



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 12:37 PM EDT

PDB ID : 3M2V
Title : Structural Insight into Methyl-Coenzyme M Reductase Chemistry using Coenzyme B Analogues
Authors : Cedervall, P.E.; Dey, M.; Ragsdale, S.W.; Wilmot, C.M.
Deposited on : 2010-03-08
Resolution : 1.80 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 types of validation reports are described at

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

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

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

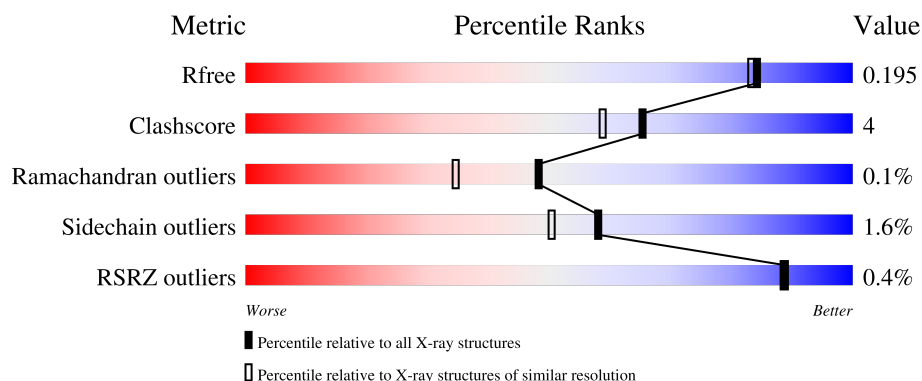
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	<div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> <div style="width: 1%;"></div> </div> <div>91% 8% .</div>
1	D	549	<div> <div style="width: 89%;"></div> <div style="width: 11%;"></div> <div style="width: 0%;"></div> </div> <div>89% 11% .</div>
2	B	442	<div> <div style="width: 89%;"></div> <div style="width: 9%;"></div> <div style="width: 2%;"></div> </div> <div>89% 9% .</div>
2	E	442	<div> <div style="width: 91%;"></div> <div style="width: 9%;"></div> <div style="width: 0%;"></div> </div> <div>91% 9%</div>
3	C	248	<div> <div style="width: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div> <div>87% 12% .</div>

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Mol	Chain	Length	Quality of chain
3	F	248	<div><div></div><div>2%</div><div>87%</div><div>11%</div><div></div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Methyl-coenzyme M reductase I subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	23	0
			4408	2785	731	871	21			
1	D	548	Total	C	N	O	S	0	19	0
			4359	2767	721	851	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	18	0
			3422	2177	559	664	22			
2	E	442	Total	C	N	O	S	0	19	0
			3431	2182	563	665	21			

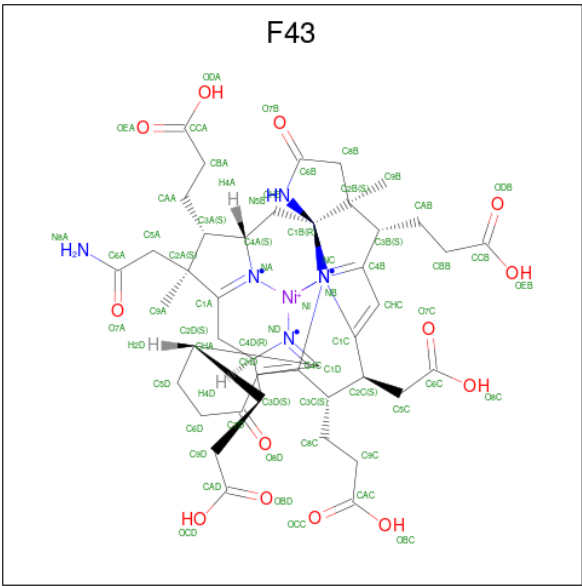
- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	8	0
			2059	1273	362	412	12			
3	F	247	Total	C	N	O	S	0	11	0
			2071	1280	367	412	12			

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

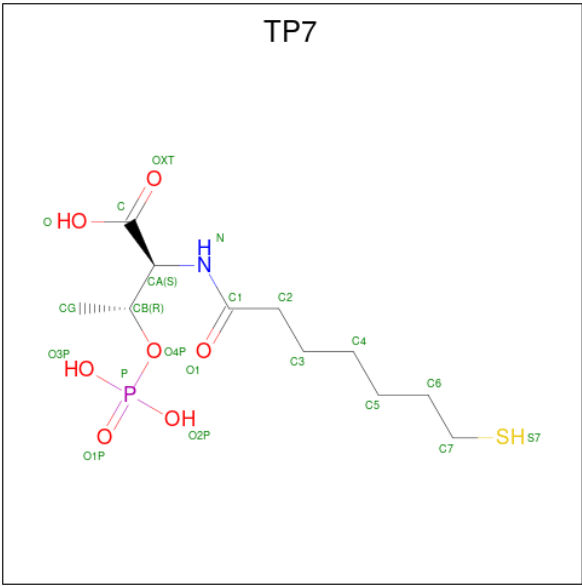
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

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



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

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



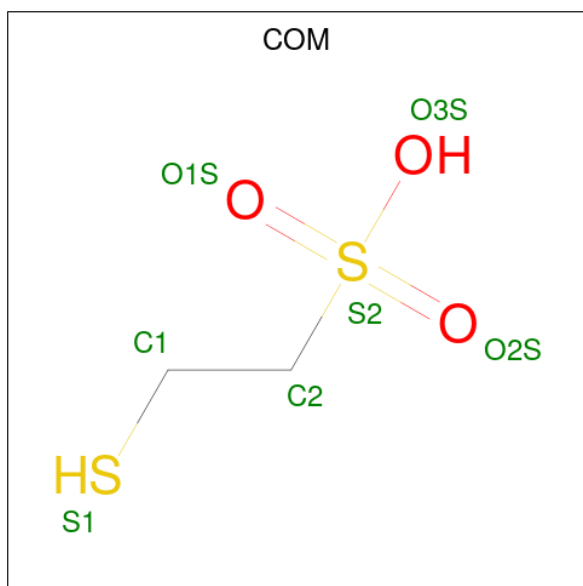
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

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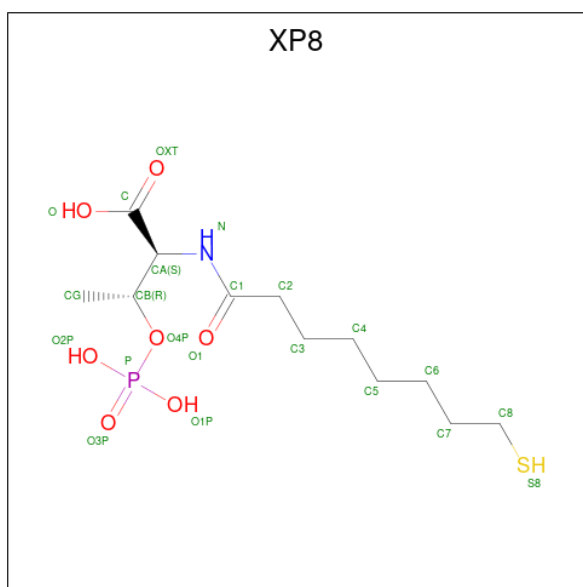
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

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



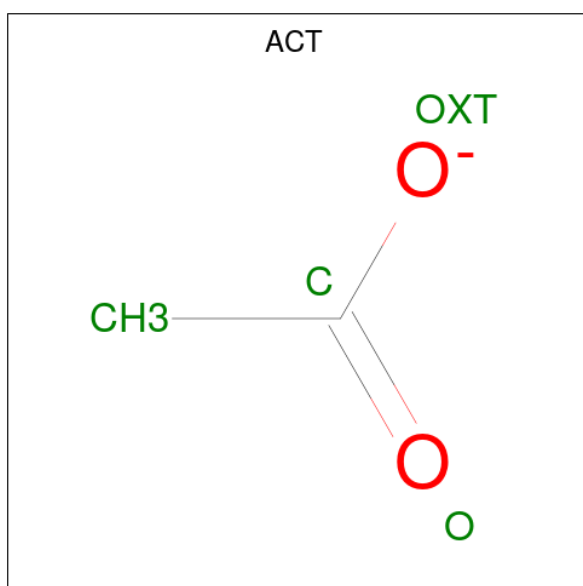
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	2	3	2		
7	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 8 is O-phosphono-N-(8-sulfanyloctanoyl)-L-threonine (three-letter code: XP8) (formula: $C_{12}H_{24}NO_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			22	12	1	7	1	1		
8	D	1	Total	C	N	O	P	S	0	1
			22	12	1	7	1	1		

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



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

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



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

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

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	427	Total	O	0	15
			435	435		
12	B	345	Total	O	0	5
			349	349		
12	C	200	Total	O	0	8
			201	201		
12	D	415	Total	O	0	9
			421	421		

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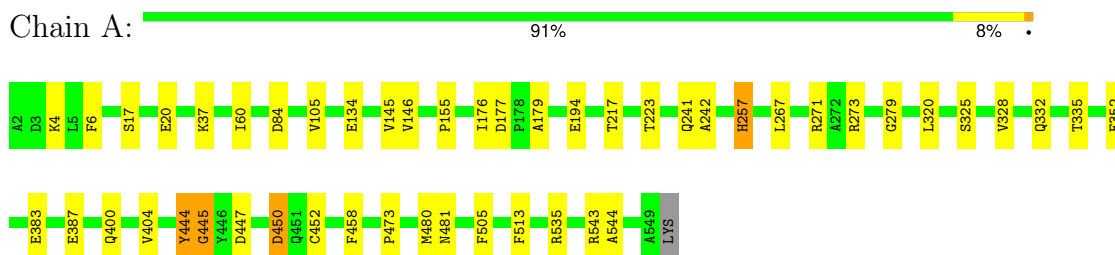
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	312	Total 314	O 314	0	6
12	F	172	Total 173	O 173	0	6

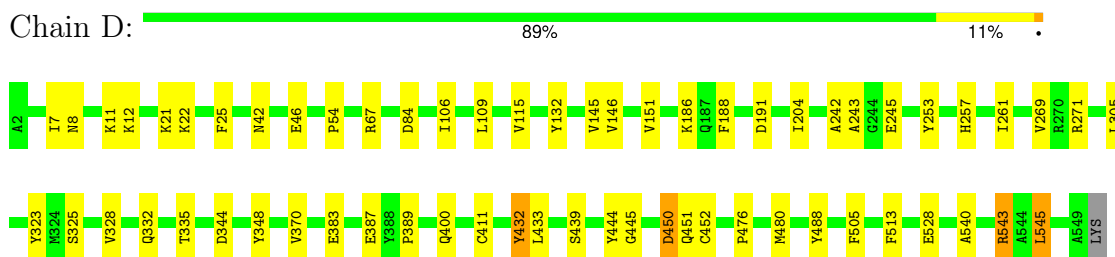
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

