3:I:153:ILE:HG22	3:I:193:GLN:HB3	2.02	0.41
3:I:149:ALA:HB2	3:I:207:PRO:HB3	2.02	0.41
3:L:131:LEU:HD23	3:L:131:LEU:C	2.41	0.41
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.85	0.41
1:G:472:GLU:HB3	1:G:508:THR:CG2	2.51	0.41
2:H:314:THR:HA	2:H:330:THR:HG21	2.02	0.41
1:J:106:LYS:HG2	1:J:280:ASN:O	2.20	0.41
1:G:226:THR:HG23	1:J:325:SER:O	2.20	0.41
1:J:435:ILE:HD11	3:L:241:HIS:HB2	2.03	0.41
1:A:158:HIS:HB3	1:A:161[A]:ILE:HG13	2.03	0.41
2:B:225:GLU:HG3	2:E:129:VAL:HB	2.02	0.41
1:D:323:LEU:HA	1:D:323:LEU:HD23	1.74	0.41
3:F:222:LYS:HA	3:F:226:ALA:HB2	2.02	0.41
1:A:155:VAL:HB	1:D:88:ASP:HA	2.01	0.40
1:G:201:LYS:NZ	9:G:2174:HOH:O	2.33	0.40
2:H:226:THR:HA	2:K:132:LEU:HD13	2.03	0.40
1:J:399:PHE:CD1	3:L:159:HIS:HE1	2.40	0.40
1:D:527:SER:HB3	1:D:530:LYS:HG3	2.02	0.40
1:A:539:GLU:HA	1:D:551:PRO:HG3	2.03	0.40
3:I:35:SER:HB2	3:I:37:GLU:OE1	2.21	0.40
1:A:472:GLU:HB3	1:A:508:THR:CG2	2.51	0.40
1:A:77:ARG:HB2	1:A:84:TYR:CZ	2.57	0.40
9:A:2235:HOH:O	2:B:186:GLU:HG2	2.19	0.40
3:C:89[A]:GLN:CD	3:C:123:ARG:NE	2.70	0.40
2:K:181:PRO:HA	2:K:182:PRO:HD3	1.94	0.40
2:E:50:LEU:HD11	2:E:112:ILE:HD11	2.04	0.40
2:E:18:LEU:HD23	2:E:18:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:LEU:HD23	2:E:92:LEU:HA	1.82	0.40
1:G:229:ARG:O	1:G:233:MET:HG2	2.21	0.40
3:L:206:GLN:HG2	3:L:207:PRO:HD2	2.04	0.40
3:F:89[A]:GLN:OE1	3:F:123:ARG:NE	2.36	0.40
2:H:65:LYS:O	2:H:66:SER:CB	2.69	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)
2:E:80:GLU:OE2	9:L:2032:HOH:O[1_445]	1.77	0.43
2:H:110:GLN:NE2	9:C:2024:HOH:O[1_564]	2.14	0.06
3:F:65:GLU:OE2	3:L:211:GLU:OE1[1_445]	2.16	0.04

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	549/554 (99%)	531 (97%)	15 (3%)	3 (0%)	29	15
1	D	549/554 (99%)	534 (97%)	14 (3%)	1 (0%)	47	33
1	G	549/554 (99%)	531 (97%)	17 (3%)	1 (0%)	47	33
1	J	549/554 (99%)	531 (97%)	17 (3%)	1 (0%)	47	33
2	B	443/443 (100%)	438 (99%)	5 (1%)	0	100	100
2	E	444/443 (100%)	440 (99%)	3 (1%)	1 (0%)	47	33
2	H	445/443 (100%)	440 (99%)	5 (1%)	0	100	100
2	K	448/443 (101%)	444 (99%)	4 (1%)	0	100	100
3	C	265/265 (100%)	259 (98%)	6 (2%)	0	100	100
3	F	263/265 (99%)	257 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	263/265 (99%)	256 (97%)	7 (3%)	0	100	100
3	L	266/265 (100%)	259 (97%)	7 (3%)	0	100	100
All	All	5033/5048 (100%)	4920 (98%)	106 (2%)	7 (0%)	51	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	SER
1	D	465	SER
1	G	465	SER
1	J	465	SER
2	E	65	LYS
1	A	248[A]	GLY
1	A	248[B]	GLY

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	440/438 (100%)	436 (99%)	4 (1%)	78	75
1	D	440/438 (100%)	437 (99%)	3 (1%)	84	81
1	G	440/438 (100%)	436 (99%)	4 (1%)	78	75
1	J	441/438 (101%)	438 (99%)	3 (1%)	84	81
2	B	348/346 (101%)	346 (99%)	2 (1%)	86	84
2	E	349/346 (101%)	348 (100%)	1 (0%)	92	91
2	H	350/346 (101%)	348 (99%)	2 (1%)	86	84
2	K	353/346 (102%)	349 (99%)	4 (1%)	73	68
3	C	234/232 (101%)	230 (98%)	4 (2%)	60	51
3	F	232/232 (100%)	229 (99%)	3 (1%)	69	62
3	I	232/232 (100%)	226 (97%)	6 (3%)	46	32
3	L	235/232 (101%)	230 (98%)	5 (2%)	53	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4094/4064 (101%)	4053 (99%)	41 (1%)	78	71

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	347	ASP
1	A	447	TYR
1	A	547	ASP
2	B	65	LYS
2	B	149	ASP
3	C	8	THR
3	C	103	ASP
3	C	192	GLU
3	C	261	ARG
1	D	122	LYS
1	D	347	ASP
1	D	447	TYR
2	E	149	ASP
3	F	8	THR
3	F	192	GLU
3	F	261	ARG
1	G	246[A]	CYS
1	G	246[B]	CYS
1	G	347	ASP
1	G	447	TYR
2	H	49	ASN
2	H	149	ASP
3	I	8	THR
3	I	103	ASP
3	I	138[A]	LYS
3	I	138[B]	LYS
3	I	192	GLU
3	I	261	ARG
1	J	347	ASP
1	J	447	TYR
1	J	547	ASP
2	K	49	ASN
2	K	65	LYS
2	K	424[A]	TYR
2	K	424[B]	TYR
3	L	8	THR

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Mol	Chain	Res	Type
3	L	89[A]	GLN
3	L	89[B]	GLN
3	L	192	GLU
3	L	261	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	GLN
2	B	110	GLN
3	C	206	GLN
1	D	210	GLN
1	D	234	GLN
2	E	107	ASN
3	F	77	GLN
1	G	134	ASN
2	H	49	ASN
2	H	107	ASN
1	J	134	ASN
2	K	49	ASN
2	K	107	ASN
2	K	111	GLN
3	L	77	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

20 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	J	448	1	2,3,4	3.81	1 (50%)	1,2,4	0.11	0
1	MHS	D	261	1	7,11,12	1.21	1 (14%)	6,14,16	1.59	2 (33%)
1	MHS	A	261	1	7,11,12	1.21	0	6,14,16	2.23	4 (66%)
1	SMC	G	455	1	5,6,7	0.96	0	2,6,8	1.87	1 (50%)
1	SMC	A	455	1	5,6,7	1.14	0	2,6,8	1.31	0
1	GL3	D	448	1	2,3,4	3.16	1 (50%)	1,2,4	0.07	0
1	SMC	D	455	1	5,6,7	1.03	0	2,6,8	0.88	0
1	GL3	A	448	1	2,3,4	4.43	1 (50%)	1,2,4	0.03	0
1	MHS	J	261	1	7,11,12	1.02	0	6,14,16	1.76	2 (33%)
1	SMC	J	455	1	5,6,7	0.93	0	2,6,8	1.22	0
1	MGN	A	403	1	6,9,10	0.90	0	5,12,14	0.80	0
1	MGN	J	403	1	6,9,10	0.90	0	5,12,14	0.54	0
1	MGN	D	403	1	6,9,10	1.10	1 (16%)	5,12,14	0.66	0
1	GL3	G	448	1	2,3,4	4.52	1 (50%)	1,2,4	0.10	0
1	AGM	D	275	1	10,11,12	2.62	3 (30%)	6,13,15	2.70	3 (50%)
1	MGN	G	403	1	6,9,10	0.95	0	5,12,14	0.59	0
1	AGM	A	275	1	10,11,12	2.34	3 (30%)	6,13,15	3.01	4 (66%)
1	AGM	G	275	1	10,11,12	2.63	3 (30%)	6,13,15	3.08	4 (66%)
1	MHS	G	261	1	7,11,12	1.07	0	6,14,16	1.60	2 (33%)
1	AGM	J	275	1	10,11,12	2.22	3 (30%)	6,13,15	3.24	4 (66%)

