



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:40 PM EDT

PDB ID : 7SUC / pdb_00007suc
Title : XFEL Serial Crystallography Reveals the Room Temperature Structure of Methyl-Coenzyme M Reductase
Authors : Ohmer, C.J.; Dasgupta, M.
Deposited on : 2021-11-16
Resolution : 1.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

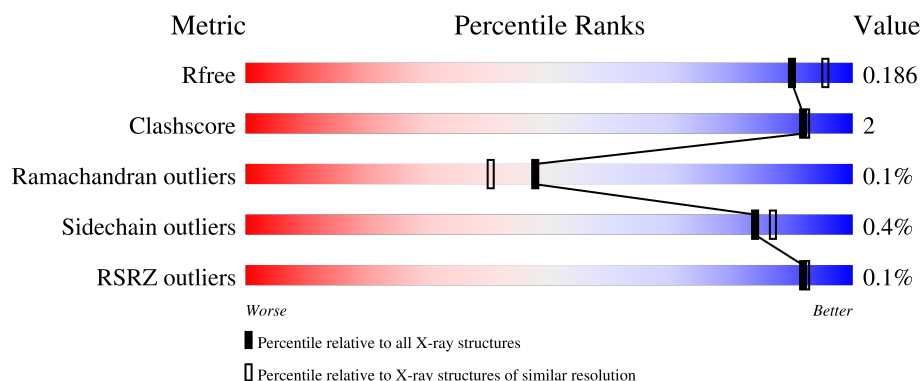
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



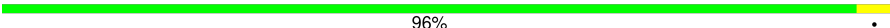
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	548	96% .
1	a	548	93% 7%
2	B	442	95% 5%
2	b	442	96% .
3	C	246	99% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	246	 96%

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
1	DYA	A	450	-	X	-	-
1	DYA	a	450	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 39730 atoms, of which 19268 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	H	N	O	S	6	16	0
			8447	2731	4133	720	843	20			
1	a	548	Total	C	H	N	O	S	13	21	0
			8547	2764	4192	720	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	H	N	O	S	0	13	0
			6768	2141	3393	555	661	18			
2	b	442	Total	C	H	N	O	S	0	22	0
			6848	2166	3434	556	671	21			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	246	Total	C	H	N	O	S	0	8	0
			3995	1259	1965	354	405	12			
3	c	246	Total	C	H	N	O	S	0	10	0
			4039	1270	1994	357	407	11			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

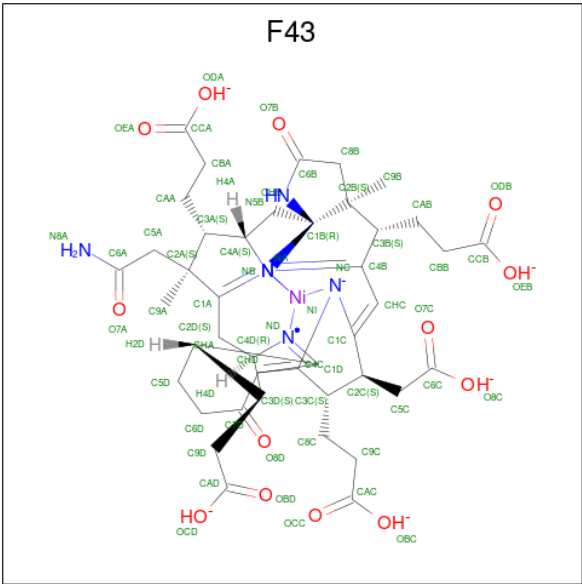
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	a	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

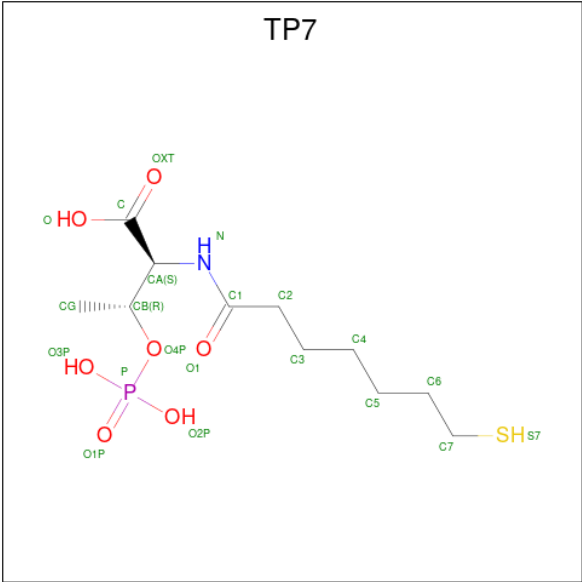
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	b	1	Total	Mg	0	0
			1	1		
4	c	1	Total	Mg	0	0
			1	1		

- Molecule 5 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$) (labeled as "Ligand of Interest" by depositor).



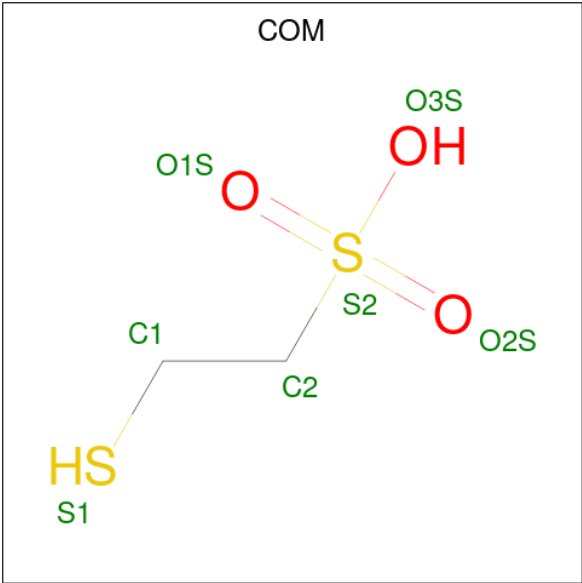
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	Ni	O	0	0
			113	42	51	6	1	13		
5	a	1	Total	C	H	N	Ni	O	0	0
			113	42	51	6	1	13		

- Molecule 6 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
6	A	1	40	11	19	1	7	1	1	0	1
6	A	1	40	11	19	1	7	1	1	0	1

- Molecule 7 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: C₂H₆O₃S₂).