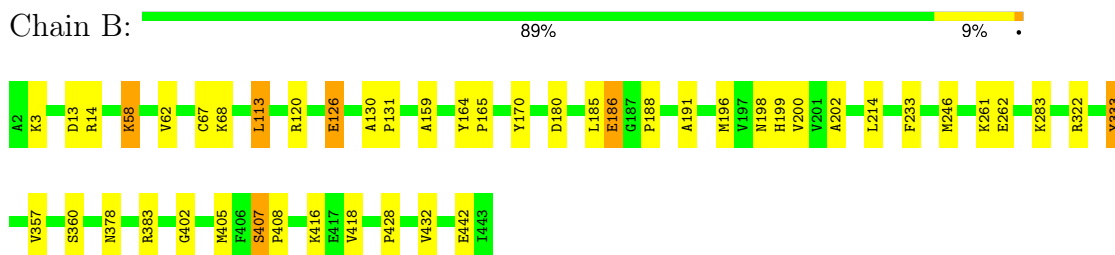
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



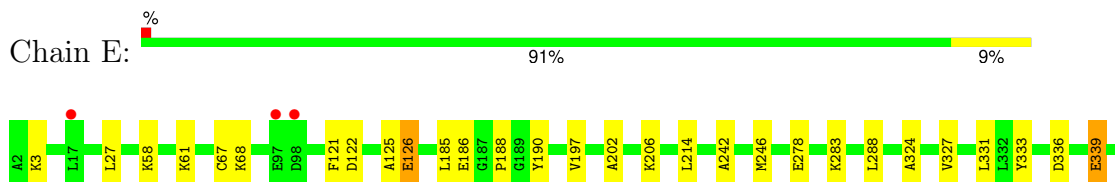
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

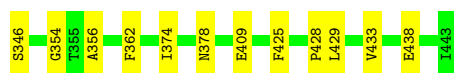


- Molecule 2: Methyl-coenzyme M reductase I subunit beta

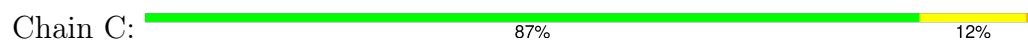


- Molecule 2: Methyl-coenzyme M reductase I subunit beta

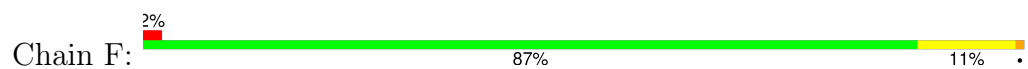




- Molecule 3: Methyl-coenzyme M reductase I subunit gamma



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	19.93 – 1.80 19.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.93-1.80) 98.2 (19.93-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.150 , 0.195 0.150 , 0.195	Depositor DCC
R_{free} test set	10624 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.010 for -h,-l,-k 0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21893	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 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GL3, ACT, MG, TP7, MGN, SMC, F43, AGM, XP8, COM, ZN, MHS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.39	7/4492 (0.2%)	1.02	3/6099 (0.0%)
1	D	1.44	14/4459 (0.3%)	1.06	5/6052 (0.1%)
2	B	1.34	7/3527 (0.2%)	1.01	4/4770 (0.1%)
2	E	1.28	7/3524 (0.2%)	0.99	2/4766 (0.0%)
3	C	1.23	3/2111 (0.1%)	1.05	7/2841 (0.2%)
3	F	1.19	3/2120 (0.1%)	1.03	3/2854 (0.1%)
All	All	1.34	41/20233 (0.2%)	1.03	24/27382 (0.1%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	62	VAL	CB-CG1	6.38	1.66	1.52
1	D	370	VAL	CB-CG1	6.15	1.65	1.52
1	D	25	PHE	CD1-CE1	5.96	1.51	1.39
1	D	411	CYS	CB-SG	5.92	1.92	1.82
1	A	458	PHE	CE1-CZ	5.85	1.48	1.37
1	D	253	TYR	CG-CD1	5.79	1.46	1.39
3	F	99	TYR	CD1-CE1	5.72	1.48	1.39
2	E	425	PHE	CE1-CZ	5.67	1.48	1.37
1	D	188	PHE	CD1-CE1	5.66	1.50	1.39
2	B	159	ALA	CA-CB	5.66	1.64	1.52
2	E	362	PHE	CB-CG	5.65	1.60	1.51
3	F	120	ARG	CG-CD	5.62	1.66	1.51
2	B	200	VAL	CB-CG1	5.62	1.64	1.52
1	A	513	PHE	CE1-CZ	5.61	1.48	1.37
2	E	197	VAL	CB-CG2	5.58	1.64	1.52
2	B	442	GLU	CG-CD	5.56	1.60	1.51
2	B	186	GLU	CD-OE2	5.55	1.31	1.25
1	D	245	GLU	CG-CD	5.54	1.60	1.51
1	A	134	GLU	CG-CD	5.49	1.60	1.51
1	A	352	GLU	CB-CG	5.43	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	407	SER	CB-OG	5.43	1.49	1.42
1	D	132	TYR	CD2-CE2	5.39	1.47	1.39
2	E	190	TYR	CG-CD1	5.30	1.46	1.39
1	A	6	PHE	CE2-CZ	5.29	1.47	1.37
3	C	208	GLU	CG-CD	5.28	1.59	1.51
2	E	339	GLU	CG-CD	5.23	1.59	1.51
1	D	543	ARG	CB-CG	5.21	1.66	1.52
3	C	157	GLY	N-CA	5.19	1.53	1.46
2	B	170	TYR	CD1-CE1	5.17	1.47	1.39
1	D	132	TYR	CD1-CE1	5.15	1.47	1.39
2	E	202	ALA	CA-CB	5.14	1.63	1.52
1	D	432	TYR	CG-CD1	5.12	1.45	1.39
1	A	37	LYS	CB-CG	5.11	1.66	1.52
1	D	513	PHE	CE2-CZ	5.07	1.47	1.37
1	A	404	VAL	CB-CG1	5.07	1.63	1.52
1	D	269	VAL	CB-CG1	5.06	1.63	1.52
1	D	323	TYR	CE1-CZ	5.04	1.45	1.38
2	E	121	PHE	CE1-CZ	5.02	1.46	1.37
3	C	219	VAL	CB-CG2	5.01	1.63	1.52
3	F	164	GLU	CG-CD	5.01	1.59	1.51
1	D	540	ALA	CA-CB	5.00	1.62	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	122	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	D	488	TYR	CB-CG-CD2	-5.99	117.41	121.00
3	C	147	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	450	ASP	N-CA-CB	5.65	120.78	110.60
3	F	161	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	545	LEU	CA-CB-CG	5.52	128.00	115.30
1	D	450	ASP	N-CA-CB	5.47	120.45	110.60
1	A	447	ASP	CB-CG-OD1	5.44	123.20	118.30
3	C	218	ARG	NE-CZ-NH1	5.44	123.02	120.30
3	C	29	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	C	193	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	528	GLU	OE1-CD-OE2	-5.39	116.83	123.30
2	E	336	ASP	CB-CG-OD1	5.39	123.15	118.30
3	C	196	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	67	ARG	NE-CZ-NH2	-5.37	117.62	120.30
3	C	168	MET	CG-SD-CE	5.26	108.61	100.20
3	F	147	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	151	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	120	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	383	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A	535	ARG	NE-CZ-NH2	5.07	122.83	120.30
3	F	128	ARG	NE-CZ-NH1	-5.06	117.77	120.30
2	B	333	TYR	CA-CB-CG	-5.02	103.86	113.40
2	B	180	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4408	0	4185	29	0
1	D	4359	0	4196	37	0
2	B	3422	0	3450	36	0
2	E	3431	0	3455	21	0
3	C	2059	0	1985	21	0
3	F	2071	0	2003	27	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	A	62	0	43	2	0
5	D	62	0	43	3	0
6	A	21	0	19	3	0
6	D	21	0	19	1	0
7	A	7	0	5	1	0
7	D	7	0	5	0	0
8	A	22	0	21	1	0
8	D	22	0	21	1	0
9	A	4	0	3	0	0
10	A	8	0	12	0	0
10	D	8	0	12	3	0
11	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	435	0	0	3	0
12	B	349	0	0	3	0
12	C	201	0	0	3	0
12	D	421	0	0	8	0
12	E	314	0	0	3	0
12	F	173	0	0	4	0
All	All	21893	0	19477	146	0