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	J	448	1	-	0/1/1/2	-
1	MHS	D	261	1	-	0/5/6/8	0/1/1/1
1	MHS	A	261	1	-	0/5/6/8	0/1/1/1
1	SMC	G	455	1	-	0/3/5/7	-
1	SMC	A	455	1	-	1/3/5/7	-
1	GL3	D	448	1	-	0/1/1/2	-
1	SMC	D	455	1	-	1/3/5/7	-
1	GL3	A	448	1	-	1/1/1/2	-
1	MHS	J	261	1	-	0/5/6/8	0/1/1/1
1	SMC	J	455	1	-	1/3/5/7	-
1	MGN	A	403	1	-	0/7/9/12	-
1	MGN	J	403	1	-	0/7/9/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MGN	D	403	1	-	0/7/9/12	-
1	GL3	G	448	1	-	0/1/1/2	-
1	AGM	D	275	1	-	2/10/11/13	-
1	MGN	G	403	1	-	0/7/9/12	-
1	AGM	A	275	1	-	3/10/11/13	-
1	AGM	G	275	1	-	3/10/11/13	-
1	MHS	G	261	1	-	0/5/6/8	0/1/1/1
1	AGM	J	275	1	-	4/10/11/13	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	275	AGM	CZ-NE1	6.84	1.45	1.33
1	G	275	AGM	CZ-NE1	6.71	1.44	1.33
1	G	448	GL3	C-S	-6.39	1.58	1.80
1	A	448	GL3	C-S	-6.27	1.59	1.80
1	A	275	AGM	CZ-NE1	5.86	1.43	1.33
1	J	275	AGM	CZ-NE1	5.42	1.42	1.33
1	J	448	GL3	C-S	-5.38	1.62	1.80
1	D	448	GL3	C-S	-4.47	1.65	1.80
1	G	275	AGM	CZ-NH2	3.77	1.47	1.32
1	J	275	AGM	CZ-NH2	3.49	1.46	1.32
1	D	275	AGM	CZ-NH2	3.36	1.45	1.32
1	A	275	AGM	CZ-NH2	3.07	1.44	1.32
1	G	275	AGM	CZ-NH1	2.67	1.45	1.34
1	A	275	AGM	CZ-NH1	2.49	1.45	1.34
1	J	275	AGM	CZ-NH1	2.42	1.44	1.34
1	D	275	AGM	CZ-NH1	2.41	1.44	1.34
1	D	403	MGN	CB1-CA	-2.16	1.52	1.55
1	D	261	MHS	CM-ND1	2.02	1.52	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	275	AGM	NH1-CZ-NE1	-5.32	107.66	119.55
1	G	275	AGM	NH1-CZ-NE1	-5.30	107.70	119.55
1	A	275	AGM	NH1-CZ-NE1	-5.10	108.15	119.55
1	D	275	AGM	NH1-CZ-NE1	-5.10	108.16	119.55
1	J	275	AGM	NE1-CZ-NH2	-4.03	113.55	120.59
1	G	275	AGM	NH1-CZ-NH2	-3.83	108.46	120.26
1	A	275	AGM	NH1-CZ-NH2	-3.68	108.94	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	MHS	CM-ND1-CG	3.16	128.65	124.44
1	J	275	AGM	NH1-CZ-NH2	-3.12	110.65	120.26
1	A	275	AGM	NE1-CZ-NH2	-2.81	115.69	120.59
1	G	261	MHS	NE2-CE1-ND1	-2.73	108.20	112.26
1	A	261	MHS	CD2-NE2-CE1	2.73	110.03	105.78
1	D	275	AGM	NH1-CZ-NH2	-2.71	111.91	120.26
1	J	261	MHS	CB-CA-C	-2.67	106.46	111.47
1	D	261	MHS	CM-ND1-CG	2.58	127.88	124.44
1	J	261	MHS	CM-ND1-CG	2.42	127.67	124.44
1	D	275	AGM	NE1-CZ-NH2	-2.42	116.36	120.59
1	A	261	MHS	NE2-CE1-ND1	-2.41	108.68	112.26
1	G	275	AGM	CE2-CD-NE1	-2.40	104.12	110.37
1	G	455	SMC	CA-CB-SG	-2.36	110.23	114.04
1	J	275	AGM	CE2-CD-NE1	-2.30	104.39	110.37
1	D	261	MHS	CB-CA-C	-2.24	107.27	111.47
1	A	275	AGM	CE2-CD-NE1	-2.19	104.67	110.37
1	G	275	AGM	NE1-CZ-NH2	-2.16	116.82	120.59
1	G	261	MHS	CD2-NE2-CE1	2.12	109.09	105.78
1	A	261	MHS	CB-CA-C	-2.07	107.59	111.47

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	275	AGM	CE2-CD-CG-CB
1	A	275	AGM	NH2-CZ-NE1-CD
1	G	275	AGM	CE2-CD-CG-CB
1	G	275	AGM	NH2-CZ-NE1-CD
1	J	275	AGM	CE2-CD-CG-CB
1	A	455	SMC	CA-CB-SG-CS
1	D	455	SMC	CA-CB-SG-CS
1	J	455	SMC	CA-CB-SG-CS
1	A	448	GL3	S-C-CA-N
1	G	275	AGM	NE1-CD-CG-CB
1	J	275	AGM	NE1-CD-CG-CB
1	D	275	AGM	NH2-CZ-NE1-CD
1	J	275	AGM	NH2-CZ-NE1-CD
1	D	275	AGM	NH1-CZ-NE1-CD
1	J	275	AGM	NH1-CZ-NE1-CD
1	A	275	AGM	NE1-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	455	SMC	1	0
1	D	455	SMC	1	0
1	G	448	GL3	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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
7	F43	D	1554	1,4	46,71,71	2.65	11 (23%)	48,118,118	1.82	11 (22%)
4	COM	D	1555	7	6,6,6	2.04	2 (33%)	7,8,8	3.57	3 (42%)
6	ACT	J	1557	-	1,3,3	1.31	0	0,3,3	0.00	-
6	ACT	A	1555	-	1,3,3	1.33	0	0,3,3	0.00	-
6	ACT	H	1444	-	1,3,3	2.56	1 (100%)	0,3,3	0.00	-
4	COM	A	1553	7	6,6,6	1.71	2 (33%)	7,8,8	4.55	4 (57%)
5	TP7	J	1556	-	16,20,20	0.86	1 (6%)	18,26,26	1.13	0
6	ACT	K	1444	-	1,3,3	1.35	0	0,3,3	0.00	-
6	ACT	E	1445	-	1,3,3	1.91	0	0,3,3	0.00	-
4	COM	G	1553	7	6,6,6	1.94	2 (33%)	7,8,8	4.28	4 (57%)
6	ACT	D	1557	-	1,3,3	1.35	0	0,3,3	0.00	-
5	TP7	A	1554	-	16,20,20	1.13	1 (6%)	18,26,26	1.02	1 (5%)
6	ACT	F	1265	-	1,3,3	0.81	0	0,3,3	0.00	-
5	TP7	D	1553	-	16,20,20	0.98	1 (6%)	18,26,26	1.52	5 (27%)
5	TP7	J	1553	-	16,20,20	0.87	1 (6%)	18,26,26	1.22	3 (16%)
6	ACT	G	1555	-	1,3,3	2.85	1 (100%)	0,3,3	0.00	-
6	ACT	L	1265	-	1,3,3	0.93	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	F43	G	1554	1,4	46,71,71	2.44	10 (21%)	48,118,118	1.71	12 (25%)
6	ACT	E	1444	-	1,3,3	2.25	1 (100%)	0,3,3	0.00	-
7	F43	J	1554	1,4	46,71,71	2.71	9 (19%)	48,118,118	1.50	8 (16%)
6	ACT	I	1265	-	1,3,3	0.55	0	0,3,3	0.00	-
7	F43	D	1556	1,4	46,71,71	2.44	10 (21%)	48,118,118	1.61	11 (22%)
4	COM	J	1555	7	6,6,6	1.55	2 (33%)	7,8,8	3.09	3 (42%)

