



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2025 – 05:07 pm BST

PDB ID : 9QQT / pdb_00009qqt
Title : Methyl-coenzyme M reductase of ANME-2d Candidatus Methanoperedens
Vercelli Strain 1 from a bioreactor enrichment culture
Authors : Mueller, M.-C.; Wagner, T.
Deposited on : 2025-04-02
Resolution : 0.98 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

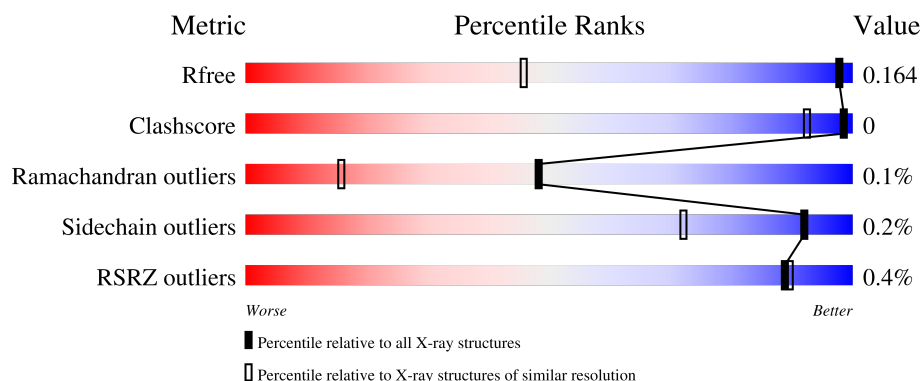
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.98 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.



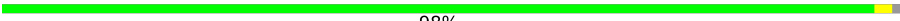
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1026 (1.02-0.94)
Clashscore	180529	1154 (1.02-0.94)
Ramachandran outliers	177936	1094 (1.02-0.94)
Sidechain outliers	177891	1095 (1.02-0.94)
RSRZ outliers	164620	1025 (1.02-0.94)

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	566	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
2	B	434	<div> <div>97%</div> <div>.</div> </div>
2	E	434	<div> <div>98%</div> <div>.</div> </div>
3	C	249	<div> <div>98%</div> <div>.</div> </div>
3	F	249	<div> <div>%</div> <div>98%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	566	 98% ..

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 43046 atoms, of which 19722 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 subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	564	Total	C	H	N	O	S	0	29	0
			8801	2828	4335	761	847	30			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	433	Total	C	H	N	O	S	0	43	0
			6868	2131	3499	575	644	19			
2	E	433	Total	C	H	N	O	S	0	35	0
			6759	2101	3434	567	639	18			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total	C	H	N	O	S	0	15	0
			4053	1281	2001	366	392	13			
3	F	248	Total	C	H	N	O	S	0	13	0
			4016	1270	1980	366	387	13			

- Molecule 4 is a protein called Methyl-coenzyme M reductase subunit alpha.

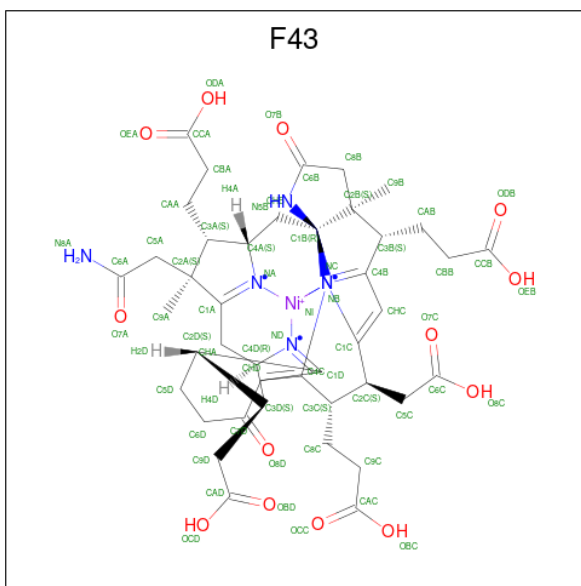
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	563	Total	C	H	N	O	S	0	31	0
			8799	2825	4341	757	845	31			

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

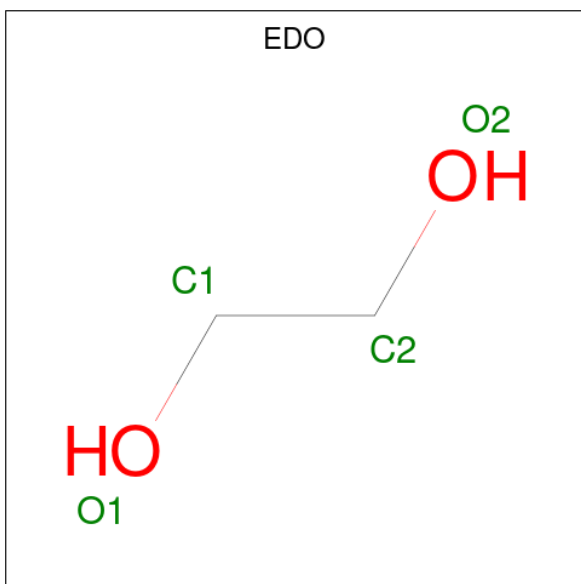
- Molecule 6 is FACTOR 430 (CCD ID: F43) (formula: C₄₂H₅₁N₆NiO₁₃) (labeled as "Ligand

of Interest" by depositor).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



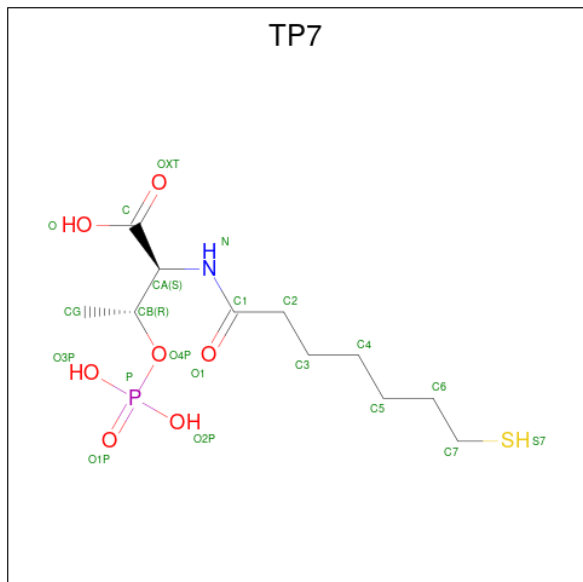
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		