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

All (146) 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:B:196[A]:MET:CE	2:B:198:ASN:HB2	1.71	1.18
1:D:432:TYR:HB2	3:F:234[B]:MET:HE3	1.18	1.16
2:B:196[A]:MET:HE1	2:B:198:ASN:HB2	1.38	1.02
1:D:432:TYR:CB	3:F:234[B]:MET:HE3	1.90	1.02
2:B:196[A]:MET:HE3	2:B:198:ASN:HB2	1.45	0.94
3:C:67[B]:ARG:HG3	3:C:67[B]:ARG:HH11	1.40	0.87
2:B:196[A]:MET:CE	2:B:198:ASN:CB	2.58	0.82
1:D:432:TYR:CB	3:F:234[B]:MET:CE	2.58	0.81
2:B:196[A]:MET:HE1	2:B:198:ASN:CB	2.12	0.79
1:D:432:TYR:HB2	3:F:234[B]:MET:CE	2.07	0.77
1:D:433:LEU:HD23	3:F:234[B]:MET:SD	2.26	0.76
1:D:42[A]:ASN:ND2	12:D:1802:HOH:O	2.21	0.73
2:B:188:PRO:HD3	12:E:1304:HOH:O	1.89	0.73
3:F:183[B]:ARG:NH1	12:F:4120:HOH:O	2.21	0.71
1:D:433:LEU:CD2	3:F:234[B]:MET:SD	2.82	0.67
2:B:196[A]:MET:HE3	2:B:198:ASN:CB	2.21	0.66
1:A:17[B]:SER:OG	1:A:20:GLU:HG3	1.96	0.65
1:D:432:TYR:HB3	3:F:234[B]:MET:CE	2.29	0.62
1:A:194[B]:GLU:HG2	12:A:2095:HOH:O	2.00	0.61
3:F:56:LEU:HA	3:F:59:MET:HG3	1.82	0.61
3:C:56:LEU:O	3:C:59[A]:MET:HB2	2.01	0.60
2:B:246[B]:MET:HE1	2:B:432:VAL:HG12	1.84	0.60
1:D:348:TYR:CZ	10:D:555:EDO:H11	2.37	0.59
1:D:432:TYR:HB3	3:F:234[B]:MET:HE2	1.84	0.59
1:D:383[B]:GLU:HG2	1:D:387[B]:GLU:OE2	2.03	0.59
3:F:56:LEU:O	3:F:59:MET:HB2	2.01	0.59
2:B:261[A]:LYS:HG3	2:B:262:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241[B]:GLN:HG3	1:A:242:ALA:O	2.03	0.58
3:F:183[B]:ARG:HB2	12:F:3972[B]:HOH:O	2.03	0.58
1:A:328:VAL:HB	5:D:551:F43:H9A1	1.86	0.57
2:B:322[B]:ARG:NH1	3:C:67[B]:ARG:HG2	2.19	0.57
3:F:178[B]:ASN:HB3	3:F:181[B]:THR:OG1	2.05	0.57
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.40	0.57
2:B:405:MET:HG3	1:D:115:VAL:HG22	1.87	0.56
2:E:186:GLU:HG3	2:E:378:ASN:O	2.06	0.56
2:B:214:LEU:HB2	2:B:428:PRO:HG3	1.89	0.55
3:F:117:LEU:HD22	3:F:120:ARG:HD3	1.88	0.55
1:A:60:ILE:HD12	12:D:3878:HOH:O	2.06	0.55
2:B:202:ALA:HB1	2:B:416:LYS:HB2	1.90	0.54
3:F:247:ASN:O	3:F:248:LEU:HB2	2.08	0.54
2:B:68[A]:LYS:HE3	12:B:1528:HOH:O	2.08	0.53
1:D:191:ASP:HB2	12:D:3703:HOH:O	2.07	0.53
1:A:267:LEU:HD12	1:A:273:ARG:HB2	1.90	0.53
3:C:67[B]:ARG:HG3	3:C:67[B]:ARG:NH1	2.14	0.53
2:B:126:GLU:HB3	2:E:126:GLU:HB3	1.91	0.53
1:D:46[B]:GLU:HG3	12:D:693:HOH:O	2.09	0.53
2:E:206:LYS:NZ	2:E:409:GLU:OE2	2.35	0.52
2:E:429:LEU:O	2:E:433:VAL:HG23	2.10	0.52
3:F:86:GLN:HG2	3:F:151:ARG:O	2.09	0.51
3:C:65:ALA:O	3:C:69:MET:HG3	2.10	0.51
1:A:105[B]:VAL:HG13	1:A:223:THR:HG22	1.91	0.51
2:E:61[A]:LYS:HG2	2:E:68[A]:LYS:HB2	1.93	0.50
5:A:1:F43:H9A1	1:D:328:VAL:HB	1.93	0.50
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:CG	2.20	0.50
3:F:82:VAL:O	3:F:83:ARG:HD2	2.11	0.50
2:B:113:LEU:C	2:B:113:LEU:HD13	2.31	0.50
2:B:196[A]:MET:HE2	2:B:199:HIS:ND1	2.26	0.50
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.47	0.50
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.47	0.50
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.47	0.50
3:C:34:GLU:HB2	12:C:1830:HOH:O	2.12	0.50
1:D:42[A]:ASN:CG	12:D:2513:HOH:O	2.49	0.50
3:C:44:ALA:HB1	3:C:45:PRO:HD2	1.94	0.49
1:A:105[B]:VAL:HG13	1:A:223:THR:CG2	2.42	0.49
2:E:61[B]:LYS:HE3	12:E:2370:HOH:O	2.13	0.49
3:C:62:PRO:O	3:C:67[A]:ARG:NH2	2.43	0.48
3:F:153:LYS:NZ	12:F:1186:HOH:O	2.34	0.48
1:D:42[A]:ASN:ND2	12:D:2513:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:HB2	3:F:84:TYR:CZ	2.48	0.48
2:B:130:ALA:HB3	2:B:131:PRO:CD	2.45	0.47
1:D:451:GLN:HB2	2:E:354:GLY:CA	2.45	0.47
1:A:445:GL3:HA2	2:B:357:VAL:HG12	1.96	0.47
3:C:67[B]:ARG:NH1	12:C:3948:HOH:O	2.38	0.47
1:A:444:TYR:CE1	2:B:360:SER:HB3	2.50	0.47
3:C:45:PRO:HB3	12:C:3636:HOH:O	2.13	0.47
3:C:82:VAL:O	3:C:83:ARG:HD2	2.14	0.47
2:E:58:LYS:HE3	12:E:1433:HOH:O	2.15	0.47
3:F:243[B]:GLN:NE2	12:F:891:HOH:O	2.46	0.46
2:E:333:TYR:HB2	3:F:106:LEU:HD22	1.98	0.46
1:A:279:GLY:HA2	1:A:473:PRO:HB2	1.97	0.46
1:A:480:MET:O	6:A:552[A]:TP7:H32C	2.15	0.46
1:D:106:ILE:HB	1:D:261:ILE:HB	1.98	0.46
2:E:214:LEU:HB2	2:E:428:PRO:HG3	1.97	0.46
2:E:331:LEU:HB3	2:E:356:ALA:HB2	1.98	0.46
1:D:8:ASN:O	1:D:12[B]:LYS:HG2	2.16	0.45
12:B:2205:HOH:O	2:E:188:PRO:HD3	2.16	0.45
2:E:242:ALA:O	2:E:246[A]:MET:HB2	2.16	0.45
1:A:145:VAL:HG23	1:A:146:VAL:HG23	1.99	0.45
1:D:305:LEU:CD1	1:D:344:ASP:HA	2.47	0.45
1:D:109:LEU:HB2	1:D:204[B]:ILE:HG23	1.98	0.44
1:A:176[B]:ILE:O	1:A:177[B]:ASP:C	2.56	0.44
1:A:383[A]:GLU:HG3	12:A:2606:HOH:O	2.17	0.44
1:A:544:ALA:HB2	12:D:3604[A]:HOH:O	2.18	0.44
2:B:186:GLU:HG3	2:B:378:ASN:O	2.18	0.44
3:C:67[A]:ARG:HE	3:C:67[A]:ARG:HB3	1.25	0.44
2:B:233[B]:PHE:CD1	3:C:248:LEU:HD12	2.53	0.44
1:D:21:LYS:HG2	1:D:389:PRO:HG2	2.00	0.44
2:B:14[A]:ARG:HH12	3:C:63:GLU:HG2	1.83	0.44
2:B:246[B]:MET:HE1	2:B:432:VAL:CG1	2.47	0.43
2:B:196[A]:MET:HE3	2:B:198:ASN:CA	2.49	0.43
2:B:322[A]:ARG:HH12	3:C:61:GLU:CD	2.21	0.43
2:B:333:TYR:HB2	3:C:106:LEU:HD22	2.01	0.43
6:A:552[A]:TP7:H42C	6:A:552[A]:TP7:H72C	1.84	0.43
1:D:12[B]:LYS:HA	1:D:12[B]:LYS:HD3	1.87	0.43
1:A:480:MET:O	8:A:554[B]:XP8:H3A	2.17	0.43
1:D:480:MET:O	8:D:553[B]:XP8:H3A	2.18	0.43
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.59	0.43
1:A:217:THR:HG23	12:D:679:HOH:O	2.19	0.43
1:D:22:LYS:NZ	10:D:554:EDO:H12	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322[B]:ARG:CZ	3:C:67[B]:ARG:HG2	2.49	0.42
1:D:7:ILE:CG2	1:D:11:LYS:HE3	2.48	0.42
10:D:554:EDO:H11	3:F:166:GLY:HA3	2.01	0.42
3:C:117:LEU:HD13	3:C:120:ARG:HG3	2.00	0.42
1:D:243:ALA:HB1	5:D:551:F43:H9B1	2.01	0.42
1:A:481:ASN:HA	6:A:552[A]:TP7:S7	2.59	0.42
1:A:177[B]:ASP:C	1:A:179:ALA:N	2.72	0.42
2:B:164:TYR:CD1	2:B:165:PRO:HA	2.54	0.42
1:D:145:VAL:HG23	1:D:146:VAL:HG23	2.01	0.42
1:D:383[B]:GLU:CG	1:D:387[B]:GLU:OE2	2.67	0.42
1:D:439:SER:HB3	3:F:97:GLN:HB3	2.02	0.42
7:A:553:COM:H12	5:D:551:F43:C1C	2.50	0.42
3:F:191:ILE:HD12	3:F:191:ILE:HA	1.91	0.42
1:A:84:ASP:HA	1:D:151:VAL:HB	2.02	0.42
2:B:13:ASP:OD1	12:B:3793:HOH:O	2.22	0.42
2:B:58:LYS:HE2	2:B:58:LYS:HB3	1.55	0.42
2:B:113:LEU:HD23	2:B:418:VAL:HG13	2.01	0.42
1:A:332:GLN:HA	1:A:335:THR:OG1	2.19	0.41
2:B:191:ALA:HB3	2:E:125:ALA:CB	2.49	0.41
3:C:99:TYR:CD1	3:C:116:THR:HG21	2.56	0.41
2:E:324:ALA:O	2:E:327:VAL:HG12	2.20	0.41
1:D:332:GLN:HA	1:D:335:THR:OG1	2.21	0.41
1:D:383[B]:GLU:OE2	1:D:387[B]:GLU:OE2	2.38	0.41
2:B:407:SER:HB2	2:B:408:PRO:CD	2.50	0.41
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.96	0.41
2:E:374:ILE:C	2:E:374:ILE:HD12	2.42	0.41
1:A:4[A]:LYS:NZ	12:A:2253:HOH:O	2.33	0.41
3:F:60:ASP:O	3:F:60:ASP:CG	2.60	0.40
1:A:257:MHS:NE2	6:D:1[A]:TP7:O1P	2.55	0.40
5:A:1:F43:C9A	5:A:1:F43:CBA	2.99	0.40
2:B:3:LYS:HZ2	2:B:3:LYS:HG3	1.74	0.40
2:E:3[A]:LYS:HB2	2:E:3[A]:LYS:HE3	1.76	0.40
2:E:339:GLU:HG3	2:E:346:SER:HB3	2.02	0.40
3:F:240:LEU:HD23	3:F:240:LEU:HA	1.98	0.40
2:E:288:LEU:HD23	2:E:288:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/549 (103%)	543 (96%)	20 (4%)	1 (0%)	44	31
1	D	560/549 (102%)	543 (97%)	16 (3%)	1 (0%)	44	31
2	B	459/442 (104%)	448 (98%)	10 (2%)	1 (0%)	44	31
2	E	459/442 (104%)	449 (98%)	10 (2%)	0	100	100
3	C	254/248 (102%)	243 (96%)	11 (4%)	0	100	100
3	F	256/248 (103%)	246 (96%)	10 (4%)	0	100	100
All	All	2552/2478 (103%)	2472 (97%)	77 (3%)	3 (0%)	48	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	325	SER
1	A	325	SER
2	B	402	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	456/434 (105%)	452 (99%)	4 (1%)	75	72
1	D	452/434 (104%)	444 (98%)	8 (2%)	54	45
2	B	360/341 (106%)	355 (99%)	5 (1%)	62	56
2	E	360/341 (106%)	354 (98%)	6 (2%)	56	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	224/216 (104%)	220 (98%)	4 (2%)	54	45
3	F	225/216 (104%)	219 (97%)	6 (3%)	40	28
All	All	2077/1982 (105%)	2044 (98%)	33 (2%)	58	50