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	TP7	J	1556	-	-	2/20/24/24	-
4	COM	D	1555	7	-	0/4/4/4	-
7	F43	D	1554	1,4	-	1/18/185/185	-
4	COM	G	1553	7	-	0/4/4/4	-
5	TP7	A	1554	-	-	1/20/24/24	-
7	F43	G	1554	1,4	-	1/18/185/185	-
7	F43	J	1554	1,4	-	1/18/185/185	-
5	TP7	D	1553	-	-	1/20/24/24	-
7	F43	D	1556	1,4	-	1/18/185/185	-
5	TP7	J	1553	-	-	2/20/24/24	-
4	COM	J	1555	7	-	4/4/4/4	-
4	COM	A	1553	7	-	0/4/4/4	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1556	F43	NI-NA	10.28	2.11	1.89
7	J	1554	F43	NI-NA	9.72	2.10	1.89
7	D	1554	F43	NI-NA	9.60	2.10	1.89
7	D	1554	F43	NI-NB	9.16	2.09	1.89
7	J	1554	F43	NI-NB	8.49	2.07	1.89
7	G	1554	F43	NI-NA	8.49	2.07	1.89
7	J	1554	F43	NI-ND	8.14	2.07	1.89
7	D	1554	F43	NI-ND	7.72	2.06	1.89
7	G	1554	F43	NI-NB	7.72	2.06	1.89
7	D	1556	F43	NI-NB	7.36	2.05	1.89
7	G	1554	F43	NI-ND	7.23	2.05	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1556	F43	NI-ND	6.46	2.03	1.89
7	J	1554	F43	C4C-NC	5.35	1.43	1.35
7	G	1554	F43	CHD-C1D	-4.62	1.37	1.43
7	J	1554	F43	CHB-C1B	3.91	1.56	1.53
5	A	1554	TP7	P-O4P	3.61	1.66	1.59
4	G	1553	COM	O1S-S2	3.46	1.55	1.45
4	D	1555	COM	C2-S2	3.44	1.82	1.77
7	G	1554	F43	C4C-NC	3.27	1.40	1.35
7	G	1554	F43	CHC-C4B	3.20	1.48	1.39
7	D	1556	F43	C6D-C7D	3.12	1.54	1.50
7	J	1554	F43	CHC-C4B	3.09	1.48	1.39
7	D	1554	F43	CHB-C1B	3.01	1.55	1.53
4	A	1553	COM	O2S-S2	2.91	1.53	1.45
6	G	1555	ACT	CH3-C	2.85	1.52	1.48
7	D	1554	F43	O8D-C7D	2.84	1.28	1.23
7	D	1556	F43	CHD-C1D	-2.80	1.39	1.43
7	G	1554	F43	C6D-C7D	2.78	1.54	1.50
7	D	1554	F43	CHC-C4B	2.78	1.47	1.39
4	J	1555	COM	O1S-S2	2.76	1.53	1.45
7	J	1554	F43	CHD-C1D	-2.72	1.39	1.43
4	D	1555	COM	O2S-S2	2.68	1.52	1.45
7	J	1554	F43	C3A-C4A	2.67	1.58	1.53
5	D	1553	TP7	P-O4P	2.67	1.64	1.59
7	D	1554	F43	C6D-C7D	2.66	1.54	1.50
7	D	1556	F43	CHC-C4B	2.58	1.46	1.39
6	H	1444	ACT	CH3-C	2.56	1.52	1.48
7	D	1556	F43	C4C-NC	2.46	1.39	1.35
4	G	1553	COM	O2S-S2	2.42	1.52	1.45
7	D	1554	F43	C4C-NC	2.38	1.39	1.35
7	G	1554	F43	CHD-C4C	-2.38	1.33	1.40
5	J	1556	TP7	P-O4P	2.27	1.63	1.59
6	E	1444	ACT	CH3-C	2.25	1.51	1.48
7	D	1554	F43	C4A-NA	2.23	1.52	1.49
7	D	1554	F43	CHD-C4C	-2.23	1.34	1.40
7	G	1554	F43	CAA-C3A	2.23	1.57	1.53
7	D	1556	F43	O8D-C7D	2.22	1.27	1.23
5	J	1553	TP7	P-O4P	2.22	1.63	1.59
4	A	1553	COM	C2-S2	2.17	1.80	1.77
4	J	1555	COM	C2-S2	2.15	1.80	1.77
7	D	1554	F43	C6A-N8A	-2.12	1.25	1.32
7	J	1554	F43	CHD-C4C	-2.08	1.34	1.40
7	D	1556	F43	C6A-N8A	-2.02	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1554	F43	O8D-C7D	2.02	1.27	1.23
7	D	1556	F43	CAA-C3A	2.01	1.57	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1553	COM	O2S-S2-C2	8.99	117.74	106.92
4	A	1553	COM	O2S-S2-C2	8.87	117.60	106.92
4	A	1553	COM	O3S-S2-O2S	-6.62	95.11	111.27
4	D	1555	COM	O2S-S2-C2	6.54	114.80	106.92
4	J	1555	COM	O2S-S2-C2	5.31	113.31	106.92
4	G	1553	COM	O2S-S2-O1S	-5.24	95.80	113.95
7	D	1554	F43	C3A-C4A-NA	-5.24	94.33	102.30
4	D	1555	COM	O3S-S2-C2	5.23	114.23	105.77
4	J	1555	COM	O3S-S2-C2	4.38	112.84	105.77
7	D	1554	F43	C4D-ND-C1D	4.21	114.05	108.51
7	G	1554	F43	C4D-ND-C1D	4.08	113.87	108.51
7	G	1554	F43	C9A-C2A-C3A	3.98	118.86	112.98
4	J	1555	COM	O3S-S2-O1S	-3.93	101.67	111.27
7	D	1554	F43	C9A-C2A-C3A	3.83	118.63	112.98
7	G	1554	F43	O8D-C7D-C6D	-3.71	114.79	120.86
4	D	1555	COM	O3S-S2-O2S	-3.69	102.26	111.27
4	A	1553	COM	O3S-S2-C2	3.63	111.64	105.77
7	J	1554	F43	C4D-ND-C1D	3.58	113.23	108.51
7	J	1554	F43	C9A-C2A-C3A	3.50	118.14	112.98
5	D	1553	TP7	C5-C6-C7	-3.47	106.91	113.09
7	D	1556	F43	C4D-ND-C1D	3.42	113.01	108.51
7	D	1556	F43	C2B-C1B-NB	3.40	106.93	101.84
7	G	1554	F43	C9B-C2B-C8B	-3.28	102.16	110.45
7	D	1556	F43	O8D-C7D-C6D	-3.27	115.50	120.86
7	J	1554	F43	C3A-C4A-NA	-3.27	97.33	102.30
4	G	1553	COM	O1S-S2-C2	3.22	110.80	106.92
7	G	1554	F43	C3A-C4A-NA	-3.19	97.45	102.30
7	D	1554	F43	C2B-C1B-NB	3.18	106.59	101.84
7	G	1554	F43	CAB-C3B-C2B	-3.14	112.45	119.09
7	D	1556	F43	O7B-C6B-C8B	-3.03	122.89	126.59
7	D	1554	F43	O8D-C7D-C6D	-2.93	116.06	120.86
7	J	1554	F43	O8D-C7D-C6D	-2.91	116.09	120.86
7	D	1556	F43	C9B-C2B-C8B	-2.70	103.62	110.45
7	D	1554	F43	CAB-C3B-C2B	-2.64	113.49	119.09
4	G	1553	COM	O3S-S2-O1S	2.63	117.71	111.27
5	J	1553	TP7	C3-C2-C1	-2.62	105.90	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	1554	F43	CAB-C3B-C2B	-2.60	113.58	119.09
7	D	1556	F43	C3A-C4A-NA	-2.58	98.37	102.30
7	D	1556	F43	C9D-C3D-C4D	-2.57	107.89	114.67
7	G	1554	F43	C9D-C3D-C4D	-2.44	108.23	114.67
7	D	1554	F43	CAA-CBA-CCA	2.44	118.83	113.59
7	D	1556	F43	C5C-C2C-C3C	-2.34	108.94	114.94
7	G	1554	F43	C2B-C1B-NB	2.32	105.31	101.84
5	D	1553	TP7	P-O4P-CB	-2.32	116.21	123.21
7	D	1554	F43	O7B-C6B-C8B	-2.31	123.77	126.59
5	J	1553	TP7	O3P-P-O1P	2.31	119.72	110.68
7	D	1554	F43	C9A-C2A-C5A	-2.30	107.02	110.80
5	A	1554	TP7	C5-C6-C7	-2.24	109.10	113.09
7	J	1554	F43	C6D-C7D-CHD	2.22	121.12	116.95
7	D	1554	F43	C9D-C3D-C4D	-2.18	108.92	114.67
5	D	1553	TP7	O3P-P-O2P	2.17	115.95	107.64
7	D	1554	F43	C5C-C2C-C3C	-2.17	109.37	114.94
5	J	1553	TP7	CG-CB-CA	2.17	117.46	113.17
7	D	1556	F43	C6D-C7D-CHD	2.16	121.01	116.95
7	D	1556	F43	C9B-C2B-C1B	2.16	117.62	113.47
5	D	1553	TP7	C3-C2-C1	-2.11	107.35	113.26
7	G	1554	F43	O7B-C6B-C8B	-2.10	124.03	126.59
7	J	1554	F43	C8C-C3C-C2C	-2.10	107.09	112.89
5	D	1553	TP7	O4P-P-O1P	-2.07	101.39	109.39
7	G	1554	F43	C9B-C2B-C3B	2.07	118.25	112.96
7	D	1556	F43	O7A-C6A-N8A	-2.06	116.88	122.50
7	J	1554	F43	C9B-C2B-C8B	-2.06	105.25	110.45
7	G	1554	F43	C9A-C2A-C5A	-2.04	107.44	110.80
4	A	1553	COM	O1S-S2-C2	2.03	109.36	106.92
7	G	1554	F43	C8C-C3C-C2C	-2.02	107.29	112.89

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1553	TP7	CB-O4P-P-O2P
5	J	1553	TP7	CB-O4P-P-O3P
4	J	1555	COM	S1-C1-C2-S2
4	J	1555	COM	C1-C2-S2-O1S
4	J	1555	COM	C1-C2-S2-O2S
4	J	1555	COM	C1-C2-S2-O3S
7	D	1556	F43	C3A-CAA-CBA-CCA
7	J	1554	F43	C3A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
7	D	1554	F43	C3A-CAA-CBA-CCA
7	G	1554	F43	C3A-CAA-CBA-CCA
5	J	1553	TP7	C2-C3-C4-C5
5	J	1556	TP7	C2-C3-C4-C5
5	J	1556	TP7	C4-C5-C6-C7
5	A	1554	TP7	CB-O4P-P-O3P

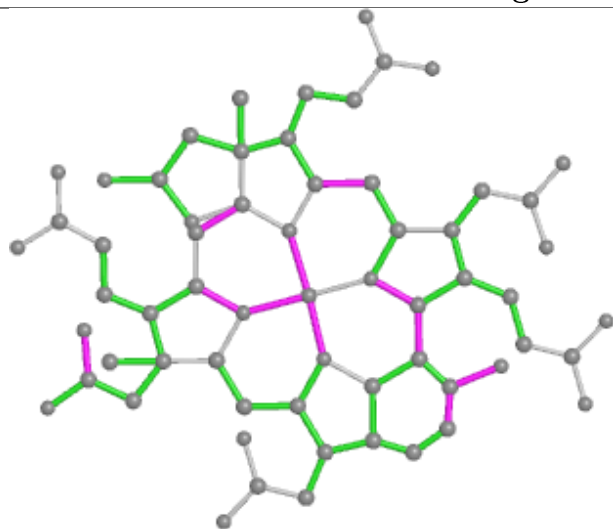
There are no ring outliers.

8 monomers are involved in 13 short contacts:

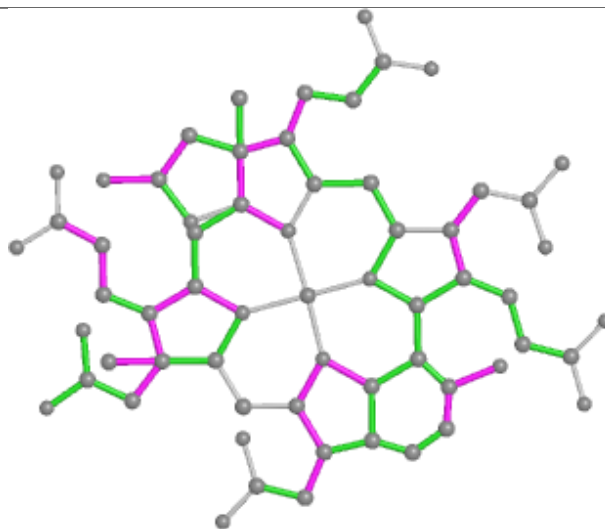
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1554	F43	3	0
4	A	1553	COM	1	0
6	E	1445	ACT	1	0
4	G	1553	COM	1	0
7	G	1554	F43	2	0
7	J	1554	F43	1	0
7	D	1556	F43	3	0
4	J	1555	COM	1	0

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 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.