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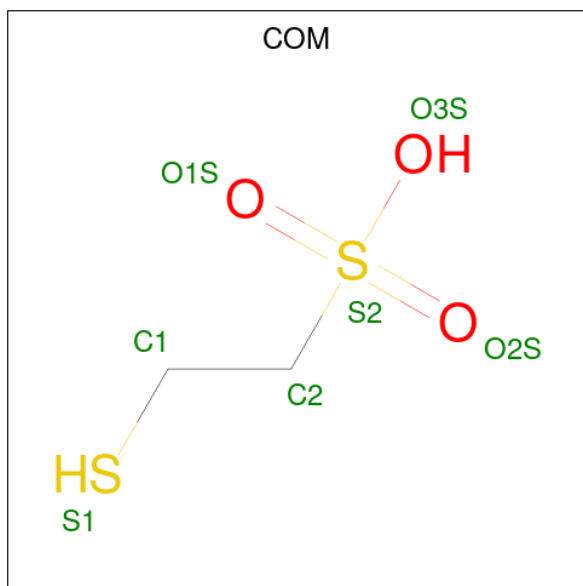
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	C	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	D	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	E	1	Total	C	H	O	0	0
			10	2	6	2		
7	F	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$) (labeled as "Ligand of Interest" by depositor).



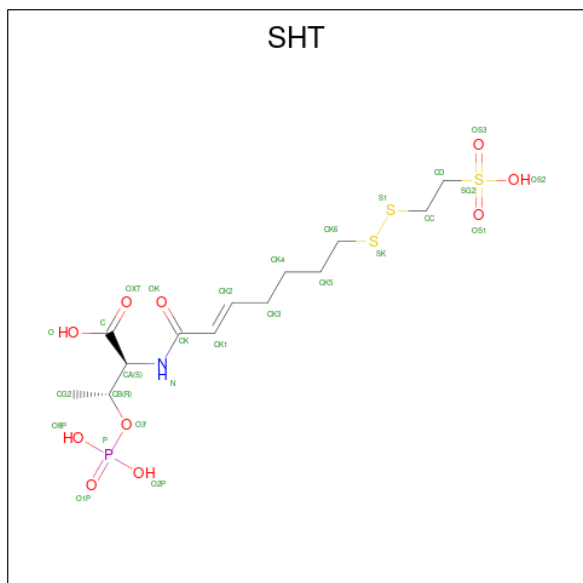
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		
8	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

- Molecule 9 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (CCD ID: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	699	Total	O	0	71
			699	699		
11	B	587	Total	O	0	96
			587	587		
11	C	391	Total	O	0	36
			391	391		
11	D	687	Total	O	0	76
			687	687		
11	E	582	Total	O	0	98
			582	582		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	F	347	Total 347	O 347	0	18

3 Residue-property plots [i](#)

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 subunit alpha

Chain A:  98%



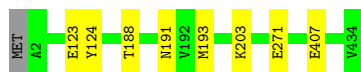
- Molecule 2: Methyl-coenzyme M reductase subunit beta

Chain B:  97%



- Molecule 2: Methyl-coenzyme M reductase subunit beta

Chain E:  98%



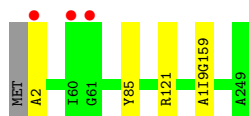
- Molecule 3: Methyl-coenzyme M reductase subunit gamma

Chain C:  98%



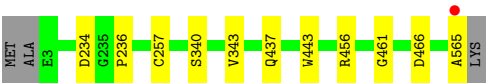
- Molecule 3: Methyl-coenzyme M reductase subunit gamma

Chain F:  98%



● Molecule 4: Methyl-coenzyme M reductase subunit alpha

Chain D:  98% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.62Å 189.82Å 83.93Å 90.00° 114.36° 90.00°	Depositor
Resolution (Å)	41.71 – 0.98 41.71 – 0.98	Depositor EDS
% Data completeness (in resolution range)	74.0 (41.71-0.98) 75.3 (41.71-0.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 0.98Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.128 , 0.148 0.153 , 0.164	Depositor DCC
R_{free} test set	66029 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	6.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	43046	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: K, F43, A1I9G, AGM, MHS, TP7, SHT, CSO, EDO, COM, DYA, GL3, TRX, SMC

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	0.58	4/4607 (0.1%)	0.77	4/6230 (0.1%)
2	B	0.52	0/3573	0.71	2/4834 (0.0%)
2	E	0.54	2/3487 (0.1%)	0.72	0/4721
3	C	0.54	0/2131	0.72	0/2876
3	F	0.50	0/2125	0.72	0/2868
4	D	0.53	0/4600	0.76	0/6217
All	All	0.54	6/20523 (0.0%)	0.74	6/27746 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
2	E	0	2
3	C	0	1
3	F	0	1
4	D	0	1
All	All	0	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78[A]	PRO	C-O	7.19	1.32	1.23
1	A	78[B]	PRO	C-O	7.19	1.32	1.23
1	A	160[A]	ILE	C-O	5.84	1.31	1.24
1	A	160[B]	ILE	C-O	5.84	1.31	1.24
2	E	193[B]	MET	C-O	5.40	1.30	1.23
2	E	193[C]	MET	C-O	5.40	1.30	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160[A]	ILE	CA-C-N	-5.94	116.90	122.66
1	A	160[A]	ILE	C-N-CA	-5.94	116.90	122.66
1	A	160[B]	ILE	CA-C-N	-5.94	116.90	122.66
1	A	160[B]	ILE	C-N-CA	-5.94	116.90	122.66
2	B	127[A]	SER	CA-C-O	5.36	126.23	120.55
2	B	127[B]	SER	CA-C-O	5.36	126.23	120.55