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	PRO
1	A	444	TYR
1	A	450	ASP
1	A	543	ARG
2	B	58	LYS
2	B	113	LEU
2	B	126	GLU
2	B	185	LEU
2	B	283	LYS
3	C	120	ARG
3	C	121	GLN
3	C	186	MET
3	C	248	LEU
1	D	54	PRO
1	D	84	ASP
1	D	186	LYS
1	D	444	TYR
1	D	450	ASP
1	D	476	PRO
1	D	543	ARG
1	D	545	LEU
2	E	126	GLU
2	E	185	LEU
2	E	278	GLU
2	E	283	LYS
2	E	438[A]	GLU
2	E	438[B]	GLU
3	F	60	ASP
3	F	61	GLU
3	F	120	ARG
3	F	121	GLN
3	F	186	MET
3	F	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
2	B	318	GLN
3	C	121	GLN
1	D	111	HIS
2	E	318	GLN
3	F	121	GLN
3	F	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MHS	A	257	1	7,11,12	2.25	2 (28%)	7,14,16	3.89	4 (57%)
1	MHS	D	257	1	7,11,12	2.33	1 (14%)	7,14,16	3.64	4 (57%)
1	SMC	A	452	1	5,6,7	0.95	0	3,6,8	2.20	1 (33%)
1	MGN	A	400	1	6,9,10	2.12	1 (16%)	7,12,14	1.74	1 (14%)
1	SMC	D	452	1	5,6,7	0.77	0	3,6,8	2.18	1 (33%)
1	MGN	D	400	1	6,9,10	1.67	1 (16%)	7,12,14	1.79	1 (14%)
1	AGM	A	271	1	10,11,12	1.38	2 (20%)	7,13,15	2.63	4 (57%)
1	GL3	D	445	1	2,3,4	3.48	1 (50%)	1,2,4	1.07	0
1	GL3	A	445	1	2,3,4	3.17	1 (50%)	1,2,4	0.12	0
1	AGM	D	271	1	10,11,12	1.62	3 (30%)	7,13,15	2.15	4 (57%)

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	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	SMC	A	452	1	-	1/3/5/7	-
1	MGN	A	400	1	-	0/7/9/12	-
1	SMC	D	452	1	-	1/3/5/7	-
1	MGN	D	400	1	-	0/7/9/12	-
1	AGM	A	271	1	-	3/10/11/13	-
1	GL3	D	445	1	-	1/1/1/2	-
1	GL3	A	445	1	-	1/1/1/2	-
1	AGM	D	271	1	-	1/10/11/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	257	MHS	CE1-NE2	5.50	1.47	1.34
1	A	257	MHS	CE1-NE2	5.07	1.46	1.34
1	D	445	GL3	C-S	-4.90	1.60	1.80
1	A	400	MGN	CB1-CA	4.61	1.60	1.55
1	A	445	GL3	C-S	-4.44	1.62	1.80
1	D	271	AGM	CG-CD	3.38	1.58	1.53
1	D	400	MGN	CB1-CA	-3.34	1.51	1.55
1	A	271	AGM	CZ-NH2	2.52	1.41	1.32
1	D	271	AGM	CB-CA	2.21	1.56	1.53
1	D	271	AGM	O-C	2.13	1.28	1.20
1	A	271	AGM	CG-CB	2.11	1.58	1.53
1	A	257	MHS	CM-ND1	2.05	1.52	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	NE2-CE1-ND1	-8.69	99.36	112.26
1	D	257	MHS	NE2-CE1-ND1	-8.19	100.11	112.26
1	A	400	MGN	CB1-CG-CD	-4.26	103.62	112.13
1	A	271	AGM	NE1-CZ-NH2	-4.13	113.50	120.58
1	D	400	MGN	CB1-CG-CD	-4.00	104.15	112.13
1	A	257	MHS	CM-ND1-CG	3.79	129.48	124.44
1	A	452	SMC	CA-CB-SG	-3.74	107.99	114.04
1	A	271	AGM	CE2-CD-CG	3.70	118.24	111.48
1	D	452	SMC	CA-CB-SG	-3.66	108.11	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	CM-ND1-CG	3.63	129.27	124.44
1	A	271	AGM	NH1-CZ-NE1	3.06	126.32	119.58
1	D	271	AGM	CE2-CD-CG	3.04	117.03	111.48
1	D	271	AGM	NH1-CZ-NE1	2.88	125.94	119.58
1	D	271	AGM	CG-CD-NE1	-2.67	105.83	110.42
1	A	257	MHS	CD2-NE2-CE1	2.59	109.82	105.72
1	A	257	MHS	CM-ND1-CE1	-2.35	114.14	125.43
1	D	257	MHS	CM-ND1-CE1	-2.18	114.92	125.43
1	D	257	MHS	CD2-NE2-CE1	2.15	109.12	105.72
1	D	271	AGM	NH1-CZ-NH2	-2.13	114.00	120.07
1	A	271	AGM	CE2-CD-NE1	-2.02	105.21	110.31

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	257	MHS	1	0
1	A	445	GL3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	COM	A	553	5	6,6,6	2.82	2 (33%)	8,8,8	2.32	2 (25%)
5	F43	A	1	7,1	63,71,71	2.47	16 (25%)	73,118,118	1.62	13 (17%)
6	TP7	A	552[A]	-	19,20,20	1.05	1 (5%)	24,26,26	1.18	1 (4%)
8	XP8	A	554[B]	-	20,21,21	0.98	1 (5%)	25,27,27	1.03	0
8	XP8	D	553[B]	-	20,21,21	0.79	0	25,27,27	0.85	1 (4%)
10	EDO	A	557	-	3,3,3	0.45	0	2,2,2	0.40	0
10	EDO	D	555	-	3,3,3	0.49	0	2,2,2	0.51	0
10	EDO	D	554	-	3,3,3	0.33	0	2,2,2	0.29	0
9	ACT	A	555[A]	4	3,3,3	0.85	0	3,3,3	1.48	0
10	EDO	A	556	-	3,3,3	0.88	0	2,2,2	0.46	0
5	F43	D	551	7,1	63,71,71	2.43	15 (23%)	73,118,118	1.92	22 (30%)
7	COM	D	552	5	6,6,6	2.68	2 (33%)	8,8,8	2.22	3 (37%)
6	TP7	D	1[A]	-	19,20,20	0.91	1 (5%)	24,26,26	0.98	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
7	COM	A	553	5	-	0/4/4/4	-
5	F43	A	1	7,1	-	9/28/185/185	-
6	TP7	A	552[A]	-	-	3/24/24/24	-
8	XP8	A	554[B]	-	-	2/25/25/25	-
8	XP8	D	553[B]	-	-	2/25/25/25	-
10	EDO	A	557	-	-	1/1/1/1	-
10	EDO	D	555	-	-	1/1/1/1	-
10	EDO	D	554	-	-	1/1/1/1	-
10	EDO	A	556	-	-	1/1/1/1	-
5	F43	D	551	7,1	-	10/28/185/185	-
7	COM	D	552	5	-	1/4/4/4	-
6	TP7	D	1[A]	-	-	2/24/24/24	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	551	F43	NI-NA	9.67	2.12	1.89
5	A	1	F43	NI-NB	9.39	2.12	1.89
5	A	1	F43	NI-NA	9.32	2.11	1.89
5	D	551	F43	NI-NB	8.88	2.10	1.89
5	A	1	F43	NI-ND	7.23	2.06	1.89
7	A	553	COM	C2-S2	-5.91	1.69	1.77
5	D	551	F43	NI-ND	5.76	2.03	1.89
7	D	552	COM	C2-S2	-5.51	1.69	1.77
5	D	551	F43	CHD-C1D	4.23	1.50	1.43
5	A	1	F43	CHB-C4A	4.18	1.57	1.51
5	D	551	F43	CHB-C1B	4.06	1.56	1.53
5	A	1	F43	CHA-C4D	3.99	1.57	1.53
5	D	551	F43	CHA-C4D	-3.84	1.49	1.53
5	A	1	F43	CHC-C4B	3.77	1.49	1.39
5	D	551	F43	CHC-C4B	3.69	1.49	1.39
5	A	1	F43	C5D-C6D	3.18	1.59	1.53
5	D	551	F43	CHB-C4A	3.05	1.56	1.51
6	A	552[A]	TP7	P-O4P	3.00	1.64	1.59
8	A	554[B]	XP8	P-O4P	2.99	1.64	1.59
5	D	551	F43	C3A-C4A	2.83	1.58	1.53
5	D	551	F43	CAB-C3B	2.77	1.60	1.54
5	D	551	F43	C9C-CAC	2.60	1.56	1.50
5	A	1	F43	CHB-C1B	2.50	1.55	1.53
5	A	1	F43	CHD-C1D	2.48	1.47	1.43
7	D	552	COM	O3S-S2	2.47	1.56	1.47
5	D	551	F43	C5C-C2C	2.46	1.57	1.53
5	A	1	F43	CAA-C3A	2.46	1.57	1.53
5	A	1	F43	C5C-C6C	2.44	1.57	1.51
7	A	553	COM	O2S-S2	2.37	1.51	1.45
5	A	1	F43	C3D-C4D	-2.35	1.49	1.53
6	D	1[A]	TP7	P-O1P	2.33	1.57	1.50
5	A	1	F43	CHA-C1A	2.30	1.55	1.50
5	D	551	F43	C2A-C3A	2.22	1.58	1.54
5	A	1	F43	C4D-ND	2.19	1.52	1.49
5	A	1	F43	ODA-CCA	-2.17	1.23	1.30
5	D	551	F43	OCD-CAD	-2.15	1.23	1.30
5	A	1	F43	C9A-C2A	-2.07	1.51	1.54
5	D	551	F43	ODA-CCA	-2.05	1.24	1.30