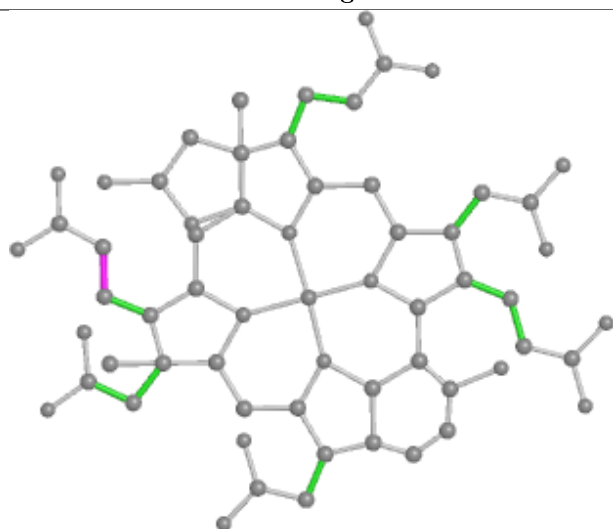
Ligand F43 D 1554



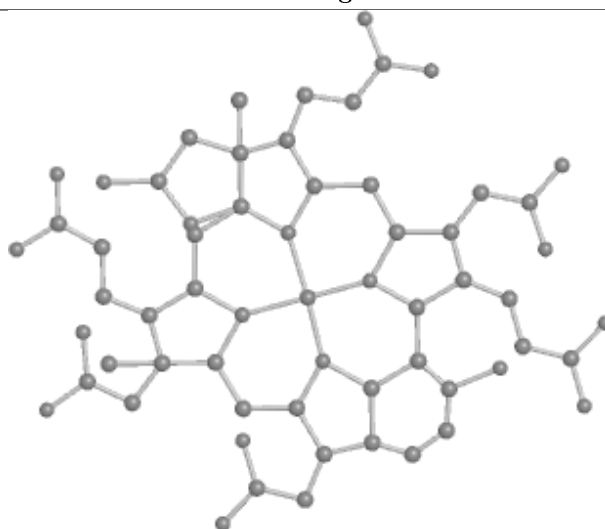
Bond lengths



Bond angles

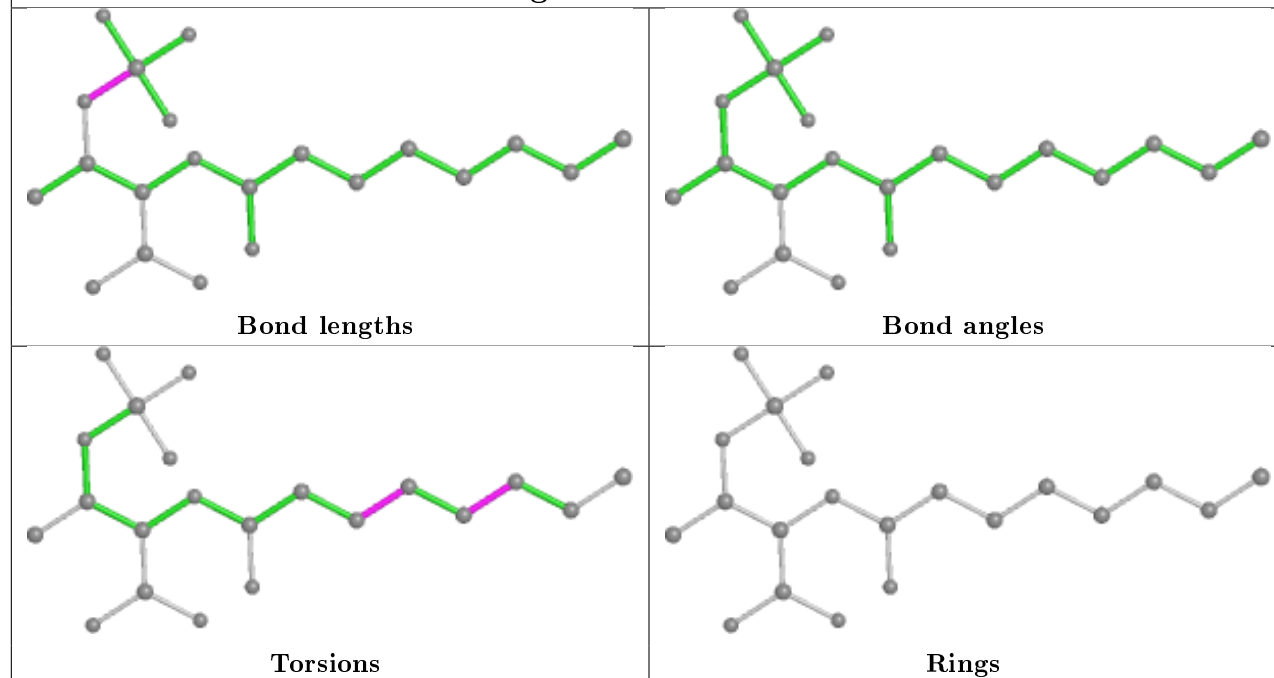


Torsions

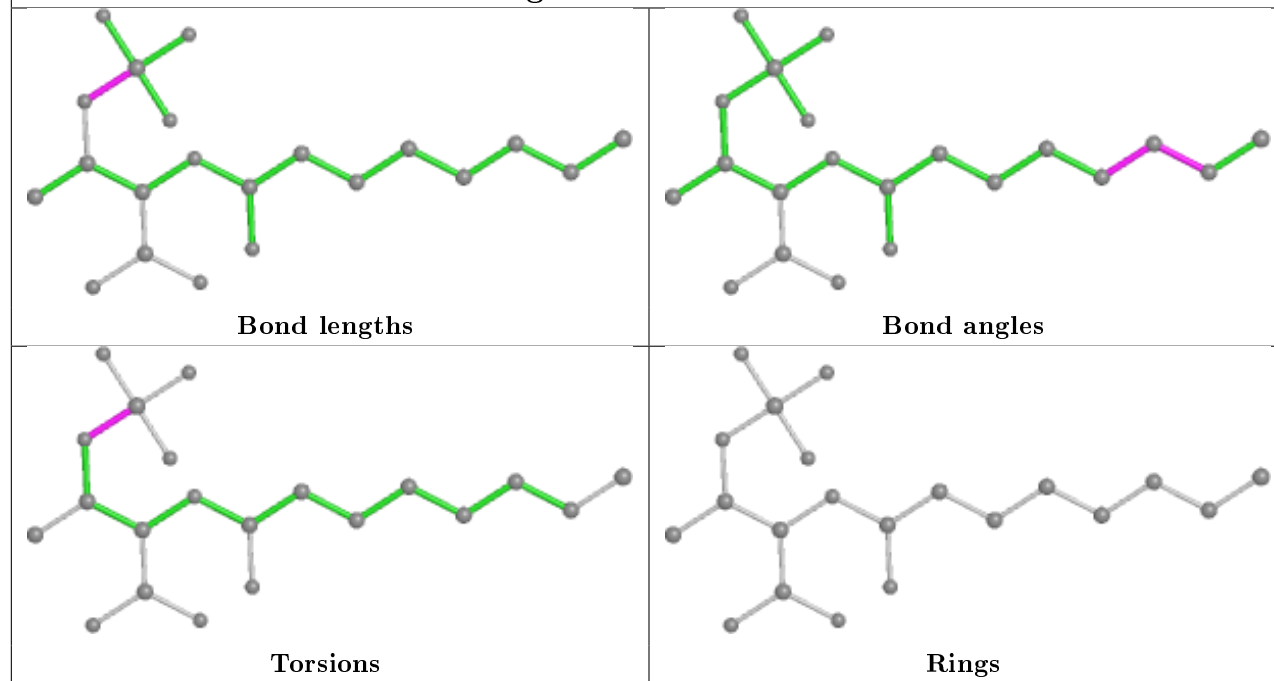


Rings

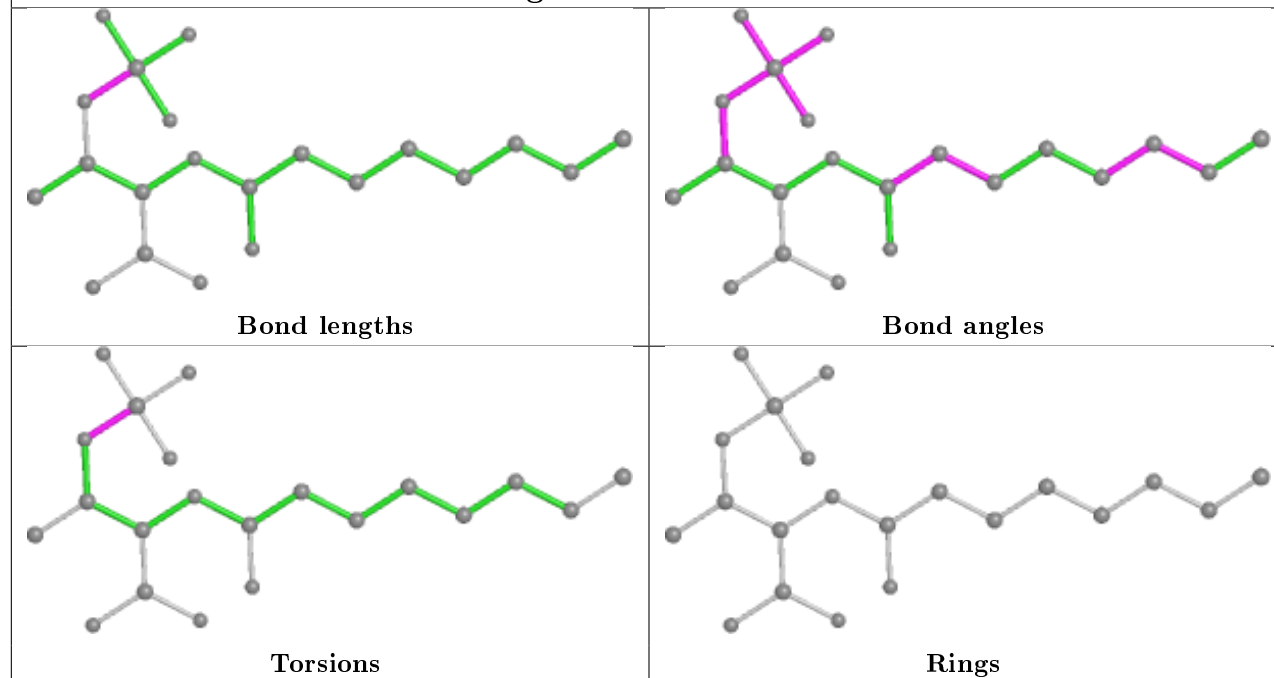
Ligand TP7 J 1556



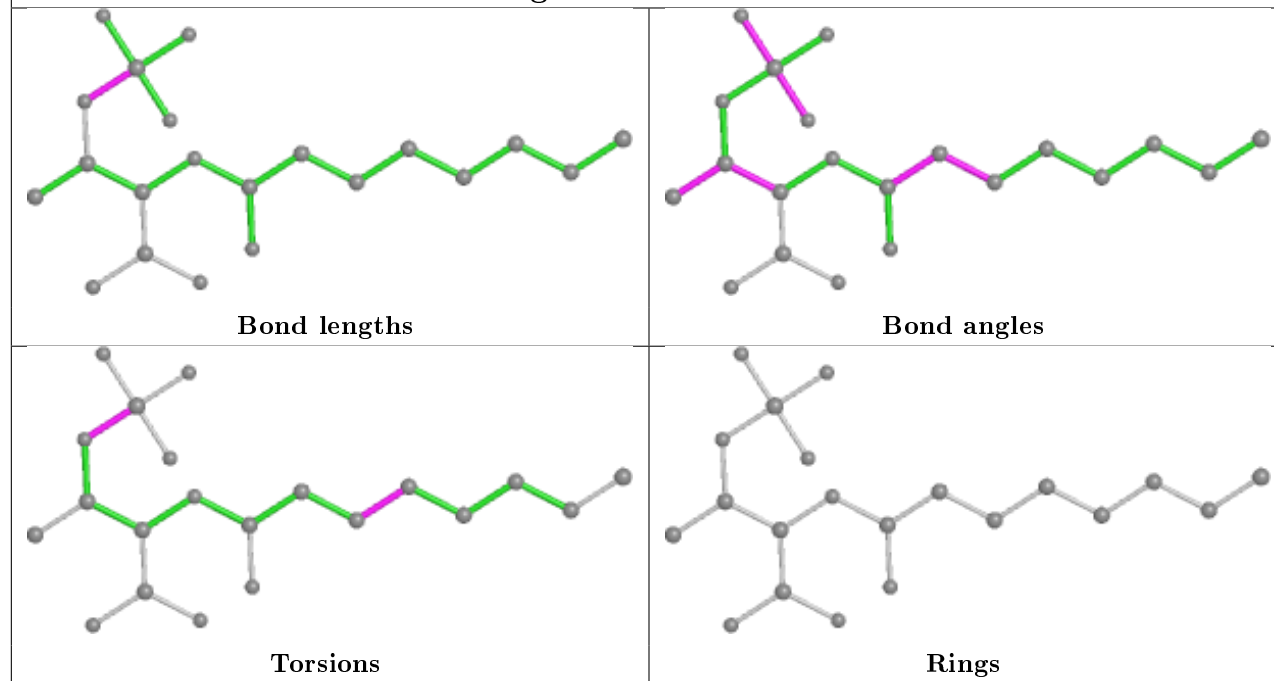
Ligand TP7 A 1554



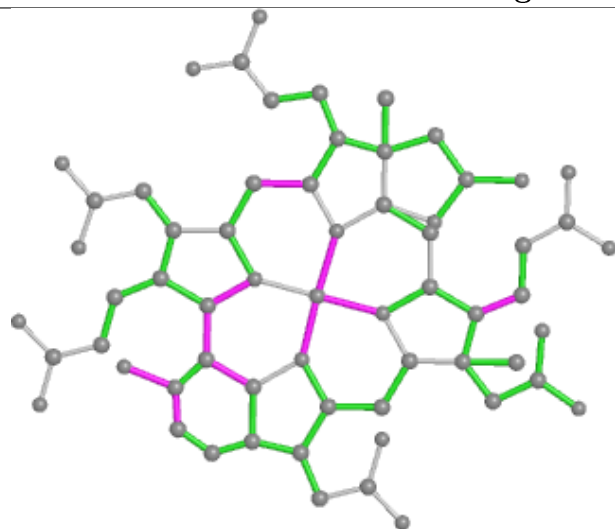
Ligand TP7 D 1553



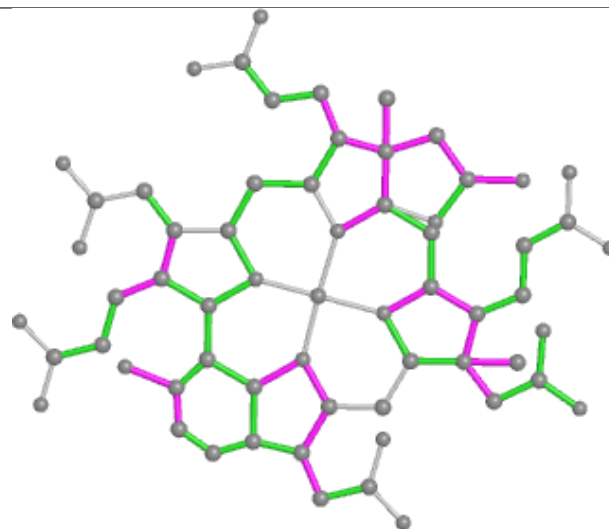
Ligand TP7 J 1553



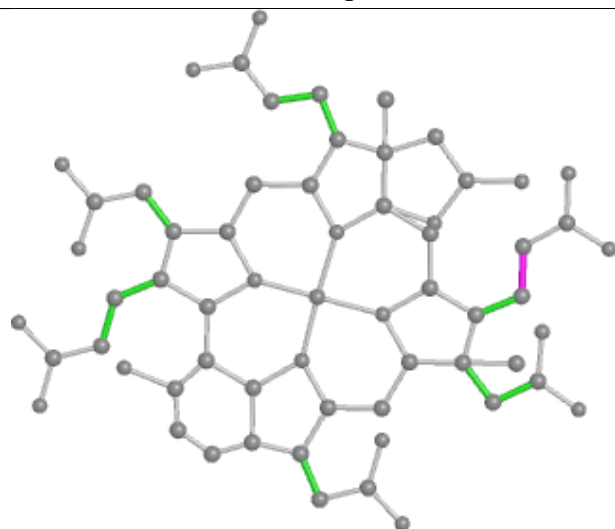
Ligand F43 G 1554



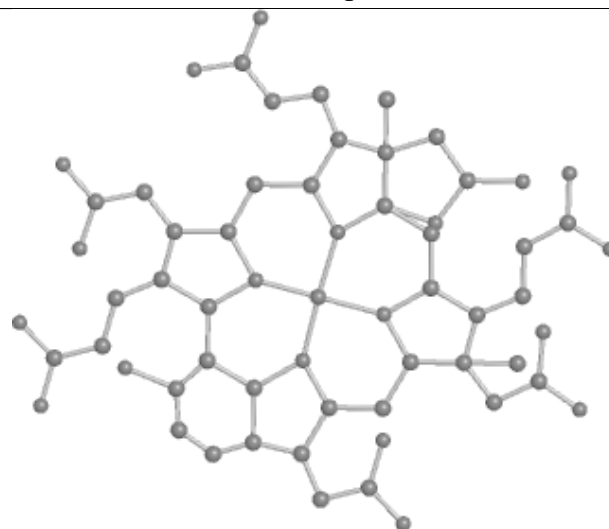
Bond lengths



Bond angles

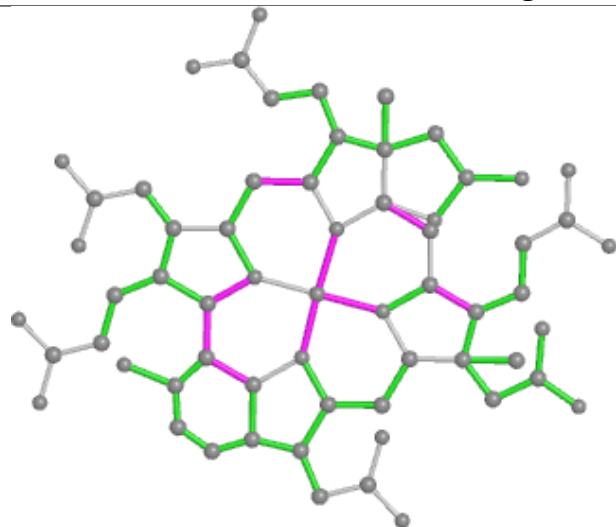


Torsions

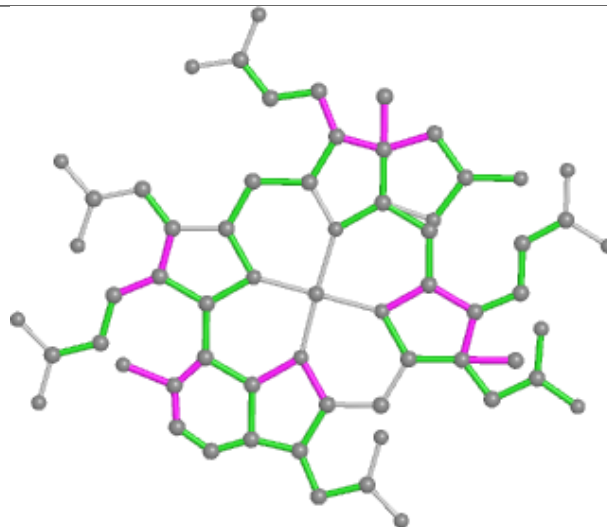


Rings

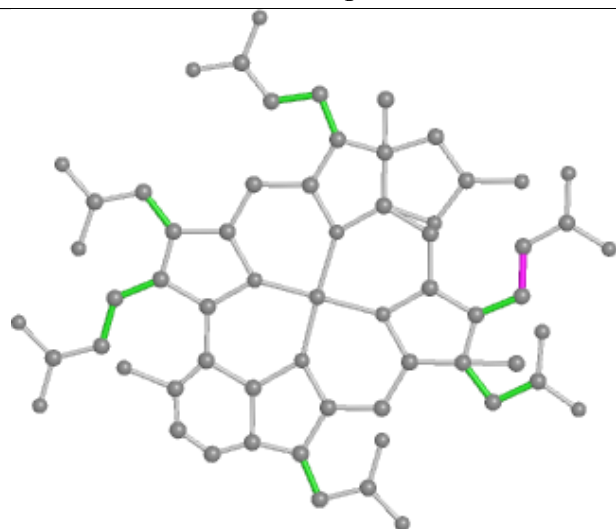
Ligand F43 J 1554



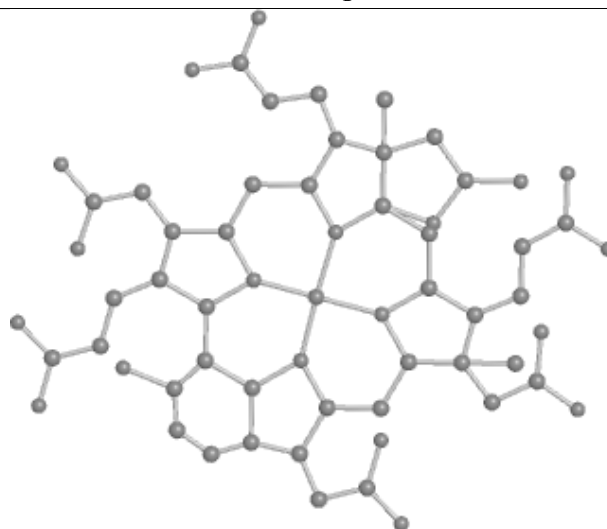
Bond lengths



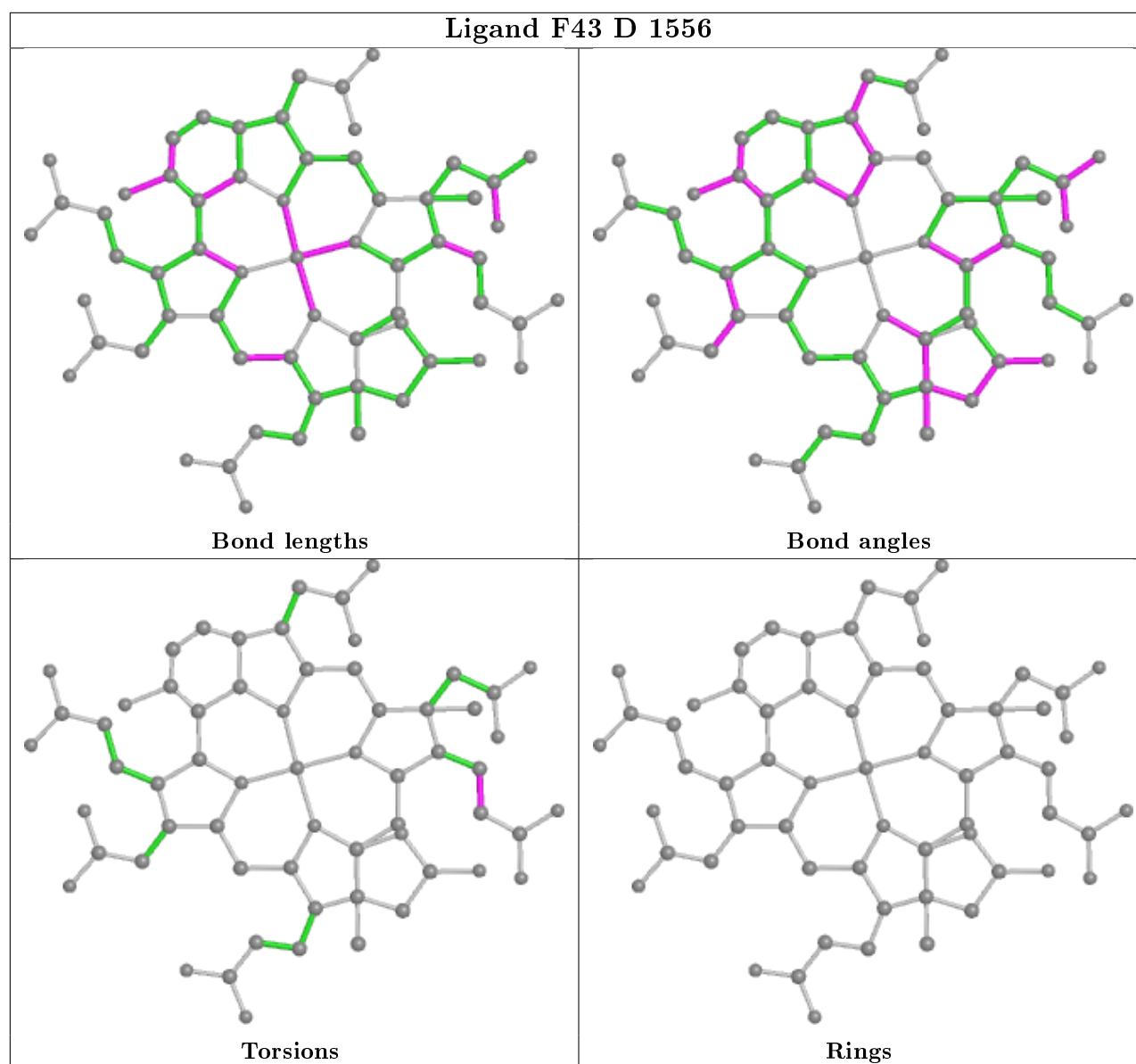
Bond angles



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, 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	543/554 (98%)	-0.03	5 (0%) 84 82	9, 14, 30, 44	1 (0%)
1	D	544/554 (98%)	-0.06	6 (1%) 80 78	8, 15, 30, 59	0
1	G	543/554 (98%)	-0.06	2 (0%) 92 90	8, 14, 29, 42	0
1	J	543/554 (98%)	-0.07	5 (0%) 84 82	9, 15, 30, 43	0