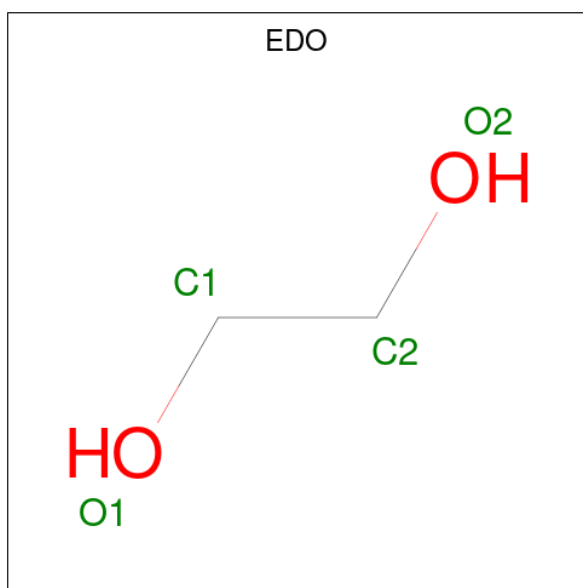
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
7	A	1	11	2	4	3	2	0	0
7	a	1	11	2	4	3	2	0	0

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	1
			7	2	3	2		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	a	1	Total	C	H	O	0	0
			10	2	6	2		

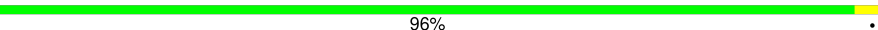
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	199	Total 199	O 199	0	0
10	B	117	Total 117	O 117	0	0
10	C	62	Total 62	O 62	0	0
10	a	178	Total 178	O 178	0	0
10	b	108	Total 108	O 108	0	0
10	c	70	Total 70	O 70	0	0

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.

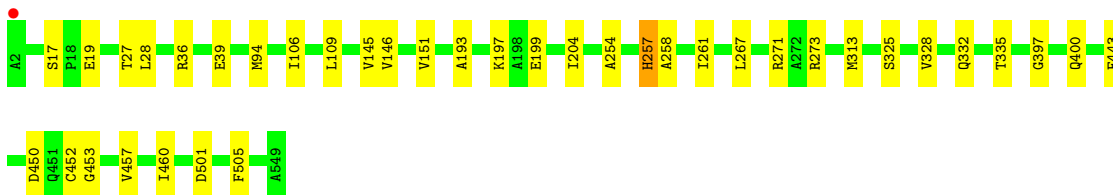
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain A:  96%

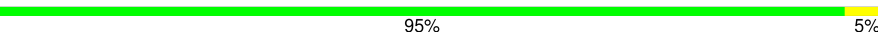


- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain a:  93% 7%

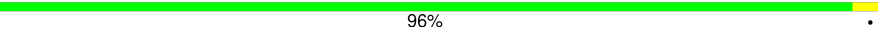


- Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain B:  95% 5%

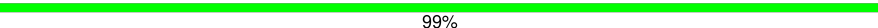


- Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain b:  96%

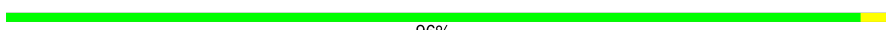


- Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C:  99%



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

Chain c:  96% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.08Å 119.78Å 123.21Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	21.25 – 1.90 21.25 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (21.25-1.90) 91.2 (21.25-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.152 , 0.186 0.152 , 0.186	Depositor DCC
R_{free} test set	2010 reflections (1.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k 0.022 for -h,-l,-k 0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	39730	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: COM, MG, ACT, GL3, EDO, SMC, MGN, TP7, F43, DYA, AGM, 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	0.20	0/4417	0.45	0/5994
1	a	0.19	0/4460	0.43	0/6052
2	B	0.18	0/3475	0.40	0/4706
2	b	0.17	0/3550	0.40	0/4805
3	C	0.19	0/2098	0.42	0/2826
3	c	0.19	0/2112	0.42	0/2844
All	All	0.19	0/20112	0.42	0/27227

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4314	4133	4080	12	0
1	a	4355	4192	4157	24	0
2	B	3375	3393	3372	13	0
2	b	3414	3434	3388	11	0
3	C	2030	1965	1955	2	0
3	c	2045	1994	1992	5	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	a	2	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
5	A	62	51	43	2	0
5	a	62	51	43	2	0
6	A	42	38	38	2	0
7	A	7	4	5	1	0
7	a	7	4	5	1	0
8	A	4	3	3	1	0
9	a	4	6	6	0	0
10	A	199	0	0	2	0
10	B	117	0	0	1	0
10	C	62	0	0	0	0
10	a	178	0	0	0	0
10	b	108	0	0	1	0
10	c	70	0	0	0	0
All	All	20462	19268	19087	62	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 2.