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	ARG	Sidechain
2	B	191[A]	ASN	Mainchain
2	B	191[B]	ASN	Mainchain
2	B	331	TYR	Sidechain
3	C	121	ARG	Sidechain
4	D	456	ARG	Sidechain
2	E	191[A]	ASN	Mainchain
2	E	191[B]	ASN	Mainchain
3	F	121	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4466	4335	4292	3	0
2	B	3369	3499	3404	6	0
2	E	3325	3434	3366	5	0
3	C	2052	2001	1977	2	0
3	F	2036	1980	1947	2	0
4	D	4458	4341	4299	4	0
5	A	1	0	0	0	0
6	A	62	0	43	1	0
6	D	62	0	43	1	0
7	A	12	18	18	0	0
7	B	28	42	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	8	12	12	0	0
7	D	28	42	42	0	0
7	E	8	12	12	0	0
7	F	4	6	6	0	0
8	A	21	0	19	0	0
8	D	21	0	19	0	0
9	A	7	0	4	0	0
9	D	7	0	5	0	0
10	A	28	0	20	0	0
10	D	28	0	20	0	0
11	A	699	0	0	0	0
11	B	587	0	0	1	0
11	C	391	0	0	0	0
11	D	687	0	0	1	0
11	E	582	0	0	0	0
11	F	347	0	0	0	0
All	All	23324	19722	19590	19	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 0.

All (19) 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:124[B]:TYR:CE1	2:B:188:THR:HG21	2.21	0.76
2:E:124[B]:TYR:CE1	2:E:188:THR:HG21	2.26	0.70
4:D:234:ASP:CG	4:D:236:PRO:HD2	2.34	0.52
3:C:85:TYR:CE1	4:D:257:CYS:HB2	2.46	0.51
4:D:343:VAL:HB	6:D:603:F43:H9A1	1.93	0.50
1:A:257:CYS:HB2	3:F:85:TYR:CE1	2.47	0.50
1:A:343:VAL:HB	6:A:602:F43:H9A1	1.94	0.49
2:B:179[B]:PRO:HG2	11:B:624:HOH:O	2.12	0.49
2:B:203[B]:LYS:NZ	2:B:407[B]:GLU:OE2	2.42	0.48
2:E:203[A]:LYS:NZ	2:E:407:GLU:OE2	2.41	0.46
1:A:234:ASP:CG	1:A:236:PRO:HD2	2.40	0.46
3:C:12:THR:HG23	3:C:226[B]:ASP:CG	2.43	0.43
2:B:193[B]:MET:HE2	2:B:196:HIS:CE1	2.53	0.43
4:D:565:ALA:C	11:D:1126[A]:HOH:O	2.63	0.42
2:E:271[A]:GLU:OE2	3:F:2:ALA:C	2.63	0.42

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	584/566 (103%)	564 (97%)	19 (3%)	1 (0%)	44	15
2	B	476/434 (110%)	466 (98%)	10 (2%)	0	100	100
2	E	466/434 (107%)	457 (98%)	9 (2%)	0	100	100
3	C	260/249 (104%)	254 (98%)	6 (2%)	0	100	100
3	F	258/249 (104%)	251 (97%)	7 (3%)	0	100	100
4	D	586/566 (104%)	566 (97%)	19 (3%)	1 (0%)	44	15
All	All	2630/2498 (105%)	2558 (97%)	70 (3%)	2 (0%)	48	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	SER
4	D	340	SER