2	B	442/443 (99%)	-0.03	7 (1%) 72 68	9, 15, 29, 52	0
2	E	442/443 (99%)	-0.03	5 (1%) 80 78	9, 15, 29, 56	1 (0%)
2	H	442/443 (99%)	0.01	6 (1%) 75 72	10, 15, 29, 56	0
2	K	442/443 (99%)	0.02	4 (0%) 84 82	10, 15, 30, 52	0
3	C	263/265 (99%)	-0.00	5 (1%) 66 63	9, 17, 35, 66	0
3	F	263/265 (99%)	-0.05	5 (1%) 66 63	9, 16, 34, 56	0
3	I	263/265 (99%)	-0.07	5 (1%) 66 63	9, 17, 35, 59	0
3	L	263/265 (99%)	0.01	7 (2%) 54 49	9, 17, 35, 62	0
All	All	4993/5048 (98%)	-0.03	62 (1%) 79 76	8, 15, 31, 66	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	552	ALA	7.5
3	L	64	PHE	7.3
3	F	64	PHE	6.0
3	C	64	PHE	5.9
3	I	64	PHE	4.7
3	C	183	GLU	4.5
3	L	264	ASP	4.3
1	G	552	ALA	4.2
1	J	552	ALA	4.2
2	B	98	ASP	4.1
1	A	552	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	443	LEU	3.9
3	I	183	GLU	3.7
3	F	264	ASP	3.7
2	B	443	LEU	3.6
2	E	98	ASP	3.5
2	H	442	GLN	3.4
3	L	183	GLU	3.2
3	F	183	GLU	3.2
2	K	98	ASP	3.1
2	H	443	LEU	3.1
2	H	98	ASP	3.0
3	I	264	ASP	3.0
1	D	5	LYS	2.9
3	C	264	ASP	2.8
2	E	442	GLN	2.8
3	F	65	GLU	2.8
2	B	357	VAL	2.8
3	C	65	GLU	2.7
2	H	441	ASP	2.6
1	J	190	LYS	2.6
2	E	424	TYR	2.5
3	L	210	GLU	2.5
2	E	441	ASP	2.5
1	D	451	LEU	2.4
2	B	442	GLN	2.4
1	A	5	LYS	2.3
2	K	2	PRO	2.3
2	B	434	LYS	2.3
3	L	167	GLU	2.3
2	B	441	ASP	2.3
3	L	63	ASP	2.2
3	I	199	ASP	2.2