All (62) 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:42[B]:ILE:HD11	2:B:178:MET:HE2	1.79	0.63
1:A:229:MET:HE1	2:b:367:TYR:HA	1.83	0.60
1:A:254:ALA:HA	1:A:258:ALA:HB3	1.86	0.56
1:a:94:MET:HB3	1:a:313:MET:SD	2.47	0.55
1:a:28[A]:LEU:N	1:a:28[A]:LEU:HD12	2.22	0.54
1:A:328:VAL:HB	5:a:603:F43:H9A1	1.89	0.54
2:b:351:LYS:NZ	10:b:601:HOH:O	2.41	0.52
2:b:246[B]:MET:HE1	2:b:432:VAL:HG12	1.92	0.51
1:a:109:LEU:HB2	1:a:204[B]:ILE:HG23	1.93	0.51
2:B:68:LYS:NZ	1:a:199:GLU:OE2	2.34	0.51
2:b:17:LEU:HD11	2:b:20[A]:GLU:HG2	1.93	0.51
1:a:94:MET:HB3	1:a:313:MET:CE	2.40	0.51
1:a:94:MET:HB3	1:a:313:MET:HE2	1.92	0.51
5:A:602:F43:H9A1	1:a:328:VAL:HB	1.93	0.50
2:B:2:ALA:N	10:B:603:HOH:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:254:ALA:HA	1:a:258:ALA:HB3	1.94	0.49
5:a:603:F43:O8D	5:a:603:F43:H3C	2.12	0.49
5:A:602:F43:H3C	5:A:602:F43:O8D	2.13	0.48
1:A:302:ARG:NH2	10:A:702:HOH:O	2.47	0.48
2:b:37:SER:OG	2:b:424[B]:GLU:OE1	2.26	0.48
1:A:432:TYR:HB3	3:C:234:MET:HE2	1.98	0.46
2:b:182:PRO:O	2:b:185:LEU:HG	2.17	0.45
2:B:214:LEU:HB2	2:B:428:PRO:HG3	1.99	0.45
1:a:145:VAL:HG23	1:a:146:VAL:HG23	1.98	0.45
3:c:234:MET:HE3	3:c:234:MET:HA	1.98	0.44
1:a:460:ILE:C	1:a:460:ILE:HD12	2.42	0.44
2:B:70:MET:HE3	1:a:501:ASP:HB3	1.98	0.44
3:C:99:TYR:CD1	3:C:116:THR:HG21	2.53	0.44
1:a:397:GLY:H	1:a:400:MGN:HN21	1.66	0.44
6:A:603[A]:TP7:O2P	1:a:257:MHS:NE2	2.52	0.43
1:a:36:ARG:NH1	1:a:39:GLU:OE1	2.50	0.43
1:a:106:ILE:HB	1:a:261:ILE:HB	2.00	0.43
3:c:82:VAL:O	3:c:83:ARG:HD2	2.18	0.43
1:A:225:ARG:O	1:A:229:MET:HG2	2.19	0.43
2:B:130:ALA:HB3	2:B:131:PRO:CD	2.48	0.43
1:a:332:GLN:HA	1:a:335:THR:OG1	2.19	0.43
8:A:605[B]:ACT:H2	10:A:890:HOH:O	2.18	0.43
1:a:193:ALA:O	1:a:197:LYS:HG3	2.19	0.43
2:b:74:LEU:HD11	2:b:152:ASP:HB3	1.99	0.43
1:A:501:ASP:HB3	2:b:70:MET:HE3	2.00	0.43
2:B:7:LYS:HD2	2:B:21:GLN:HE21	1.84	0.43
3:c:95:PRO:HA	3:c:214:THR:HA	2.01	0.43
1:A:505:PHE:CE1	2:b:67:CYS:HB3	2.54	0.43
1:a:17:SER:OG	1:a:19:GLU:OE1	2.36	0.42
1:A:83:GLY:HA3	1:a:151:VAL:HG11	2.01	0.42
3:c:155:VAL:O	3:c:156:HIS:C	2.61	0.42
2:B:335:ASN:OD1	2:B:346:SER:HB2	2.19	0.42
1:a:453:GLY:O	1:a:457:VAL:HG23	2.19	0.41
2:b:190:TYR:CE1	2:b:226:MET:HE3	2.55	0.41
2:B:42[B]:ILE:CD1	2:B:178:MET:HE2	2.47	0.41
1:A:312:ALA:O	1:A:316:ASP:HB2	2.20	0.41
1:A:481:ASN:HA	6:A:603[A]:TP7:S7	2.59	0.41
2:B:311:MET:HG3	2:B:315:MET:HE3	2.02	0.41
1:a:443:PHE:HB2	7:a:604:COM:O1S	2.19	0.41
1:a:267:LEU:HD12	1:a:273:ARG:HB2	2.03	0.41
2:B:272:LEU:HD13	2:B:272:LEU:C	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:54:PRO:O	3:c:59:MET:HE3	2.22	0.40
2:B:67:CYS:HB3	1:a:505:PHE:CE1	2.56	0.40
1:a:28[A]:LEU:N	1:a:28[A]:LEU:CD1	2.84	0.40
1:A:443:PHE:HB2	7:A:604:COM:O1S	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	556/548 (102%)	536 (96%)	19 (3%)	1 (0%)	43	36
1	a	561/548 (102%)	540 (96%)	20 (4%)	1 (0%)	43	36
2	B	453/442 (102%)	443 (98%)	9 (2%)	1 (0%)	43	36
2	b	462/442 (104%)	455 (98%)	7 (2%)	0	100	100
3	C	252/246 (102%)	243 (96%)	9 (4%)	0	100	100
3	c	254/246 (103%)	247 (97%)	7 (3%)	0	100	100
All	All	2538/2472 (103%)	2464 (97%)	71 (3%)	3 (0%)	48	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	a	325	SER
2	B	402	GLY

5.3.2 Protein sidechains [i](#)

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	447/432 (104%)	445 (100%)	2 (0%)	84	87
1	a	452/432 (105%)	450 (100%)	2 (0%)	84	87
2	B	354/341 (104%)	350 (99%)	4 (1%)	65	67
2	b	363/341 (106%)	361 (99%)	2 (1%)	78	81
3	C	222/214 (104%)	222 (100%)	0	100	100
3	c	224/214 (105%)	222 (99%)	2 (1%)	70	73
All	All	2062/1974 (104%)	2050 (99%)	12 (1%)	84	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	545[A]	LEU
1	A	545[B]	LEU
2	B	83[A]	GLU
2	B	83[B]	GLU
2	B	126	GLU
2	B	147	ASP
1	a	27[A]	THR
1	a	27[B]	THR
2	b	297[A]	ASP
2	b	297[B]	ASP
3	c	194[A]	GLU
3	c	194[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	296	ASN
1	A	437	GLN
1	A	449	GLN
2	B	21	GLN
2	B	174	ASN
2	B	421	GLN
3	C	178	ASN
1	a	456	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	477	ASN
2	b	94	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AGM	A	271	1	10,11,12	1.31	1 (10%)	7,13,15	1.37	1 (14%)
1	MGN	a	400	1	6,9,10	0.76	0	7,12,14	0.75	0
1	DYA	A	450	1	6,7,8	2.51	2 (33%)	6,8,10	3.72	3 (50%)
1	GL3	a	445	1	2,3,4	1.40	0	1,2,4	0.51	0
1	MHS	A	257	1	10,11,12	1.81	3 (30%)	5,14,16	1.13	1 (20%)
1	AGM	a	271	1	10,11,12	1.20	1 (10%)	7,13,15	0.95	0
1	MGN	A	400	1	6,9,10	0.75	0	7,12,14	0.93	0
1	GL3	A	445	1	2,3,4	1.46	1 (50%)	1,2,4	0.20	0
1	SMC	a	452	1	5,6,7	0.93	0	3,6,8	1.50	1 (33%)
1	DYA	a	450	1	6,7,8	2.50	2 (33%)	6,8,10	3.98	3 (50%)
1	SMC	A	452	1	5,6,7	0.93	0	3,6,8	1.89	1 (33%)
1	MHS	a	257	1	10,11,12	1.78	2 (20%)	5,14,16	1.49	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGM	A	271	1	-	2/10/11/13	-
1	MGN	a	400	1	-	2/7/9/12	-
1	DYA	A	450	1	-	4/4/6/8	-
1	GL3	a	445	1	-	1/1/1/2	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	AGM	a	271	1	-	1/10/11/13	-
1	MGN	A	400	1	-	1/7/9/12	-
1	GL3	A	445	1	-	0/1/1/2	-
1	SMC	a	452	1	-	1/3/5/7	-
1	DYA	a	450	1	-	4/4/6/8	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MHS	a	257	1	-	0/5/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	450	DYA	C-CA	4.38	1.52	1.45
1	a	450	DYA	C-CA	4.23	1.52	1.45
1	A	257	MHS	CD2-CG	3.76	1.41	1.36
1	a	257	MHS	CD2-CG	3.70	1.41	1.36
1	A	271	AGM	CZ-NE1	2.91	1.38	1.33
1	a	450	DYA	CB-CA	-2.90	1.28	1.36
1	A	450	DYA	CB-CA	-2.54	1.29	1.36
1	a	271	AGM	CZ-NE1	2.44	1.37	1.33
1	a	257	MHS	CG-ND1	2.25	1.41	1.38
1	A	257	MHS	CG-ND1	2.11	1.41	1.38
1	A	445	GL3	C-S	-2.05	1.72	1.80
1	A	257	MHS	CE1-ND1	2.04	1.40	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	450	DYA	CB-CA-N	-7.14	110.28	123.25
1	A	450	DYA	CB-CA-N	-6.10	112.17	123.25
1	A	450	DYA	O-C-CA	-5.77	118.16	125.39
1	a	450	DYA	O-C-CA	-5.69	118.26	125.39
1	A	450	DYA	CA-CB-CG	2.96	135.66	126.27
1	a	257	MHS	ND1-CE1-NE2	-2.79	111.28	112.94
1	A	452	SMC	CA-CB-SG	-2.78	109.54	114.04
1	a	450	DYA	CA-CB-CG	2.57	134.42	126.27
1	A	271	AGM	NH1-CZ-NE1	2.27	124.58	119.58
1	a	452	SMC	CB-CA-C	-2.23	104.75	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	ND1-CE1-NE2	-2.21	111.63	112.94