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	551	F43	C5D-C2D-C1D	5.92	118.15	110.43
7	A	553	COM	O1S-S2-C2	5.71	115.35	106.73
5	D	551	F43	O8D-C7D-C6D	-4.16	114.05	120.87
5	D	551	F43	C2C-C5C-C6C	-4.05	106.38	113.95
5	D	551	F43	C6D-C7D-CHD	3.91	124.16	116.94
5	A	1	F43	C2B-C1B-NB	3.82	107.53	101.86
7	D	552	COM	O2S-S2-C2	3.74	112.38	106.73
7	D	552	COM	O1S-S2-C2	3.71	112.33	106.73
5	A	1	F43	OBC-CAC-C9C	3.65	125.53	114.00
5	A	1	F43	C2C-C5C-C6C	-3.57	107.26	113.95
5	D	551	F43	C2B-C1B-NB	3.42	106.94	101.86
5	D	551	F43	CAB-C3B-C2B	-3.28	111.76	119.00
5	A	1	F43	CAB-C3B-C2B	-3.27	111.78	119.00
5	D	551	F43	C1D-CHD-C4C	-3.22	116.23	125.28
5	D	551	F43	C9A-C2A-C3A	3.18	117.56	112.99
5	D	551	F43	OBC-CAC-C9C	3.11	123.84	114.00
5	D	551	F43	CHA-C4D-C3D	-3.08	109.21	117.90
5	A	1	F43	C3A-C2A-C1A	-3.07	96.91	99.97
5	D	551	F43	C4B-CHC-C1C	3.04	130.76	125.84
5	D	551	F43	C5C-C2C-C3C	-3.02	107.58	115.05
5	A	1	F43	OCC-CAC-C9C	-2.97	113.66	123.09
7	A	553	COM	O3S-S2-O2S	-2.97	103.96	111.40
5	A	1	F43	ODB-CCB-CBB	-2.90	113.89	123.09
5	A	1	F43	C9B-C2B-C8B	-2.89	103.33	110.61
6	A	552[A]	TP7	C5-C6-C7	-2.89	107.95	113.09
5	D	551	F43	C7D-CHD-C4C	2.71	127.43	121.76
5	A	1	F43	C4B-CHC-C1C	2.69	130.19	125.84
7	D	552	COM	O3S-S2-O2S	-2.66	104.75	111.40
5	D	551	F43	C1B-C2B-C3B	2.65	105.36	101.51
5	A	1	F43	O8D-C7D-C6D	-2.57	116.66	120.87
5	A	1	F43	O7B-C6B-C8B	-2.53	121.83	126.92
5	D	551	F43	C9D-C3D-C4D	-2.47	108.15	114.63
5	A	1	F43	C9A-C2A-C5A	2.44	114.88	110.74
5	D	551	F43	C9C-C8C-C3C	-2.41	106.61	113.79
5	A	1	F43	ODA-CCA-CBA	2.32	121.33	114.00
5	D	551	F43	ODB-CCB-CBB	-2.29	115.83	123.09
5	D	551	F43	CHC-C1C-NC	2.25	128.02	124.39
5	D	551	F43	C5D-C2D-C3D	-2.15	114.34	118.26
5	D	551	F43	OCC-CAC-C9C	-2.14	116.29	123.09
5	D	551	F43	C2D-C1D-CHD	-2.14	119.20	121.85
8	D	553[B]	XP8	O2P-P-O1P	2.05	115.50	107.80
5	D	551	F43	OEB-CCB-ODB	2.01	128.49	123.33

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	552	COM	C1-C2-S2-O2S
8	D	553[B]	XP8	C6-C7-C8-S8
5	D	551	F43	C3A-CAA-CBA-CCA
5	A	1	F43	C3A-CAA-CBA-CCA
10	D	554	EDO	O1-C1-C2-O2
10	D	555	EDO	O1-C1-C2-O2
6	D	1[A]	TP7	C2-C3-C4-C5
8	A	554[B]	XP8	C6-C7-C8-S8
10	A	556	EDO	O1-C1-C2-O2
6	A	552[A]	TP7	C2-C3-C4-C5
8	D	553[B]	XP8	C2-C3-C4-C5
5	A	1	F43	C2C-C5C-C6C-O8C
10	A	557	EDO	O1-C1-C2-O2
6	A	552[A]	TP7	CB-O4P-P-O3P
6	D	1[A]	TP7	CB-O4P-P-O3P
8	A	554[B]	XP8	C2-C3-C4-C5
5	A	1	F43	CAA-CBA-CCA-OEA
5	D	551	F43	CAA-CBA-CCA-ODA
5	D	551	F43	CAA-CBA-CCA-OEA
5	A	1	F43	CAA-CBA-CCA-ODA
5	A	1	F43	CAB-CBB-CCB-OEB
6	A	552[A]	TP7	C4-C5-C6-C7
5	A	1	F43	C8C-C9C-CAC-OCC
5	D	551	F43	CAB-CBB-CCB-OEB
5	D	551	F43	C3D-C9D-CAD-OB
5	D	551	F43	C3D-C9D-CAD-OC
5	A	1	F43	C8C-C9C-CAC-OBC
5	A	1	F43	CAB-CBB-CCB-OD
5	A	1	F43	C2C-C5C-C6C-O7C
5	D	551	F43	C2C-C5C-C6C-O7C
5	D	551	F43	C8C-C9C-CAC-OBC
5	D	551	F43	C2C-C5C-C6C-O8C
5	D	551	F43	CAB-CBB-CCB-OD

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	553	COM	1	0
5	A	1	F43	2	0
6	A	552[A]	TP7	3	0

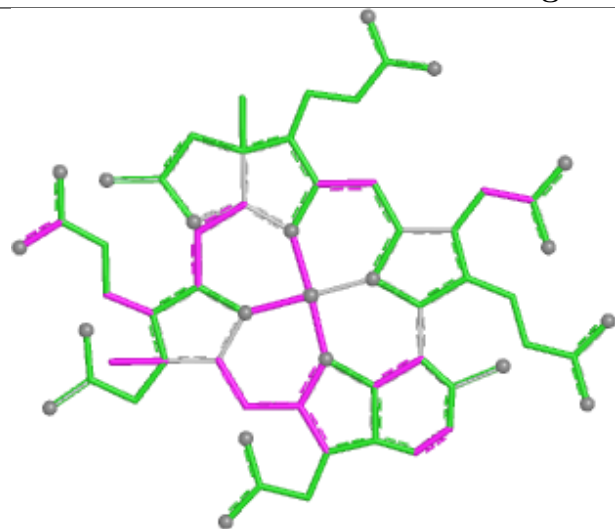
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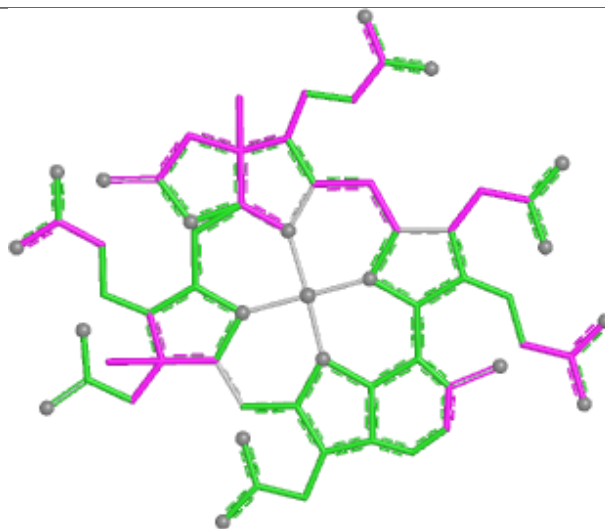
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	554[B]	XP8	1	0
8	D	553[B]	XP8	1	0
10	D	555	EDO	1	0
10	D	554	EDO	2	0
5	D	551	F43	3	0
6	D	1[A]	TP7	1	0

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.