2	K	184	LEU	2.2
3	I	167	GLU	2.2
1	A	45	GLU	2.2
3	F	63	ASP	2.2
2	K	443	LEU	2.2
1	D	301	ASP	2.2
3	C	199	ASP	2.2
2	H	277	GLU	2.1
1	J	18	GLY	2.1
1	J	49	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	247	ALA	2.1
2	H	424	TYR	2.1
2	B	409	GLU	2.1
3	L	263	GLY	2.1
1	D	190	LYS	2.1
1	A	48	LYS	2.0
1	A	247	ALA	2.0
1	D	52	GLU	2.0
1	J	5	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	AGM	J	275	12/13	0.93	0.15	6,13,18,18	0
1	AGM	D	275	12/13	0.94	0.14	8,11,14,18	0
1	AGM	G	275	12/13	0.94	0.15	10,13,14,14	0
1	MHS	G	261	11/12	0.94	0.11	11,16,22,23	0
1	MHS	D	261	11/12	0.94	0.10	15,17,20,20	0
1	MHS	J	261	11/12	0.95	0.11	11,16,21,24	0
1	MHS	A	261	11/12	0.95	0.09	13,17,21,21	0
1	AGM	A	275	12/13	0.95	0.15	8,10,14,16	0
1	SMC	J	455	7/8	0.97	0.14	12,12,14,15	0
1	MGN	G	403	10/11	0.97	0.11	7,8,11,12	0
1	MGN	A	403	10/11	0.97	0.12	7,8,12,13	0
1	SMC	A	455	7/8	0.98	0.13	10,13,16,17	0
1	SMC	D	455	7/8	0.98	0.14	11,13,13,13	0
1	MGN	J	403	10/11	0.98	0.12	7,9,11,13	0
1	MGN	D	403	10/11	0.98	0.10	6,9,12,12	0
1	SMC	G	455	7/8	0.98	0.12	9,10,14,14	0
1	GL3	J	448	4/5	0.99	0.10	8,10,10,11	0
1	GL3	G	448	4/5	0.99	0.10	8,9,11,13	0
1	GL3	A	448	4/5	0.99	0.11	9,10,10,13	0
1	GL3	D	448	4/5	0.99	0.08	6,7,10,11	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