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	450	DYA	N-CA-CB-CG
1	A	450	DYA	O-C-CA-CB
1	A	450	DYA	CA-CB-CG-OD1
1	A	452	SMC	CA-CB-SG-CS
1	a	450	DYA	N-CA-CB-CG
1	a	450	DYA	O-C-CA-CB
1	a	452	SMC	CA-CB-SG-CS
1	A	450	DYA	CA-CB-CG-OD2
1	a	450	DYA	CA-CB-CG-OD1
1	a	450	DYA	CA-CB-CG-OD2
1	A	271	AGM	NE1-CD-CG-CB
1	a	400	MGN	OE1-CD-CG-CB1
1	a	445	GL3	S-C-CA-N
1	A	271	AGM	CE2-CD-CG-CB
1	a	400	MGN	NE2-CD-CG-CB1
1	a	271	AGM	NE1-CD-CG-CB
1	A	400	MGN	NE2-CD-CG-CB1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	400	MGN	1	0
1	a	257	MHS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	TP7	A	606[A]	-	19,20,20	1.62	3 (15%)	24,26,26	1.09	2 (8%)
9	EDO	a	605	-	3,3,3	0.46	0	2,2,2	0.34	0
7	COM	A	604	5	6,6,6	1.62	2 (33%)	8,8,8	1.19	1 (12%)
5	F43	A	602	7,1	63,71,71	1.85	4 (6%)	73,118,118	1.28	11 (15%)
7	COM	a	604	5	6,6,6	1.44	0	8,8,8	1.62	2 (25%)
5	F43	a	603	7,1	63,71,71	1.78	4 (6%)	73,118,118	1.26	10 (13%)
6	TP7	A	603[A]	-	19,20,20	1.15	1 (5%)	24,26,26	1.08	2 (8%)
8	ACT	A	605[B]	-	3,3,3	1.16	0	3,3,3	1.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TP7	A	606[A]	-	-	0/24/24/24	-
9	EDO	a	605	-	-	0/1/1/1	-
7	COM	A	604	5	-	0/4/4/4	-
5	F43	A	602	7,1	-	8/28/185/185	-
7	COM	a	604	5	-	0/4/4/4	-
5	F43	a	603	7,1	-	6/28/185/185	-
6	TP7	A	603[A]	-	-	2/24/24/24	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	F43	NI-NA	8.90	2.10	1.89
5	a	603	F43	NI-NA	8.64	2.10	1.89
5	A	602	F43	NI-NB	8.33	2.09	1.89
5	a	603	F43	NI-NB	8.08	2.08	1.89
5	A	602	F43	NI-ND	6.66	2.05	1.89
5	a	603	F43	NI-ND	6.41	2.04	1.89
6	A	606[A]	TP7	OXT-C	4.35	1.35	1.22
6	A	606[A]	TP7	P-O1P	3.58	1.61	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603[A]	TP7	P-O1P	3.56	1.61	1.50
6	A	606[A]	TP7	O-C	-2.97	1.21	1.30
7	A	604	COM	O2S-S2	2.67	1.52	1.45
5	A	602	F43	CHB-C1B	2.45	1.54	1.53
5	a	603	F43	CHB-C1B	2.17	1.54	1.53
7	A	604	COM	C2-S2	2.14	1.80	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	F43	C3A-C2A-C1A	3.90	103.87	99.97
5	a	603	F43	C5D-C2D-C1D	-3.76	105.52	110.43
5	A	602	F43	C2A-C3A-C4A	-3.73	96.71	102.36
5	a	603	F43	C2A-C3A-C4A	-3.55	96.99	102.36
7	a	604	COM	O2S-S2-C2	3.24	111.62	106.73
5	a	603	F43	C3A-C2A-C1A	3.13	103.10	99.97
5	a	603	F43	C9D-C3D-C4D	-2.93	106.93	114.63
5	A	602	F43	C3A-C4A-NA	2.70	106.40	102.30
5	A	602	F43	C4B-CHC-C1C	2.69	130.19	125.84
5	A	602	F43	C5D-C2D-C1D	-2.67	106.95	110.43
5	a	603	F43	C5D-C2D-C3D	-2.57	113.59	118.26
5	A	602	F43	C9D-C3D-C4D	-2.56	107.91	114.63
6	A	606[A]	TP7	C-CA-N	-2.55	104.57	110.17
5	a	603	F43	C4B-CHC-C1C	2.54	129.95	125.84
6	A	603[A]	TP7	C-CA-N	-2.50	104.69	110.17
5	A	602	F43	C3D-C4D-ND	2.48	106.19	102.34
5	A	602	F43	C5D-C2D-C3D	-2.44	113.81	118.26
5	a	603	F43	C3D-C4D-ND	2.39	106.06	102.34
5	A	602	F43	CHA-C4D-C3D	-2.29	111.45	117.90
5	a	603	F43	C3A-C4A-NA	2.24	105.71	102.30
6	A	606[A]	TP7	O-C-CA	2.20	121.78	114.15
5	A	602	F43	C4A-NA-C1A	-2.10	106.22	109.08
5	a	603	F43	C2B-C1B-NB	2.10	104.98	101.86
7	a	604	COM	O1S-S2-C2	2.06	109.85	106.73
5	A	602	F43	C2B-C1B-NB	2.06	104.92	101.86
5	a	603	F43	CHA-C4D-C3D	-2.06	112.10	117.90
6	A	603[A]	TP7	C3-C2-C1	-2.04	107.55	113.19
7	A	604	COM	O3S-S2-C2	2.02	109.96	106.00

There are no chirality outliers.