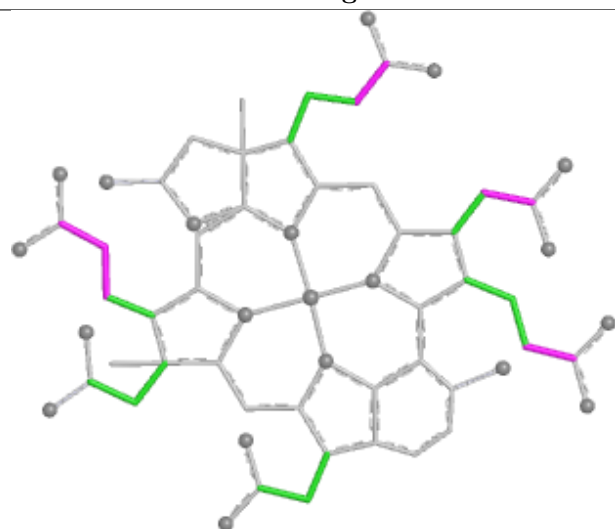
Ligand F43 A 1



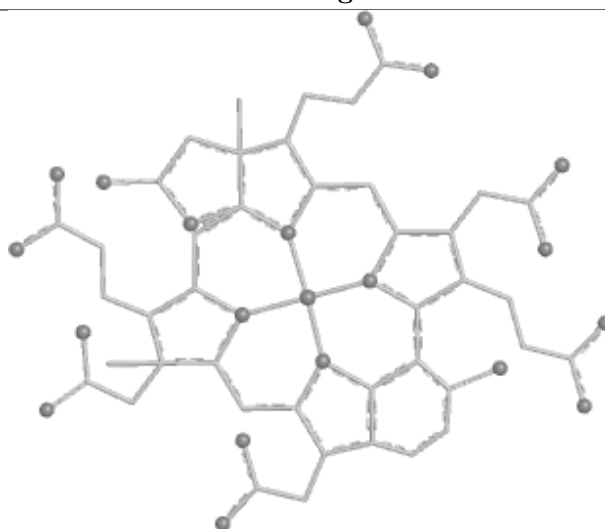
Bond lengths



Bond angles

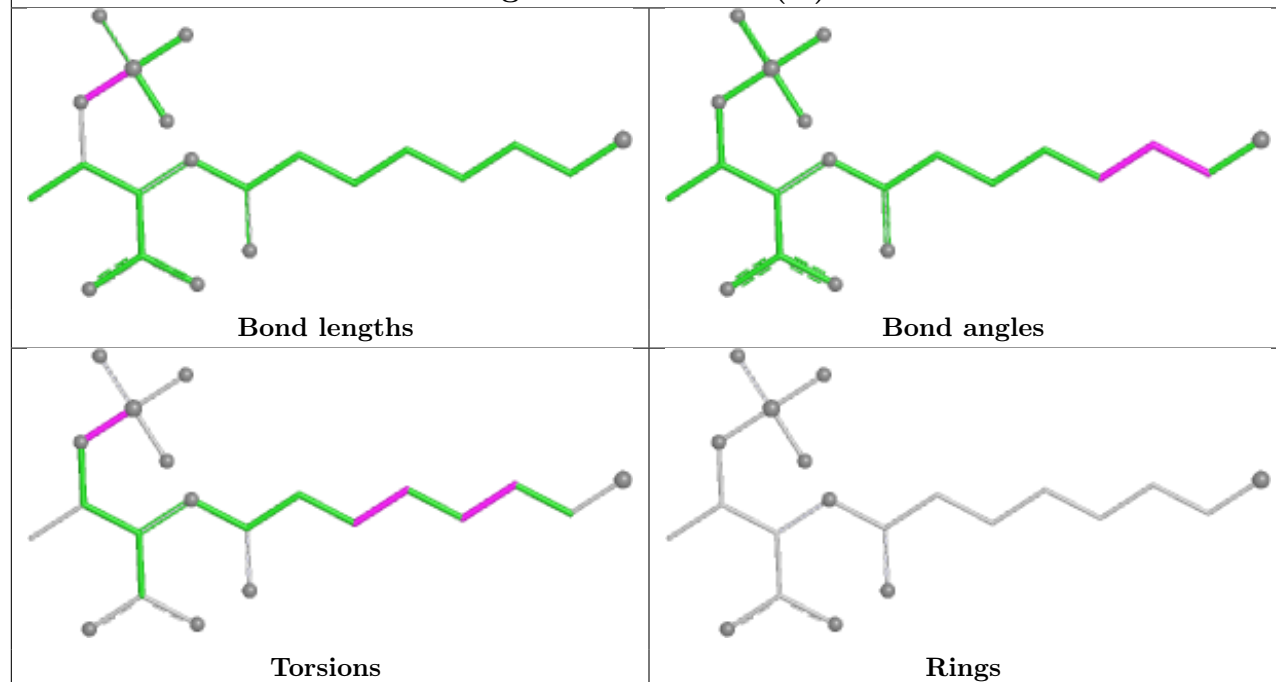


Torsions

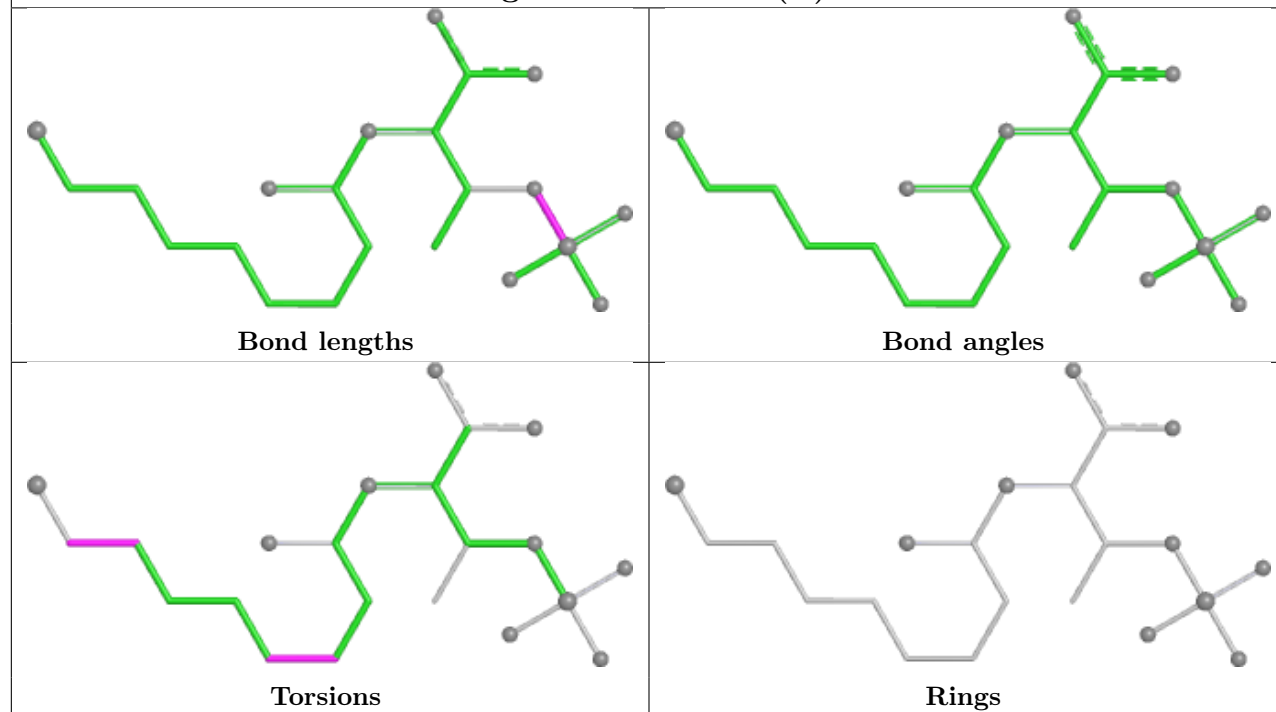


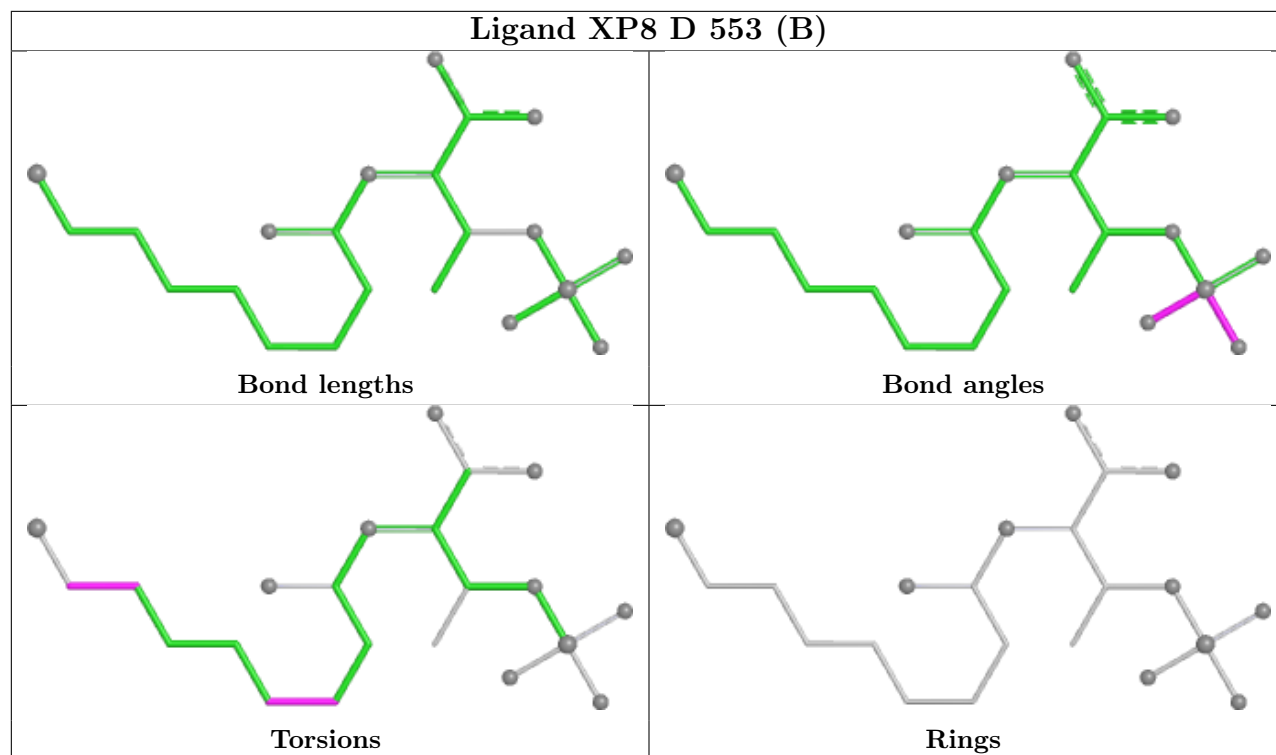
Rings

Ligand TP7 A 552 (A)

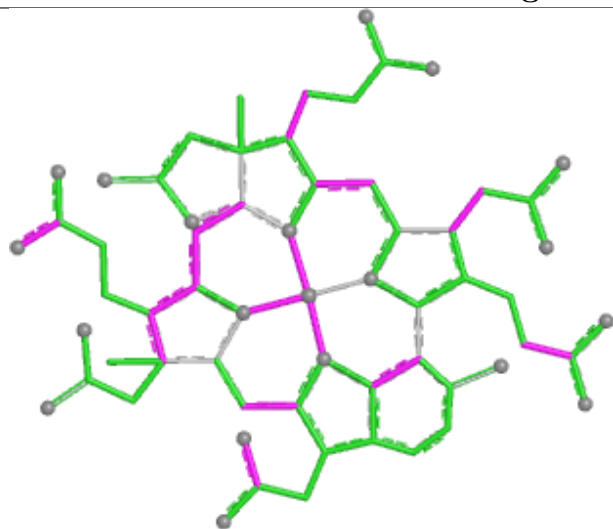


Ligand XP8 A 554 (B)