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	461/435 (106%)	461 (100%)	0	100	100
2	B	377/335 (112%)	373 (99%)	4 (1%)	70	37
2	E	367/335 (110%)	365 (100%)	2 (0%)	86	63
3	C	222/210 (106%)	222 (100%)	0	100	100
3	F	221/210 (105%)	221 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	463/436 (106%)	462 (100%)	1 (0%)	92	72
All	All	2111/1961 (108%)	2104 (100%)	7 (0%)	92	72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	123[A]	GLU
2	B	123[B]	GLU
2	B	179[A]	PRO
2	B	179[B]	PRO
4	D	437	GLN
2	E	123[A]	GLU
2	E	123[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	ASN
2	B	87	ASN
2	B	104	ASN
2	B	112	GLN
4	D	332	GLN
4	D	366	ASN
4	D	376	ASN
4	D	465	GLN
4	D	472	ASN
4	D	493	ASN
2	E	112	GLN
2	E	207	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 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	272	1	7,11,12	0.83	0	6,14,16	0.64	0
4	AGM	D	286	4	10,11,12	0.76	0	6,13,15	0.74	0
1	DYA	A	466	1	7,7,8	1.41	1 (14%)	5,8,10	2.18	2 (40%)
1	GL3	A	461	1	2,3,4	2.22	1 (50%)	1,2,4	0.14	0
1	SMC	A	468	1	5,6,7	0.49	0	2,6,8	1.09	0
1	AGM	A	286	1	10,11,12	0.91	0	6,13,15	0.73	0
4	TRX	D	443	4	14,16,17	0.65	0	15,22,24	1.03	1 (6%)
1	CSO	A	55	1	3,6,7	0.81	0	0,6,8	-	-
4	GL3	D	461	4	2,3,4	3.20	1 (50%)	1,2,4	0.44	0
4	SMC	D	468	4	5,6,7	0.67	0	2,6,8	1.18	0
3	A1I9G	F	159	3	5,11,12	0.77	0	8,14,16	1.64	1 (12%)
4	DYA	D	466	4	7,7,8	1.04	0	5,8,10	1.95	2 (40%)
4	MHS	D	272	4	7,11,12	0.74	0	6,14,16	0.71	0
3	A1I9G	C	159	3	5,11,12	0.70	0	8,14,16	2.09	2 (25%)
1	TRX	A	443	1	14,16,17	0.73	0	15,22,24	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MHS	A	272	1	-	0/5/6/8	0/1/1/1
4	AGM	D	286	4	-	2/10/11/13	-
1	DYA	A	466	1	-	3/4/6/8	-
1	GL3	A	461	1	-	1/1/1/2	-
1	SMC	A	468	1	-	1/3/5/7	-
1	AGM	A	286	1	-	3/10/11/13	-
4	TRX	D	443	4	-	0/4/6/8	0/2/2/2
1	CSO	A	55	1	-	0/1/5/7	-
4	GL3	D	461	4	-	0/1/1/2	-
4	SMC	D	468	4	-	1/3/5/7	-
3	A1I9G	F	159	3	-	2/6/10/12	0/1/1/1
4	DYA	D	466	4	-	3/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MHS	D	272	4	-	0/5/6/8	0/1/1/1
3	A1I9G	C	159	3	-	2/6/10/12	0/1/1/1
1	TRX	A	443	1	-	0/4/6/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	461	GL3	C-S	-4.52	1.65	1.80
1	A	461	GL3	C-S	-3.13	1.69	1.80
1	A	466	DYA	CA-N	2.27	1.40	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	159	A1I9G	CB-CG-ND1	4.40	128.14	120.16
3	F	159	A1I9G	CB-CG-ND1	3.62	126.74	120.16
1	A	466	DYA	O-C-CA	-3.61	120.80	125.39
4	D	466	DYA	O-C-CA	-3.04	121.52	125.39
3	C	159	A1I9G	CD2-CG-CB	-2.45	125.48	129.25
4	D	443	TRX	CH2-CZ2-CE2	-2.28	116.88	119.29
1	A	466	DYA	OD2-CG-CB	-2.18	116.95	123.89
4	D	466	DYA	OD2-CG-CB	-2.10	117.22	123.89

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	DYA	O-C-CA-CB
1	A	466	DYA	CA-CB-CG-OD1
1	A	468	SMC	CA-CB-SG-CS
4	D	466	DYA	O-C-CA-CB
4	D	466	DYA	CA-CB-CG-OD1
4	D	468	SMC	CA-CB-SG-CS
3	C	159	A1I9G	O-C-CA-CB
3	F	159	A1I9G	O-C-CA-CB
1	A	466	DYA	CA-CB-CG-OD2
4	D	466	DYA	CA-CB-CG-OD2
3	C	159	A1I9G	CF-CB-CG-CD2
3	F	159	A1I9G	CF-CB-CG-CD2
1	A	286	AGM	CE2-CD-NE1-CZ
4	D	286	AGM	CE2-CD-NE1-CZ