All (16) torsion outliers are listed below:

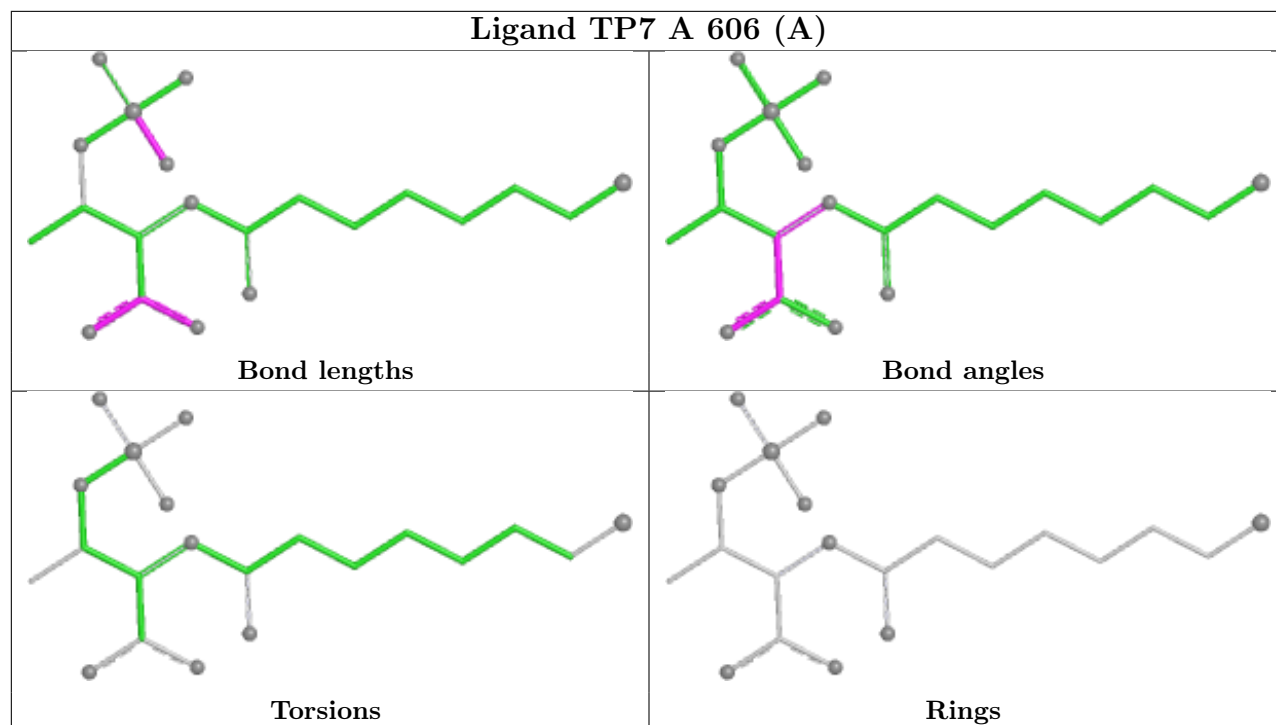
Mol	Chain	Res	Type	Atoms
5	A	602	F43	C3A-CAA-CBA-CCA
5	a	603	F43	C3A-CAA-CBA-CCA
5	a	603	F43	C2C-C5C-C6C-O8C
5	A	602	F43	C2C-C5C-C6C-O8C
5	a	603	F43	CAA-CBA-CCA-OEA
5	A	602	F43	CAA-CBA-CCA-OEA
5	a	603	F43	CAB-CBB-CCB-OEB
5	a	603	F43	CAA-CBA-CCA-ODA
5	A	602	F43	CAB-CBB-CCB-OEB
5	A	602	F43	C8C-C9C-CAC-OBC
5	A	602	F43	CAA-CBA-CCA-ODA
6	A	603[A]	TP7	CB-O4P-P-O3P
5	A	602	F43	C3D-C9D-CAD-OB
5	A	602	F43	CAB-CBB-CCB-OD
6	A	603[A]	TP7	C2-C3-C4-C5
5	a	603	F43	C3D-C9D-CAD-OD

There are no ring outliers.

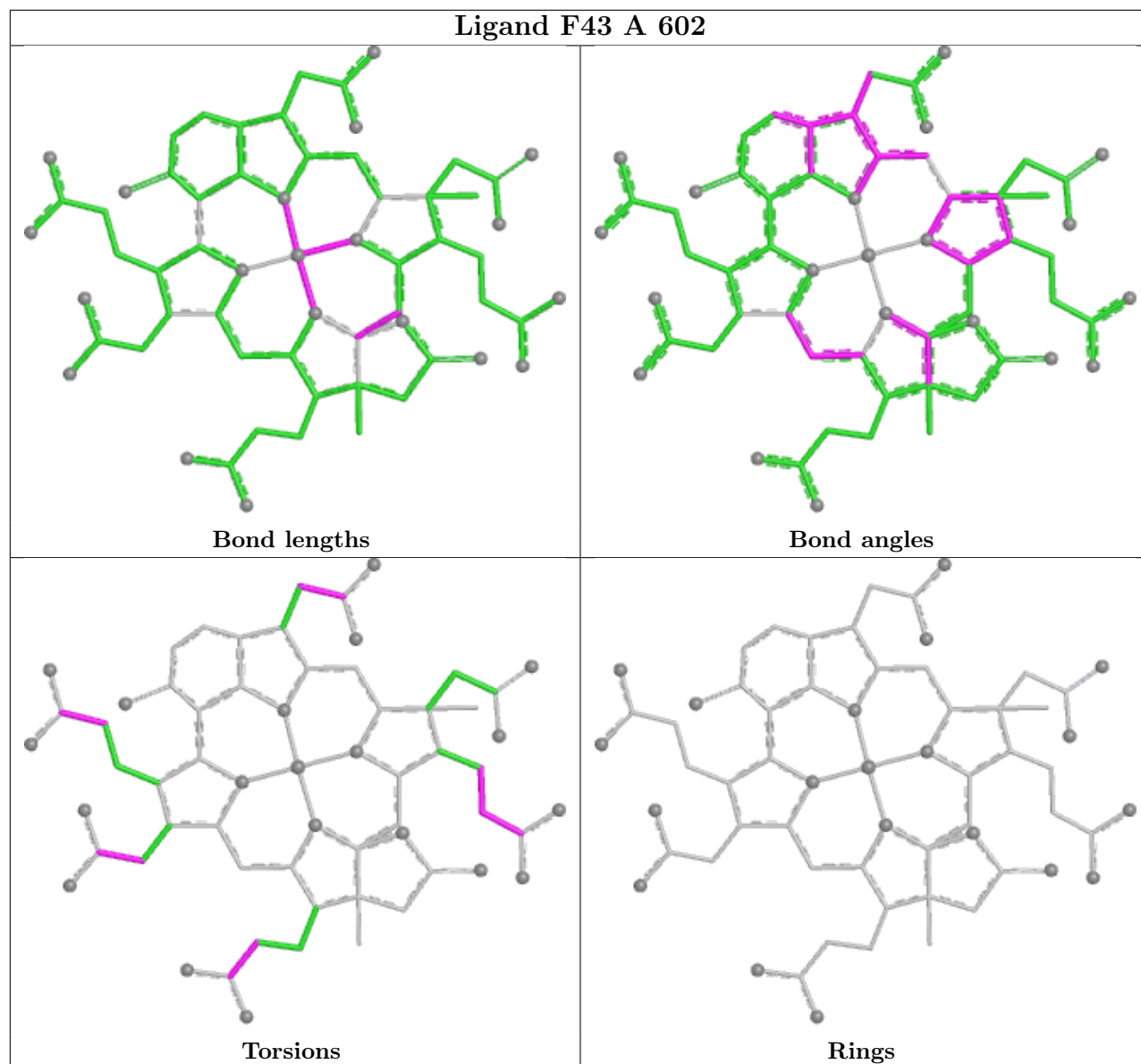
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	604	COM	1	0
5	A	602	F43	2	0
7	a	604	COM	1	0
5	a	603	F43	2	0
6	A	603[A]	TP7	2	0
8	A	605[B]	ACT	1	0