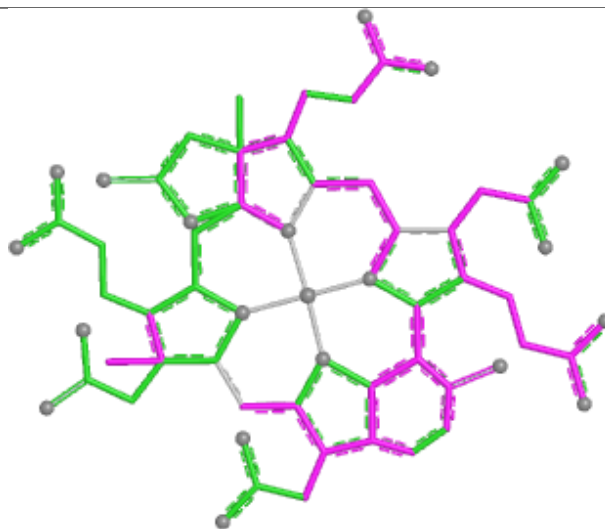




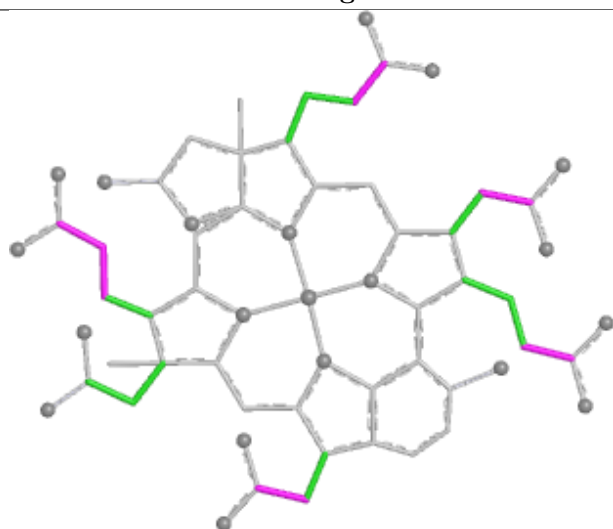
Ligand F43 D 551



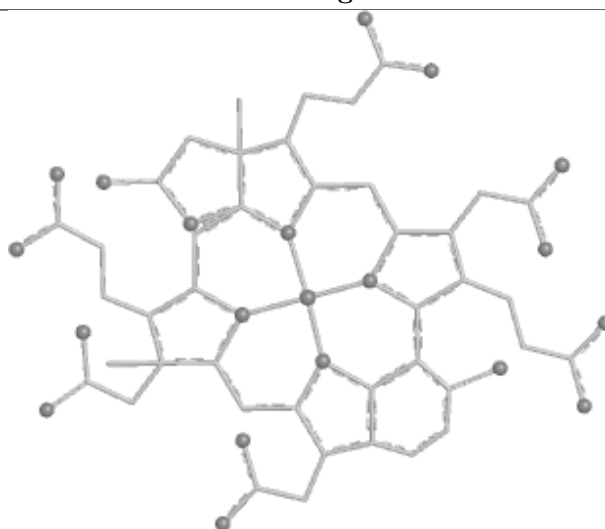
Bond lengths



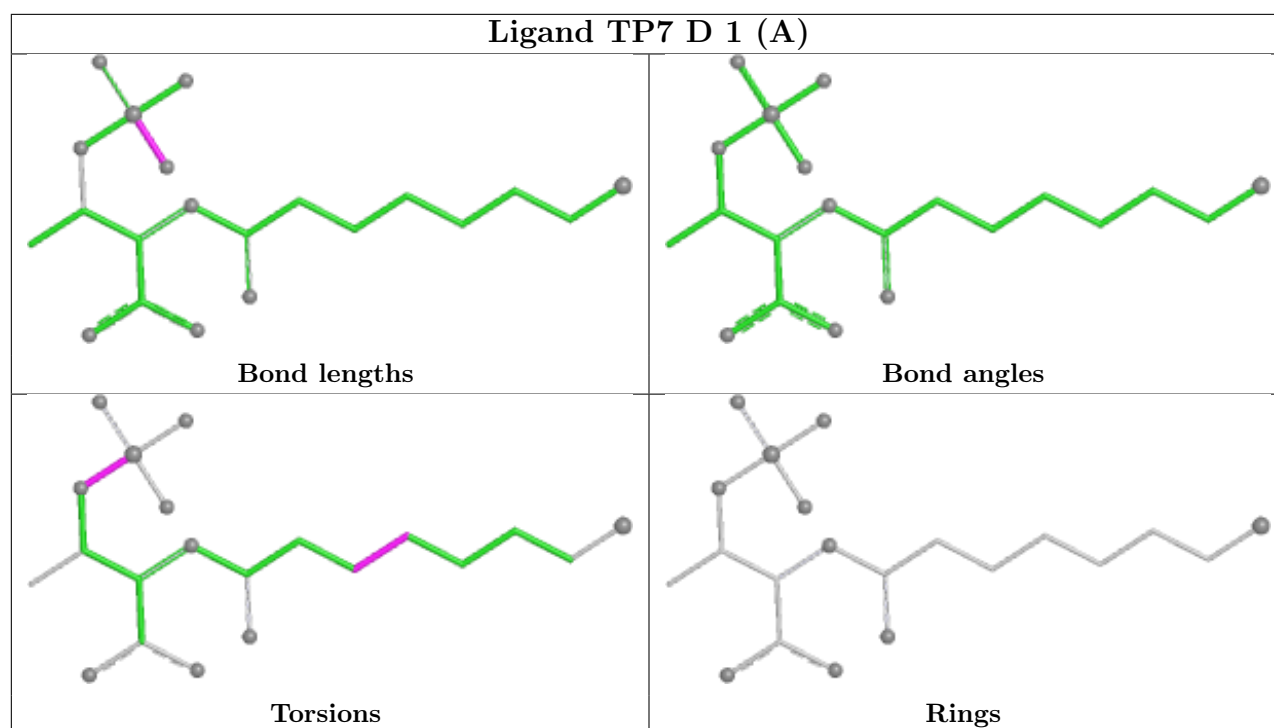
Bond angles



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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	543/549 (98%)	-0.98	0	100	100	4, 11, 24, 39	22 (4%)
1	D	543/549 (98%)	-0.95	0	100	100	3, 11, 24, 40	19 (3%)
2	B	442/442 (100%)	-0.67	0	100	100	5, 16, 27, 43	18 (4%)
2	E	442/442 (100%)	-0.41	3 (0%)	84	84	6, 19, 36, 53	19 (4%)
3	C	248/248 (100%)	-0.57	1 (0%)	89	88	7, 18, 34, 58	8 (3%)
3	F	247/248 (99%)	-0.29	5 (2%)	64	63	8, 22, 41, 63	11 (4%)
All	All	2465/2478 (99%)	-0.71	9 (0%)	89	88	3, 15, 31, 63	97 (3%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	62	PRO	3.0
3	F	59	MET	2.6
3	F	45	PRO	2.5
2	E	97	GLU	2.5
3	C	45	PRO	2.4
2	E	17	LEU	2.3
3	F	66	ILE	2.2
2	E	98	ASP	2.1
3	F	65	ALA	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MHS	A	257	11/12	0.95	0.06	15,18,21,22	0
1	MHS	D	257	11/12	0.95	0.06	15,18,20,21	0
1	AGM	D	271	12/13	0.97	0.04	7,9,11,13	0
1	SMC	A	452	7/8	0.98	0.05	7,8,11,12	0
1	AGM	A	271	12/13	0.98	0.04	7,9,10,11	0
1	MGN	A	400	10/11	0.98	0.03	6,6,11,11	0
1	MGN	D	400	10/11	0.98	0.03	7,9,10,12	0
1	SMC	D	452	7/8	0.99	0.04	9,10,13,16	0
1	GL3	D	445	4/5	1.00	0.02	7,8,9,10	0
1	GL3	A	445	4/5	1.00	0.02	6,6,7,10	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

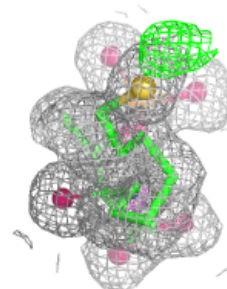
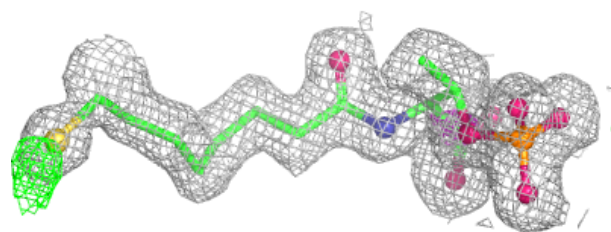
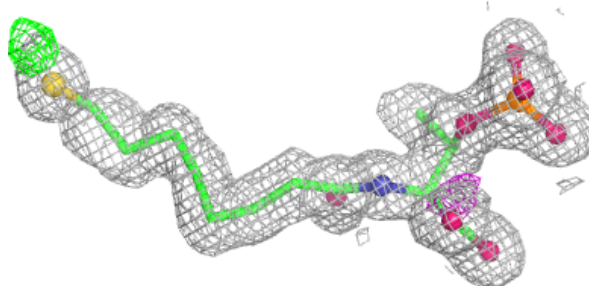
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	D	555	4/4	0.84	0.12	39,43,43,45	0
4	MG	B	444	1/1	0.87	0.09	30,30,30,30	1
10	EDO	A	556	4/4	0.89	0.11	31,31,31,34	0
10	EDO	D	554	4/4	0.91	0.11	33,38,38,38	0
10	EDO	A	557	4/4	0.91	0.12	40,42,43,44	0
4	MG	B	1	1/1	0.93	0.05	41,41,41,41	0
4	MG	A	551	1/1	0.94	0.07	22,22,22,22	1
8	XP8	A	554[B]	22/22	0.94	0.06	11,14,18,18	22
8	XP8	D	553[B]	22/22	0.94	0.07	12,14,17,19	22
9	ACT	A	555[A]	4/4	0.94	0.07	21,21,21,22	4
6	TP7	A	552[A]	21/21	0.96	0.06	10,14,16,17	21
6	TP7	D	1[A]	21/21	0.96	0.06	12,14,17,19	21
4	MG	C	250	1/1	0.96	0.06	32,32,32,32	0
4	MG	F	250	1/1	0.97	0.06	28,28,28,28	0
7	COM	D	552	7/7	0.98	0.06	14,16,18,22	0
7	COM	A	553	7/7	0.99	0.04	12,15,17,20	0
5	F43	A	1	62/62	0.99	0.03	5,9,14,19	0
5	F43	D	551	62/62	0.99	0.03	3,8,12,16	0
11	ZN	D	556	1/1	1.00	0.01	14,14,14,14	1