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Mol	Chain	Res	Type	Atoms
1	A	461	GL3	S-C-CA-N
1	A	286	AGM	CE2-CD-CG-CB
1	A	286	AGM	NE1-CD-CG-CB
4	D	286	AGM	NE1-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	EDO	A	603	-	3,3,3	0.33	0	2,2,2	0.29	0
7	EDO	D	605	-	3,3,3	0.53	0	2,2,2	0.22	0
7	EDO	D	607	-	3,3,3	0.51	0	2,2,2	0.31	0
7	EDO	E	502	-	3,3,3	0.13	0	2,2,2	0.28	0
7	EDO	C	302	-	3,3,3	0.45	0	2,2,2	0.48	0
7	EDO	E	501	-	3,3,3	0.52	0	2,2,2	0.21	0
7	EDO	D	608	-	3,3,3	0.14	0	2,2,2	0.39	0
7	EDO	B	504	-	3,3,3	0.16	0	2,2,2	0.79	0
7	EDO	F	301	-	3,3,3	0.39	0	2,2,2	0.44	0
6	F43	A	602	4,9,10	61,71,71	2.16	5 (8%)	64,118,118	1.18	7 (10%)
7	EDO	D	602	-	3,3,3	0.31	0	2,2,2	0.24	0
7	EDO	B	503	-	3,3,3	0.51	0	2,2,2	0.38	0
9	COM	A	607[A]	6	6,6,6	2.88	1 (16%)	7,8,8	1.54	1 (14%)
6	F43	D	603	1,9,10	61,71,71	2.12	5 (8%)	64,118,118	1.23	7 (10%)
7	EDO	C	301	-	3,3,3	0.89	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	D	609	-	3,3,3	0.07	0	2,2,2	0.17	0
10	SHT	A	608[C]	6	26,27,27	1.62	1 (3%)	30,36,36	1.39	3 (10%)
7	EDO	A	606	-	3,3,3	0.16	0	2,2,2	0.11	0
7	EDO	D	611	-	3,3,3	0.12	0	2,2,2	0.24	0
7	EDO	B	502	-	3,3,3	0.57	0	2,2,2	0.23	0
7	EDO	B	505	-	3,3,3	0.25	0	2,2,2	0.53	0
7	EDO	B	501	-	3,3,3	0.47	0	2,2,2	0.22	0
7	EDO	D	606	-	3,3,3	0.49	0	2,2,2	0.41	0
10	SHT	D	610[C]	6	26,27,27	1.61	1 (3%)	30,36,36	1.32	2 (6%)
7	EDO	B	506	-	3,3,3	0.07	0	2,2,2	0.25	0
7	EDO	B	507	-	3,3,3	0.08	0	2,2,2	0.25	0
8	TP7	A	604[A]	-	19,20,20	0.83	0	24,26,26	0.77	0
7	EDO	A	605	-	3,3,3	0.52	0	2,2,2	0.36	0
8	TP7	D	604[A]	-	19,20,20	0.95	0	24,26,26	0.63	0
9	COM	D	601[A]	6	6,6,6	1.18	1 (16%)	7,8,8	2.08	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	603	-	-	0/1/1/1	-
7	EDO	D	605	-	-	0/1/1/1	-
7	EDO	D	607	-	-	0/1/1/1	-
7	EDO	E	502	-	-	1/1/1/1	-
7	EDO	C	302	-	-	0/1/1/1	-
7	EDO	E	501	-	-	0/1/1/1	-
7	EDO	D	608	-	-	0/1/1/1	-
7	EDO	B	504	-	-	1/1/1/1	-
7	EDO	F	301	-	-	0/1/1/1	-
6	F43	A	602	4,9,10	-	7/28/185/185	-
7	EDO	D	602	-	-	0/1/1/1	-
7	EDO	B	503	-	-	0/1/1/1	-
9	COM	A	607[A]	6	-	0/4/4/4	-
6	F43	D	603	1,9,10	-	8/28/185/185	-
7	EDO	C	301	-	-	0/1/1/1	-
7	EDO	D	609	-	-	0/1/1/1	-
10	SHT	A	608[C]	6	-	4/31/31/31	-
7	EDO	A	606	-	-	0/1/1/1	-
7	EDO	D	611	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	502	-	-	0/1/1/1	-
7	EDO	B	505	-	-	0/1/1/1	-
7	EDO	B	501	-	-	0/1/1/1	-
7	EDO	D	606	-	-	0/1/1/1	-
10	SHT	D	610[C]	6	-	4/31/31/31	-
7	EDO	B	506	-	-	0/1/1/1	-
7	EDO	B	507	-	-	1/1/1/1	-
8	TP7	A	604[A]	-	-	0/24/24/24	-
7	EDO	A	605	-	-	0/1/1/1	-
8	TP7	D	604[A]	-	-	1/24/24/24	-
9	COM	D	601[A]	6	-	0/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	F43	NI-NA	8.94	2.08	1.89
6	A	602	F43	NI-NB	8.51	2.07	1.89
6	D	603	F43	NI-NA	8.47	2.07	1.89
6	D	603	F43	NI-NB	8.19	2.07	1.89
10	A	608[C]	SHT	CK1-CK2	7.59	1.51	1.32
10	D	610[C]	SHT	CK1-CK2	7.58	1.51	1.32
6	A	602	F43	NI-ND	7.33	2.05	1.89
6	D	603	F43	NI-ND	7.14	2.04	1.89
9	A	607[A]	COM	C2-S2	-6.82	1.67	1.77
6	D	603	F43	CHD-C1D	-5.36	1.36	1.43
6	A	602	F43	CHD-C1D	-5.14	1.36	1.43
6	A	602	F43	CHC-C4B	3.15	1.48	1.39
6	D	603	F43	CHC-C4B	3.07	1.47	1.39
9	D	601[A]	COM	O1S-S2	2.27	1.51	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	608[C]	SHT	CK3-CK2-CK1	-5.83	113.35	125.85
10	D	610[C]	SHT	CK3-CK2-CK1	-5.75	113.52	125.85
9	D	601[A]	COM	O1S-S2-C2	3.48	111.10	106.92
9	D	601[A]	COM	O3S-S2-C2	3.37	111.22	105.77
6	D	603	F43	O8D-C7D-C6D	-3.22	115.59	120.86
9	A	607[A]	COM	O3S-S2-C2	2.97	110.58	105.77
6	D	603	F43	O7B-C6B-C8B	-2.83	123.13	126.59
6	A	602	F43	C4D-ND-C1D	2.64	111.99	108.51
6	A	602	F43	C2B-C1B-NB	2.61	105.75	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	603	F43	C4D-ND-C1D	2.58	111.90	108.51
6	D	603	F43	C2B-C1B-NB	2.45	105.50	101.84
9	D	601[A]	COM	O2S-S2-O1S	-2.43	105.52	113.95
6	A	602	F43	O7B-C6B-C8B	-2.31	123.77	126.59
6	A	602	F43	O8D-C7D-C6D	-2.28	117.12	120.86
10	A	608[C]	SHT	O3'-P-O1P	-2.24	100.75	109.39
10	D	610[C]	SHT	OS2-SG2-CD	-2.15	102.29	105.77
6	D	603	F43	OBC-CAC-C9C	2.10	120.77	114.03
6	D	603	F43	CAB-C3B-C2B	-2.10	114.65	119.09
6	A	602	F43	CAB-C3B-C2B	-2.07	114.71	119.09
6	A	602	F43	OBC-CAC-C9C	2.05	120.61	114.03
10	A	608[C]	SHT	OS2-SG2-OS1	-2.04	106.30	111.27
6	A	602	F43	C3A-C4A-NA	-2.01	99.24	102.30
6	D	603	F43	OCC-CAC-C9C	-2.01	116.63	123.08

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	608[C]	SHT	S1-CC-CD-SG2
10	D	610[C]	SHT	S1-CC-CD-SG2
7	B	507	EDO	O1-C1-C2-O2
10	D	610[C]	SHT	CK1-CK2-CK3-CK4
10	A	608[C]	SHT	CK1-CK2-CK3-CK4
8	D	604[A]	TP7	CB-O4P-P-O3P
10	A	608[C]	SHT	CK5-CK6-SK-S1
7	B	504	EDO	O1-C1-C2-O2
7	D	611	EDO	O1-C1-C2-O2
7	E	502	EDO	O1-C1-C2-O2
6	D	603	F43	CAB-CBB-CCB-ODB
6	A	602	F43	CAB-CBB-CCB-ODB
10	D	610[C]	SHT	CK5-CK6-SK-S1
6	D	603	F43	CAB-CBB-CCB-OEB
6	A	602	F43	CAB-CBB-CCB-OEB
6	D	603	F43	C3A-CAA-CBA-CCA
6	A	602	F43	C3A-CAA-CBA-CCA
6	D	603	F43	C3D-C9D-CAD-OCD
6	A	602	F43	CAA-CBA-CCA-ODA
6	A	602	F43	CAA-CBA-CCA-OEA
6	D	603	F43	CAA-CBA-CCA-ODA
6	D	603	F43	CAA-CBA-CCA-OEA
6	A	602	F43	C2D-C3D-C9D-CAD