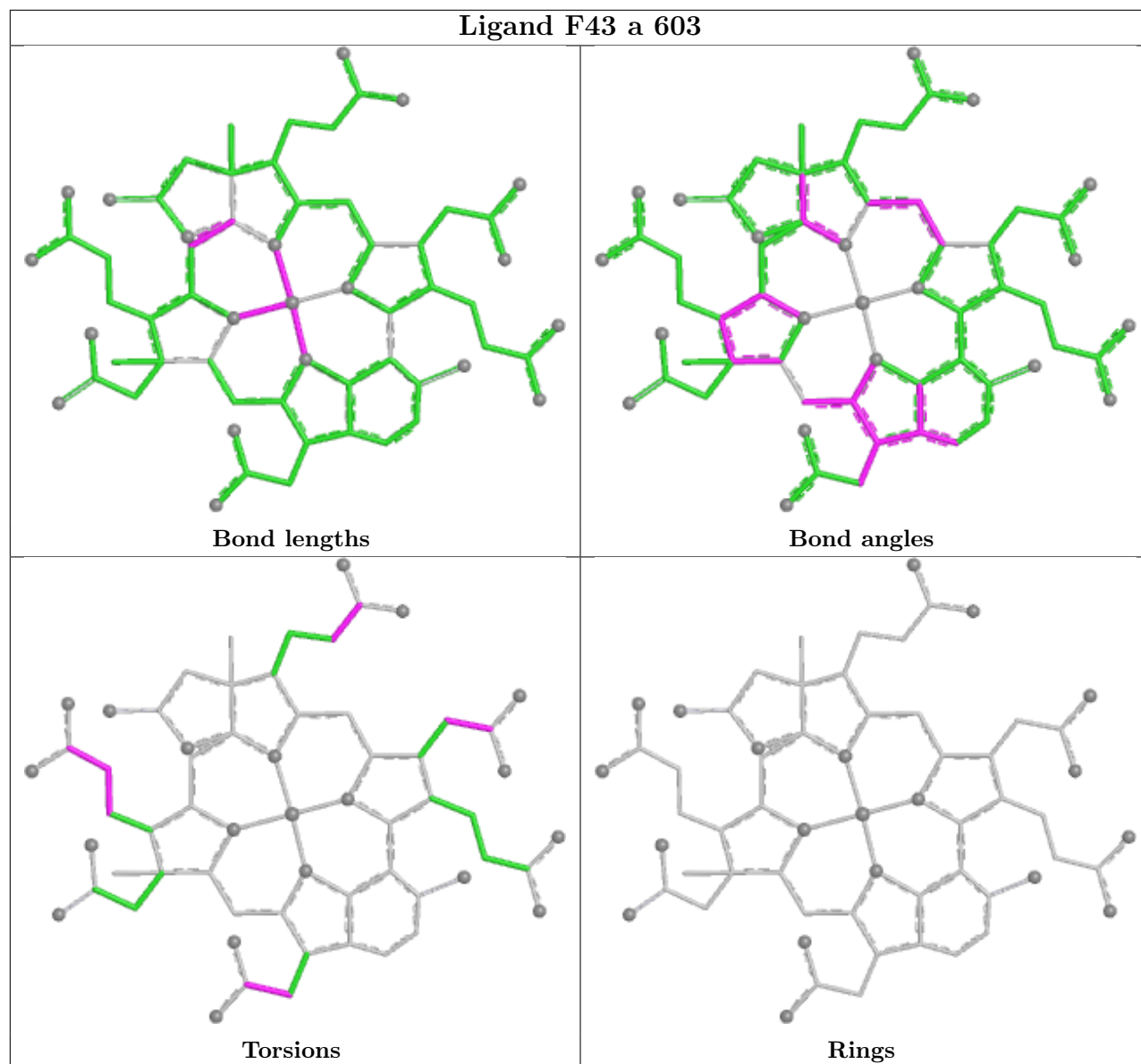
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