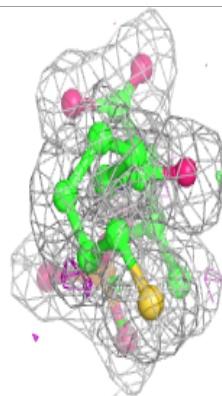
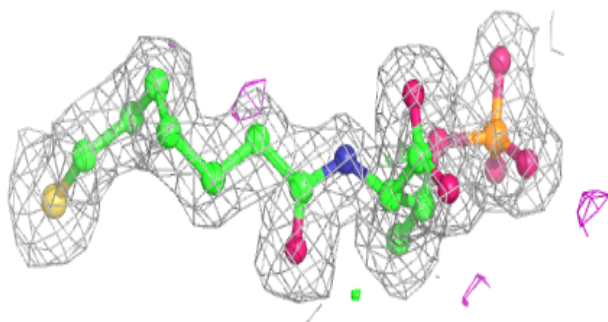
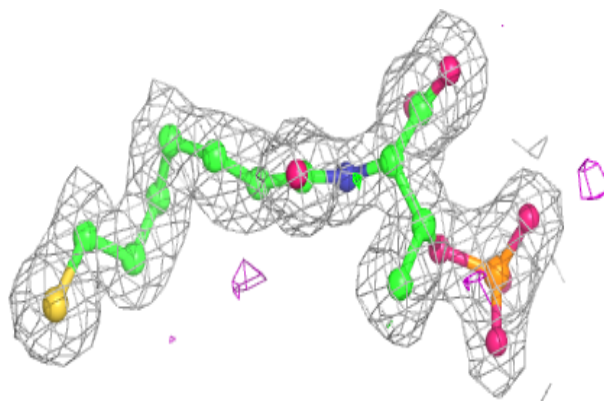
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ACT	G	1555	4/4	0.67	0.24	30,32,35,35	0
6	ACT	E	1444	4/4	0.69	0.21	48,51,52,52	0
6	ACT	E	1445	4/4	0.76	0.21	39,41,43,47	0
6	ACT	A	1555	4/4	0.80	0.20	34,37,38,39	0
6	ACT	F	1265	4/4	0.80	0.18	27,33,34,34	0
6	ACT	L	1265	4/4	0.81	0.19	31,37,37,39	0
6	ACT	K	1444	4/4	0.81	0.21	44,46,47,48	0
6	ACT	H	1444	4/4	0.84	0.27	35,36,38,42	0
6	ACT	I	1265	4/4	0.88	0.13	31,38,38,38	0
6	ACT	D	1557	4/4	0.90	0.19	38,39,40,41	0
6	ACT	J	1557	4/4	0.91	0.19	35,39,41,42	0
4	COM	D	1555	7/7	0.94	0.19	4,10,13,20	7
4	COM	G	1553	7/7	0.95	0.21	5,9,14,17	7
5	TP7	J	1553	21/21	0.95	0.12	9,14,20,21	0
8	NA	F	1270	1/1	0.95	0.09	37,37,37,37	0
4	COM	A	1553	7/7	0.95	0.19	8,13,18,20	7
4	COM	J	1555	7/7	0.95	0.16	8,11,18,23	7
5	TP7	J	1556	21/21	0.96	0.11	10,15,20,20	0
5	TP7	D	1553	21/21	0.96	0.12	10,15,18,20	0
5	TP7	A	1554	21/21	0.96	0.13	9,15,21,21	0
7	F43	J	1554	62/62	0.97	0.11	3,11,16,19	0
7	F43	D	1554	62/62	0.97	0.11	1,9,16,18	0
7	F43	D	1556	62/62	0.97	0.13	3,10,17,19	0
7	F43	G	1554	62/62	0.97	0.11	4,10,16,18	0

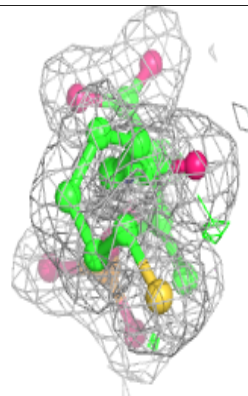
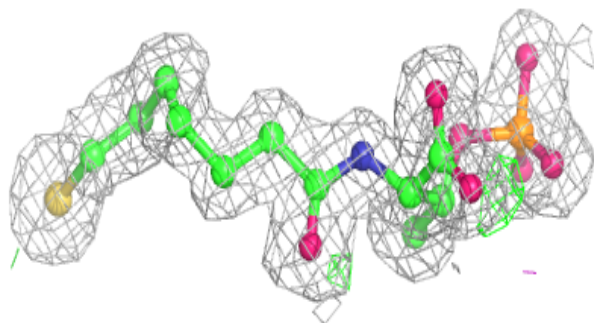
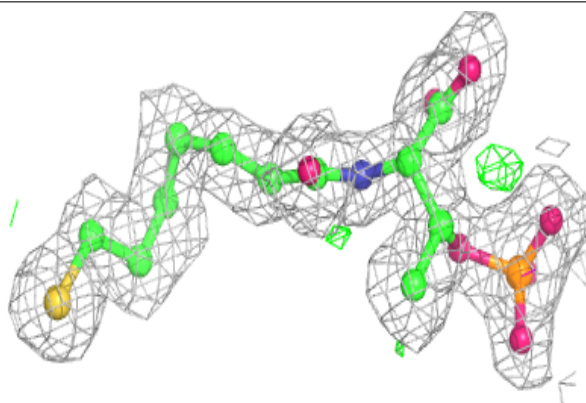
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TP7 J 1553:

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

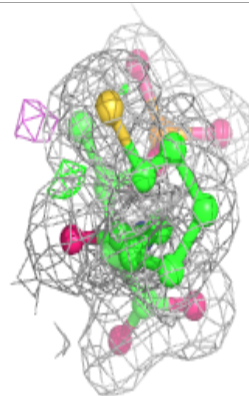
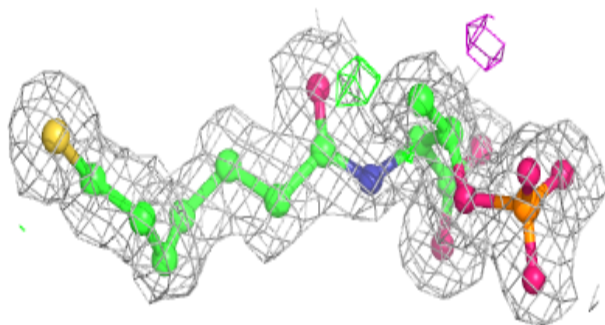
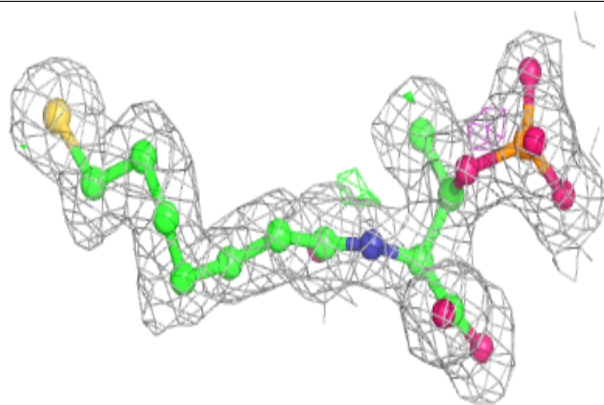
**Electron density around TP7 J 1556:**

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

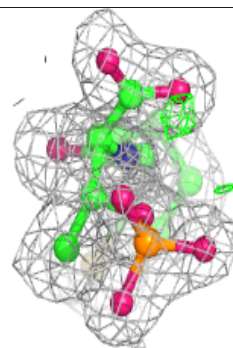
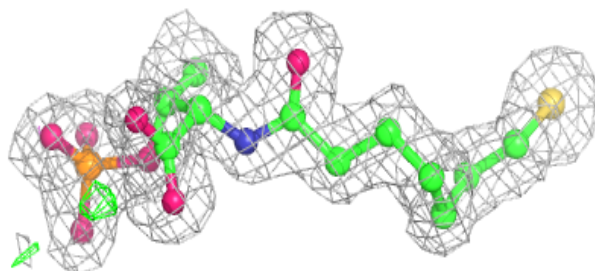
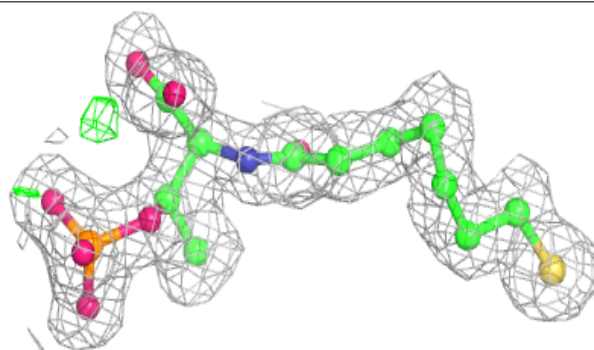


Electron density around TP7 D 1553:

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

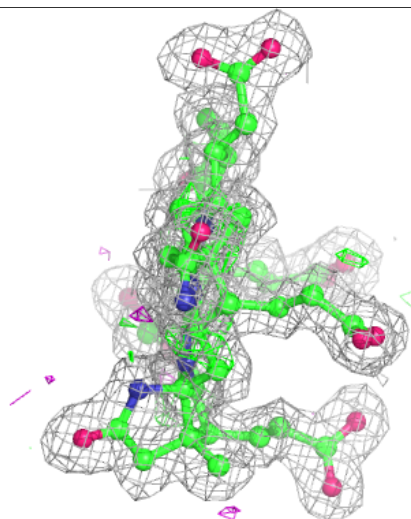
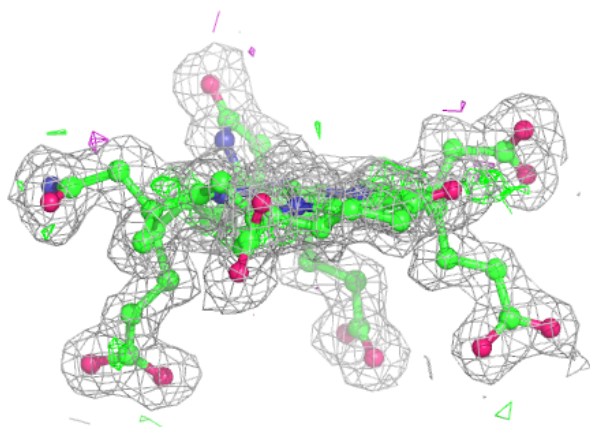
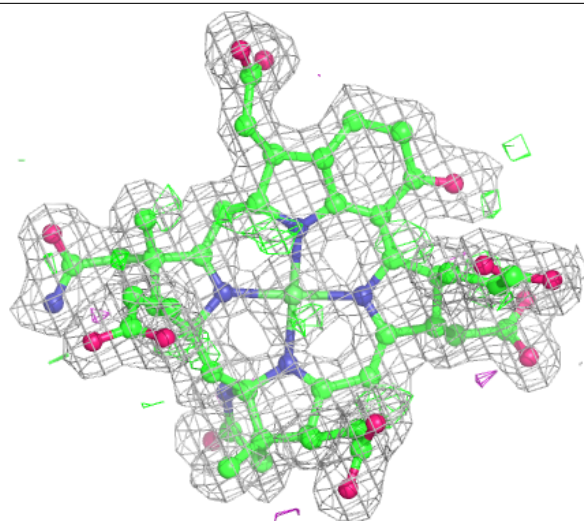
**Electron density around TP7 A 1554:**

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



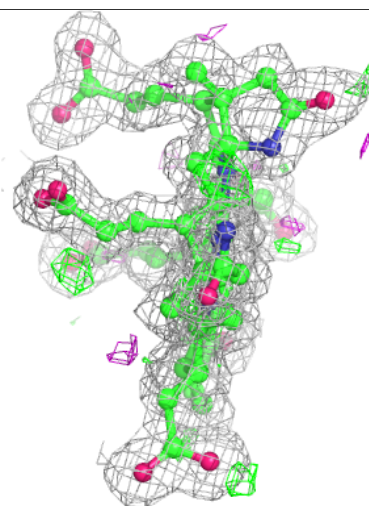
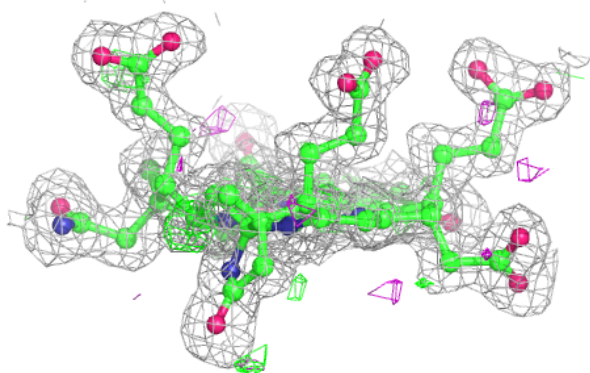
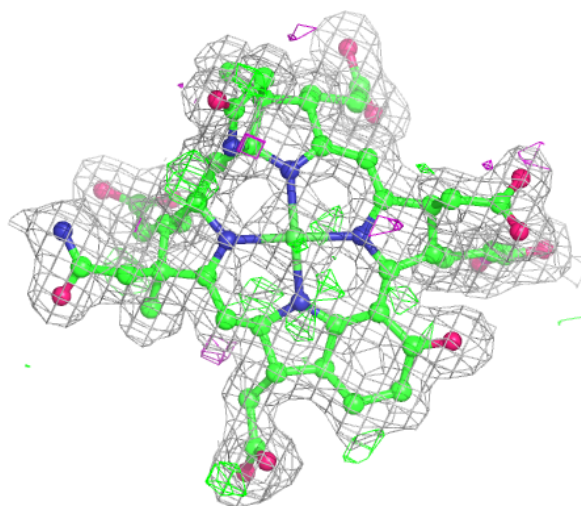
Electron density around F43 J 1554:

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



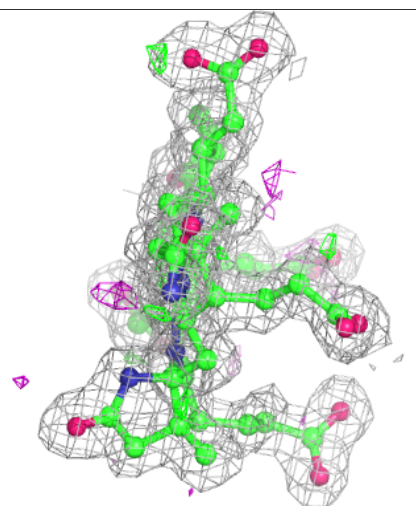
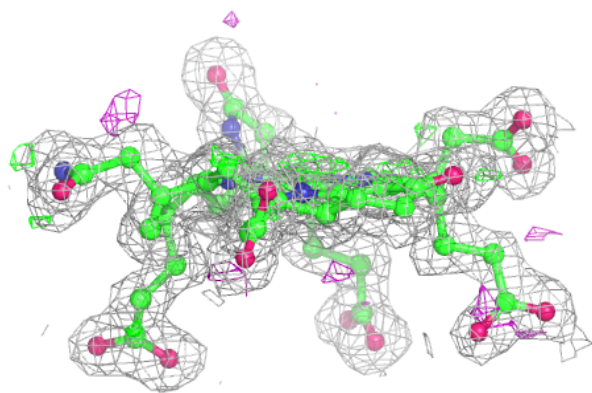
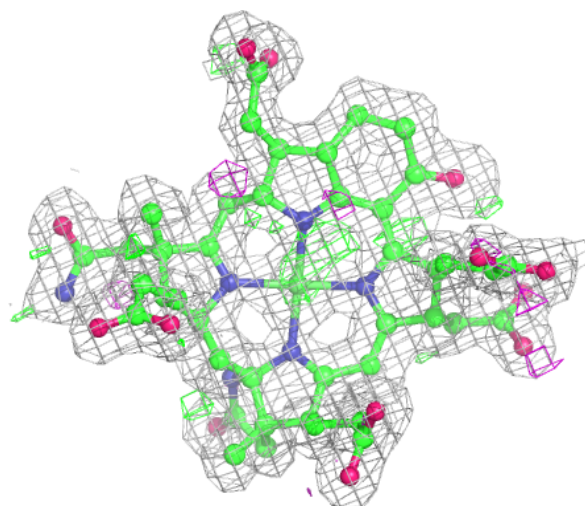
Electron density around F43 D 1554:

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



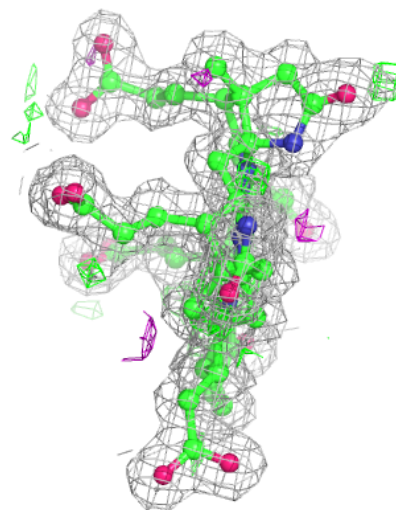
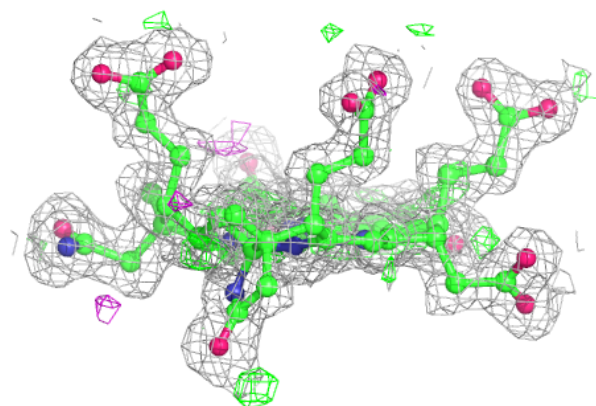
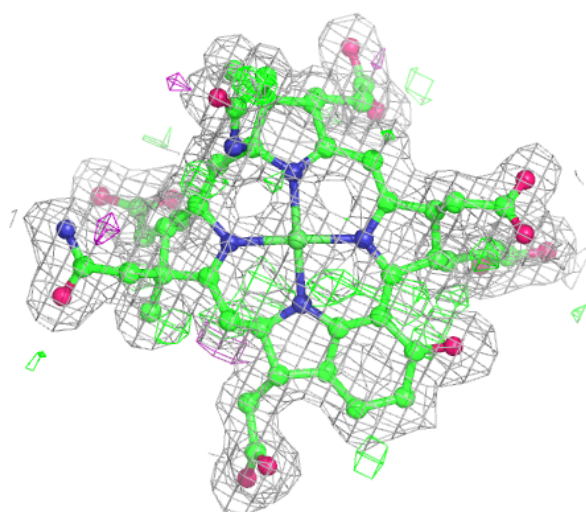
Electron density around F43 D 1556:

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



Electron density around F43 G 1554:

$2mF_o-DF_c$ (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.