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Mol	Chain	Res	Type	Atoms
6	A	602	F43	C4D-C3D-C9D-CAD
6	D	603	F43	C2D-C3D-C9D-CAD
10	A	608[C]	SHT	CD-CC-S1-SK
10	D	610[C]	SHT	CD-CC-S1-SK
6	D	603	F43	C3D-C9D-CAD-OB

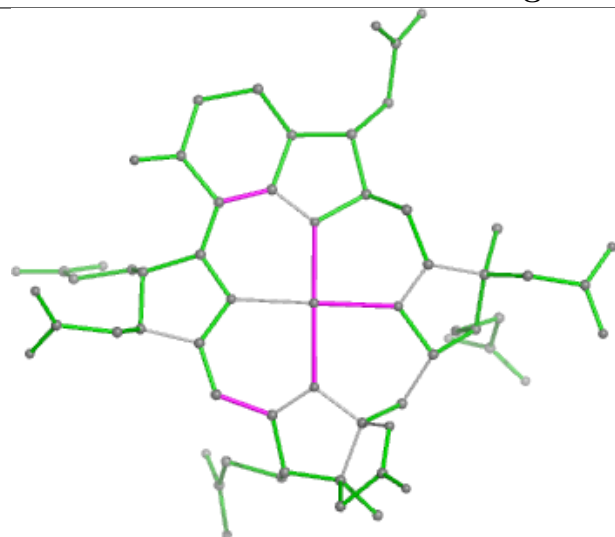
There are no ring outliers.

2 monomers are involved in 2 short contacts:

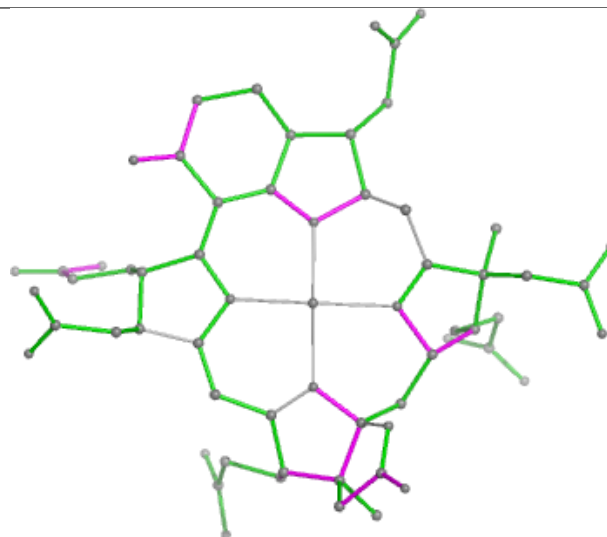
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	F43	1	0
6	D	603	F43	1	0