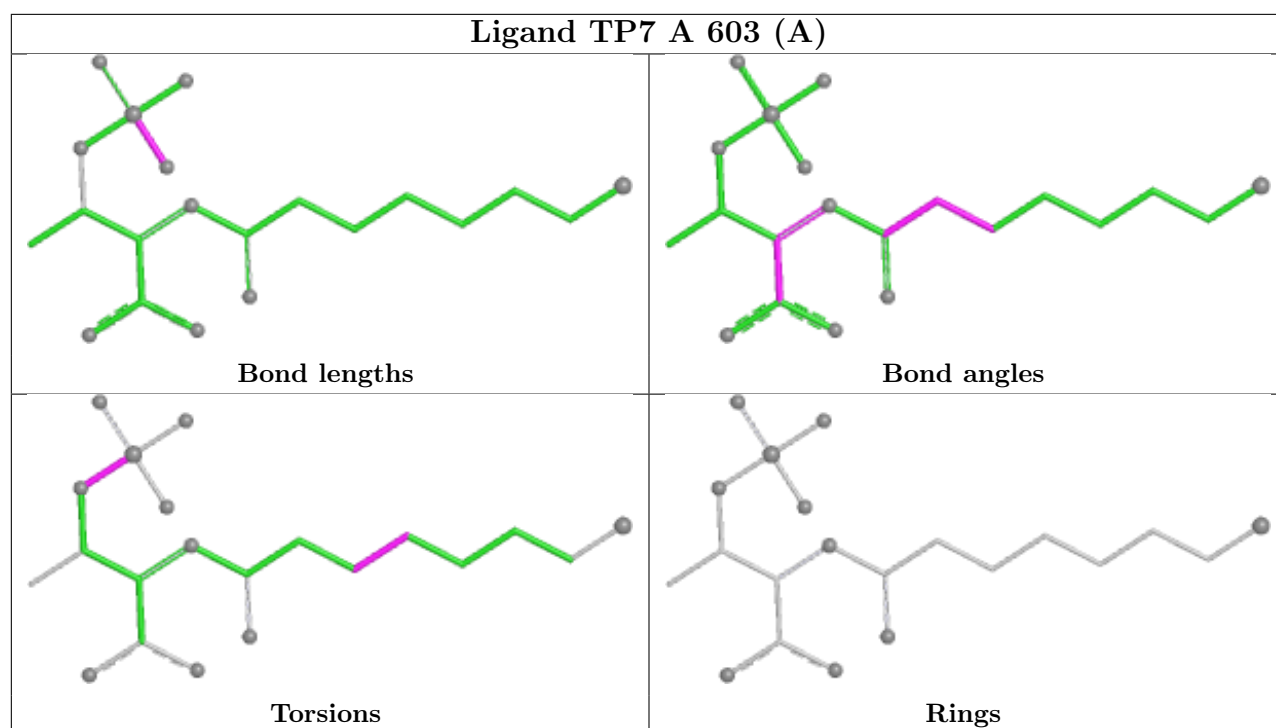


Ligand F43 A 602



Ligand F43 a 603





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(Å ²)	Q<0.9
1	A	542/548 (98%)	-0.61	0 100 100	13, 27, 43, 82	11 (2%)
1	a	542/548 (98%)	-0.65	1 (0%) 91 92	11, 26, 42, 85	18 (3%)
2	B	442/442 (100%)	-0.37	0 100 100	16, 33, 49, 80	11 (2%)
2	b	442/442 (100%)	-0.32	1 (0%) 91 92	17, 34, 54, 70	17 (3%)
3	C	246/246 (100%)	-0.19	0 100 100	16, 36, 61, 96	7 (2%)
3	c	246/246 (100%)	-0.12	0 100 100	15, 37, 63, 89	10 (4%)
All	All	2460/2472 (99%)	-0.43	2 (0%) 92 92	11, 31, 51, 96	74 (3%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	2	ALA	3.0
2	b	2	ALA	2.2

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	DYA	A	450	8/9	0.92	0.07	20,23,23,23	0
1	MHS	A	257	11/12	0.94	0.06	27,34,44,44	0
1	DYA	a	450	8/9	0.94	0.06	19,21,22,22	0
1	MHS	a	257	11/12	0.95	0.07	25,32,40,40	0
1	AGM	A	271	12/13	0.96	0.05	18,22,26,26	0
1	AGM	a	271	12/13	0.97	0.05	18,21,25,26	0
1	MGN	a	400	10/11	0.97	0.05	17,22,24,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MGN	A	400	10/11	0.97	0.05	19,22,25,25	0
1	GL3	A	445	4/5	0.99	0.04	19,22,23,28	0
1	GL3	a	445	4/5	0.99	0.04	19,20,27,27	0
1	SMC	A	452	7/8	0.99	0.04	19,23,27,27	0
1	SMC	a	452	7/8	0.99	0.04	20,23,27,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

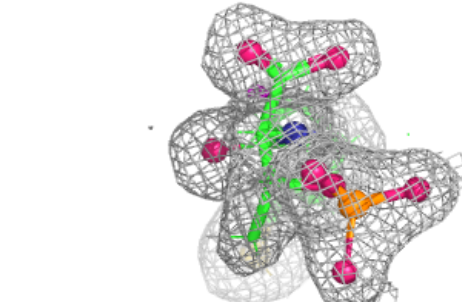
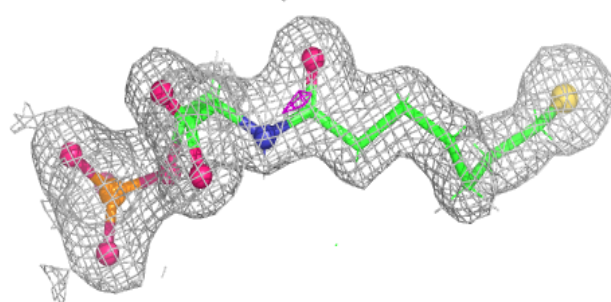
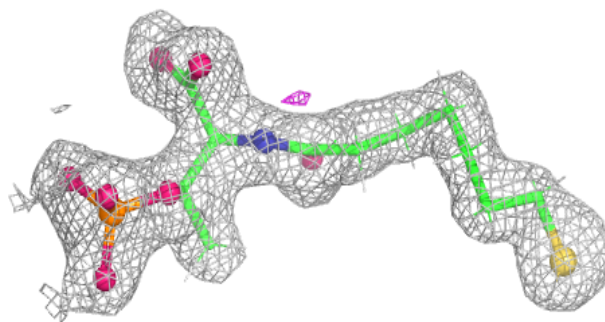
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ACT	A	605[B]	4/4	0.70	0.25	29,32,37,37	7
4	MG	A	601	1/1	0.74	0.12	59,59,59,59	0
9	EDO	a	605	4/4	0.75	0.14	52,64,74,77	0
4	MG	C	301	1/1	0.80	0.08	56,56,56,56	0
4	MG	a	602	1/1	0.80	0.10	61,61,61,61	0
4	MG	a	601	1/1	0.82	0.13	55,55,55,55	0
4	MG	B	501	1/1	0.82	0.14	63,63,63,63	0
4	MG	b	501	1/1	0.86	0.12	66,66,66,66	0
4	MG	c	301	1/1	0.96	0.05	52,52,52,52	0
6	TP7	A	603[A]	21/21	0.98	0.06	20,25,29,29	40
6	TP7	A	606[A]	21/21	0.98	0.05	19,26,31,32	0
7	COM	A	604	7/7	0.99	0.07	22,23,28,28	0
7	COM	a	604	7/7	0.99	0.08	24,25,31,31	0
5	F43	A	602	62/62	0.99	0.04	17,23,27,33	0
5	F43	a	603	62/62	0.99	0.04	17,22,27,30	0

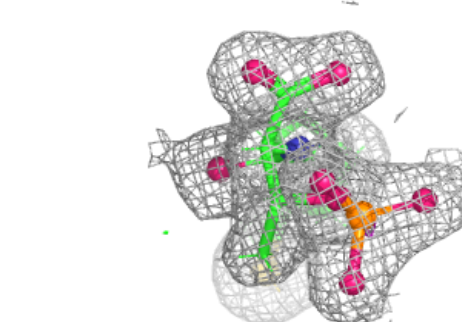
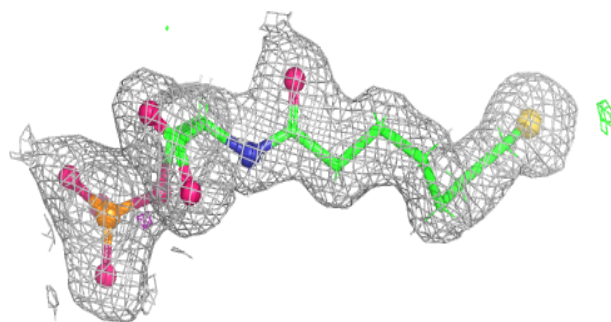
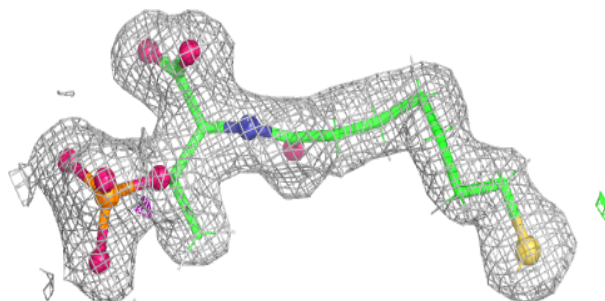
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TP7 A 603 (A):