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

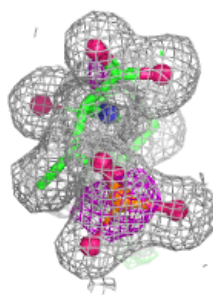
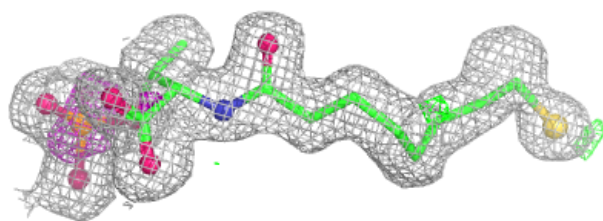
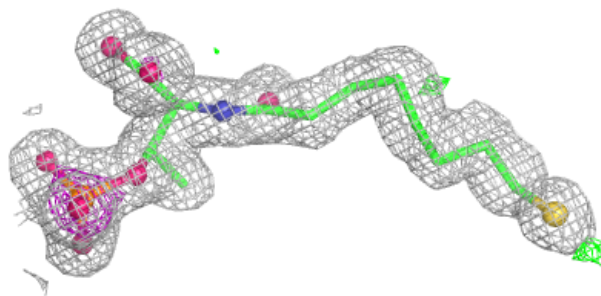
Electron density around XP8 A 554 (B):

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

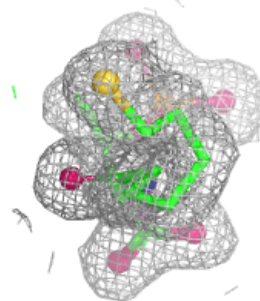
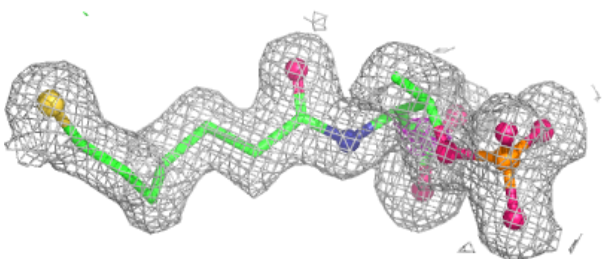
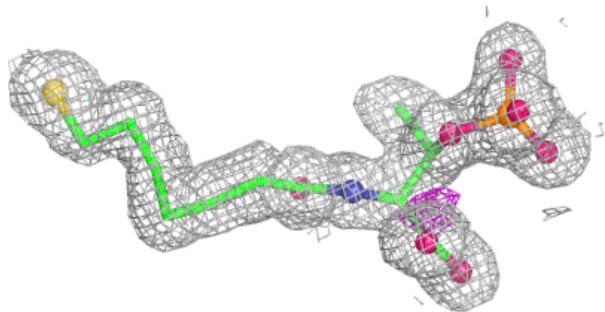


Electron density around XP8 D 553 (B):

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

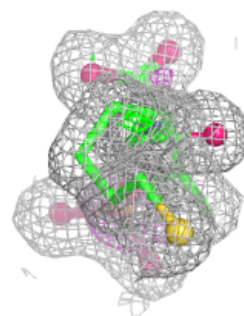
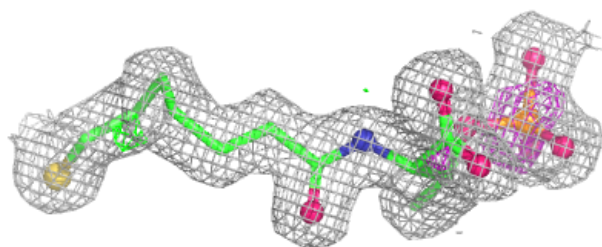
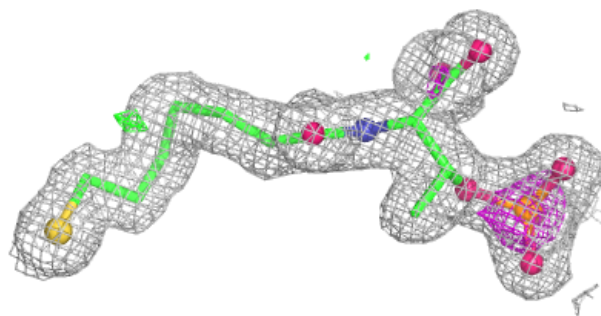
**Electron density around TP7 A 552 (A):**

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



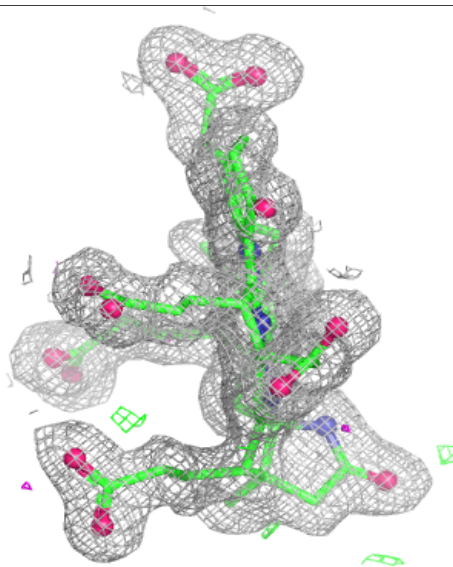
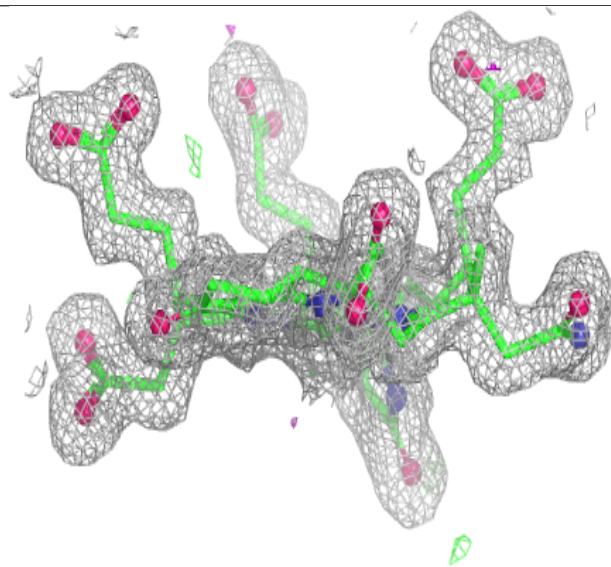
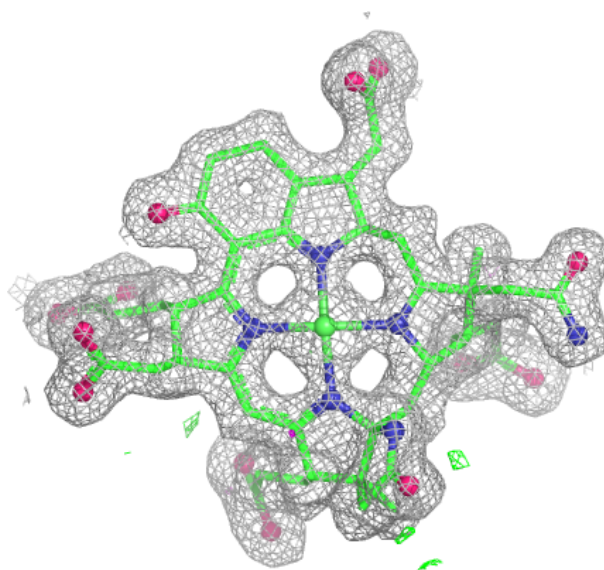
Electron density around TP7 D 1 (A):

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



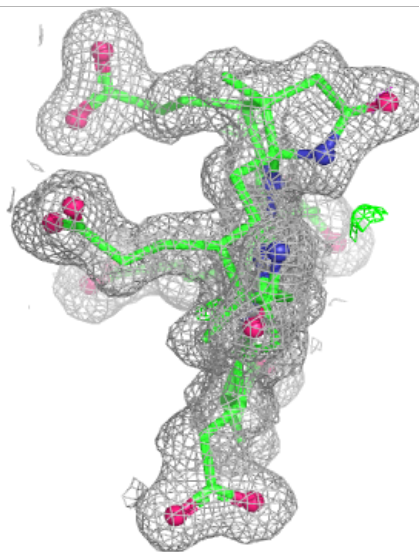
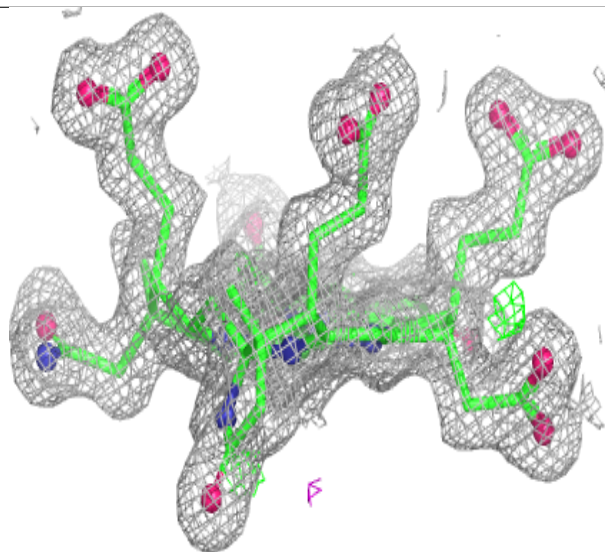
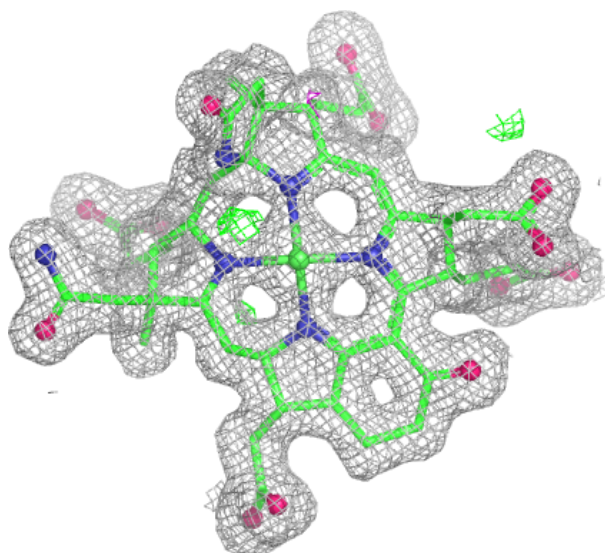
Electron density around F43 A 1:

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



Electron density around F43 D 551:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.