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

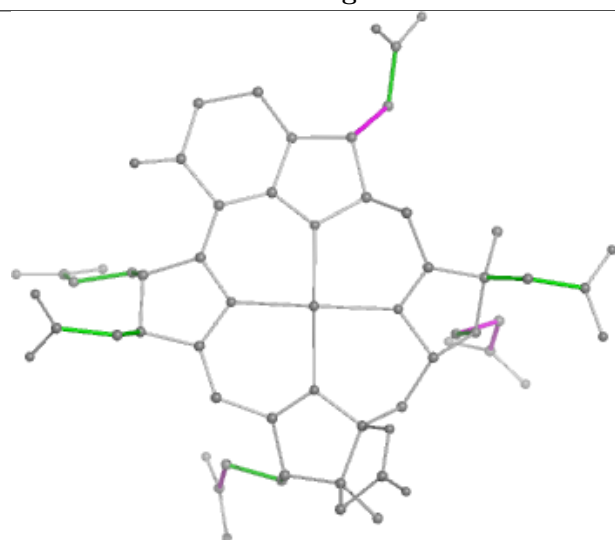
Ligand F43 A 602



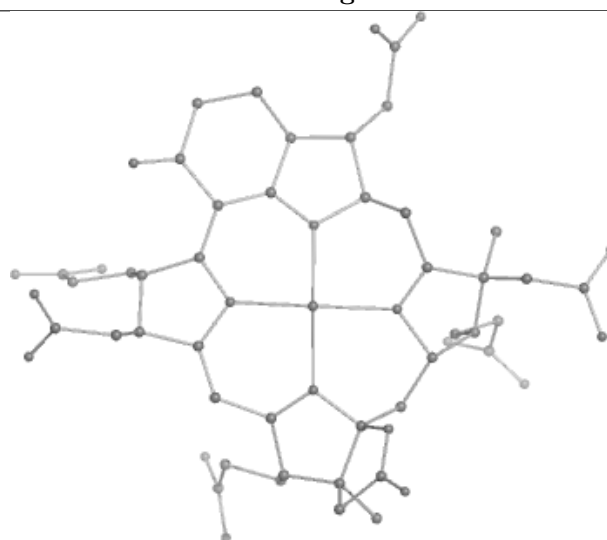
Bond lengths



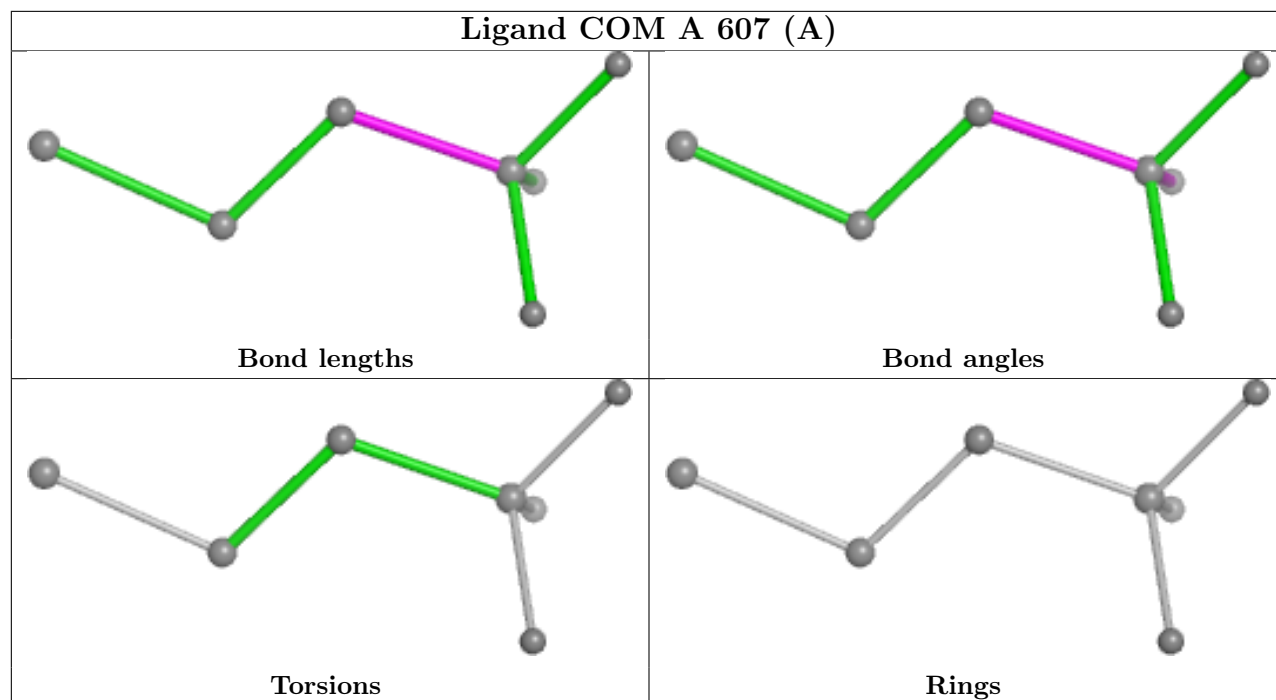
Bond angles



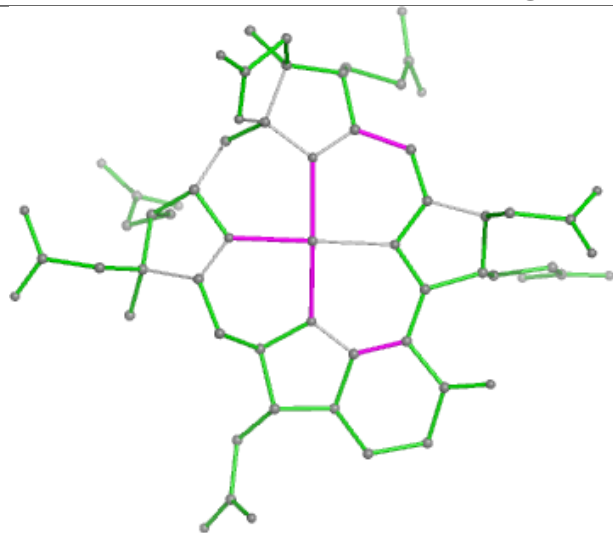
Torsions