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

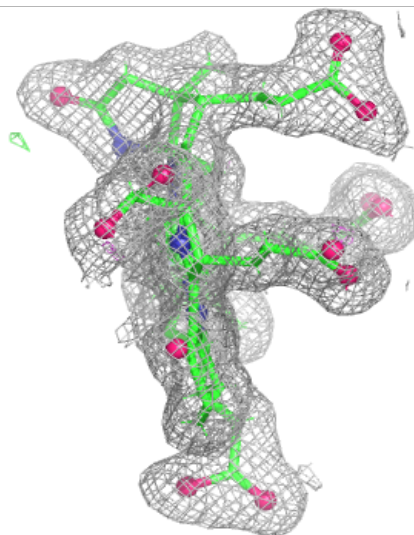
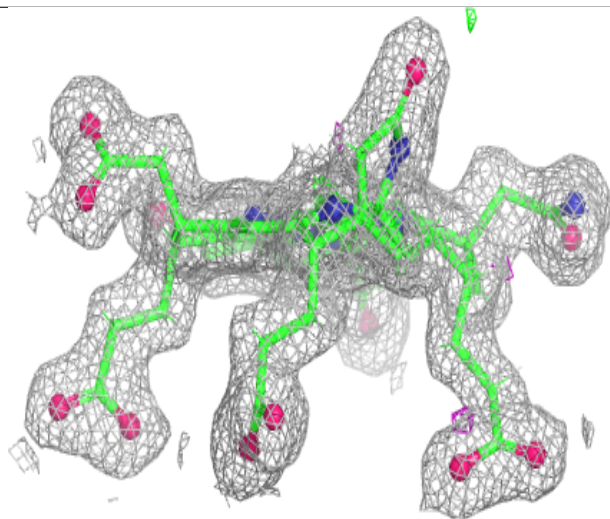
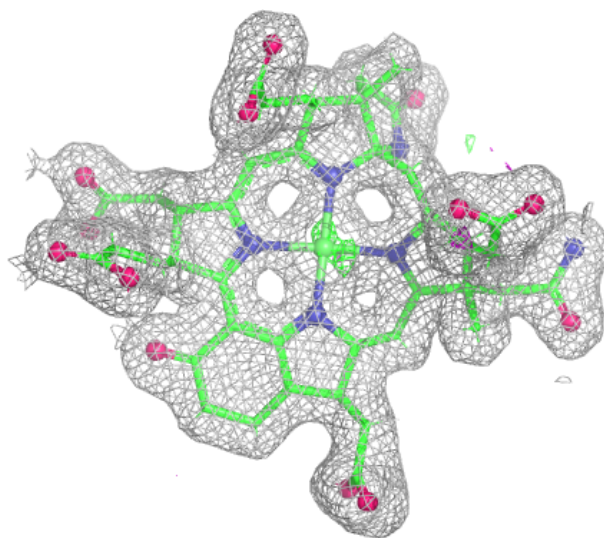
**Electron density around TP7 A 606 (A):**

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



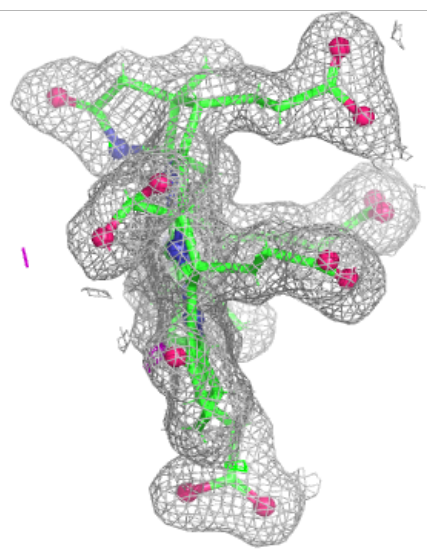
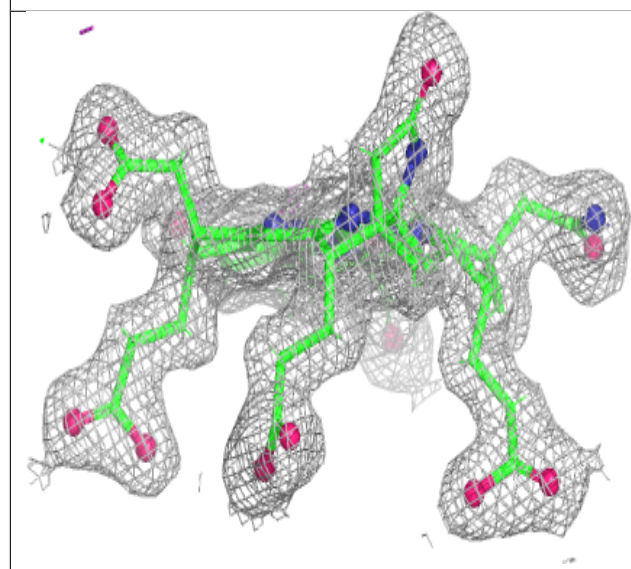
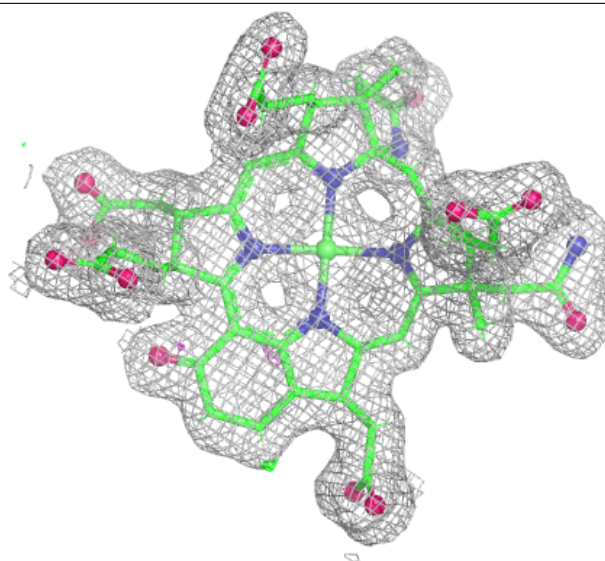
Electron density around F43 A 602:

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



Electron density around F43 a 603:

$2mF_o-DF_c$ (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.