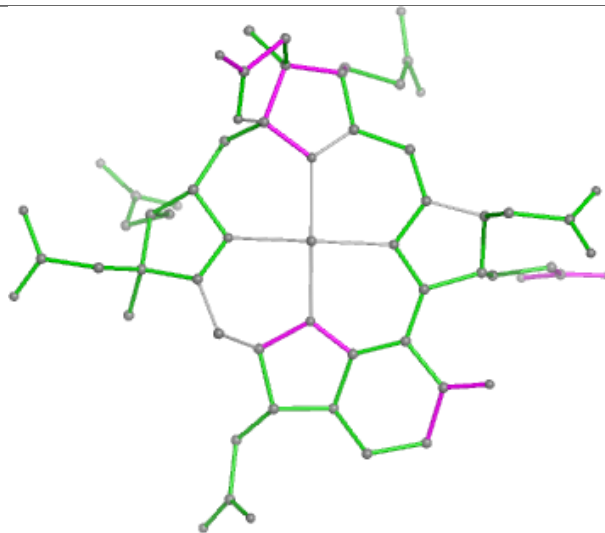
Rings



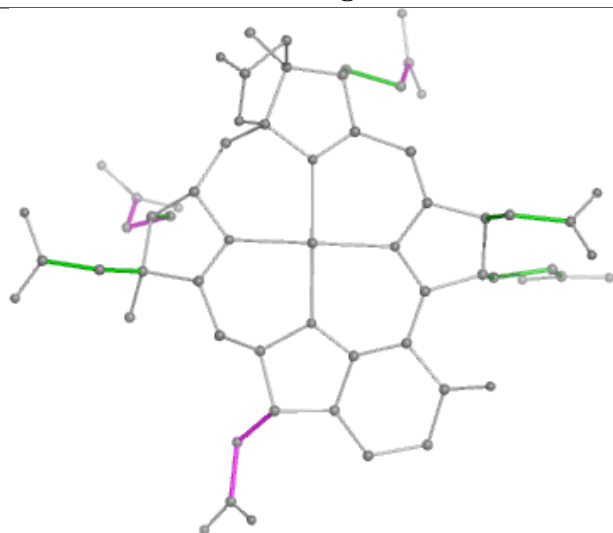
Ligand F43 D 603



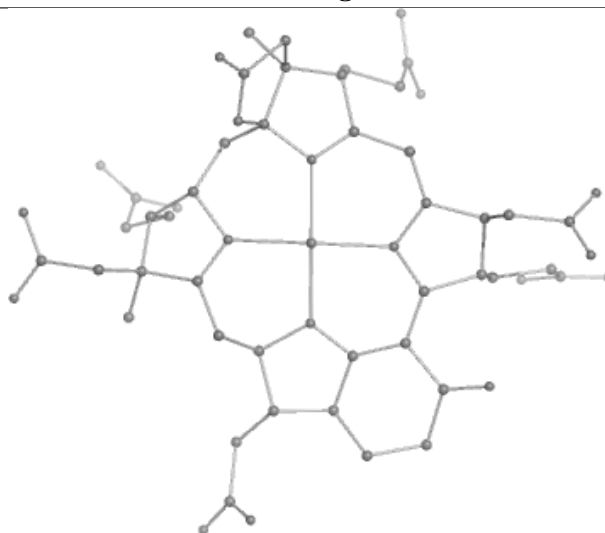
Bond lengths



Bond angles

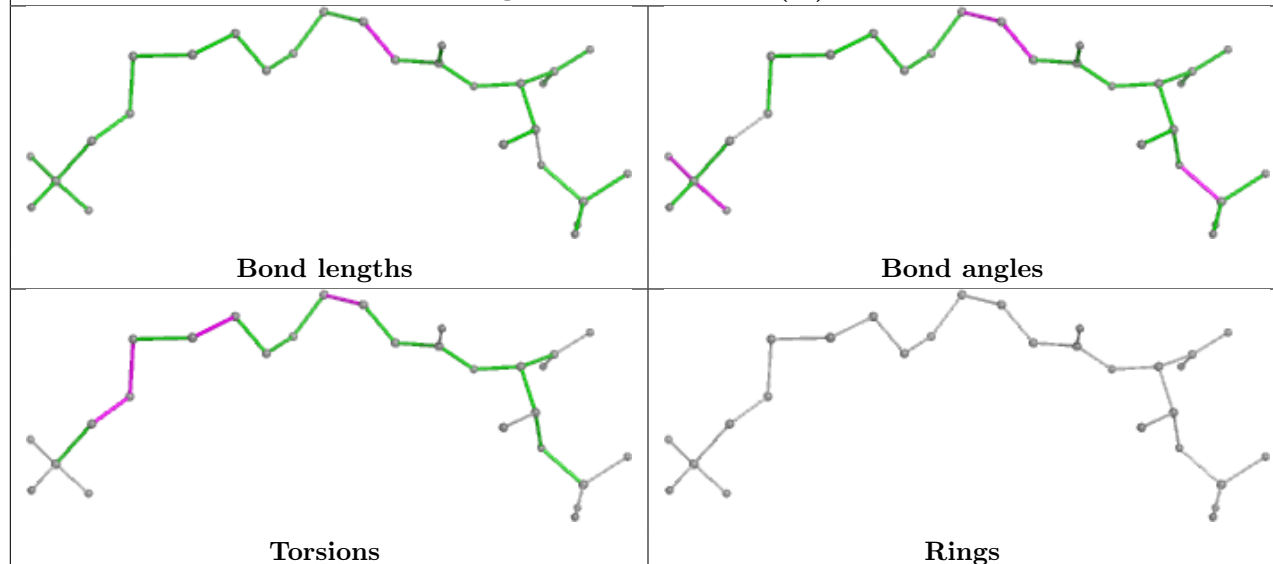


Torsions

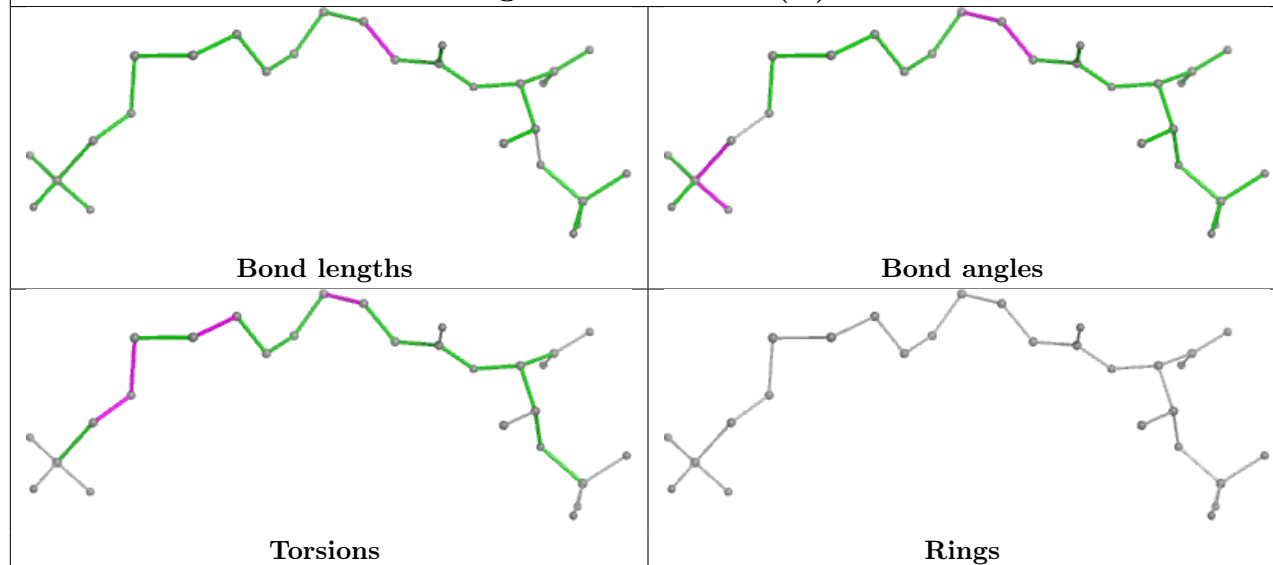


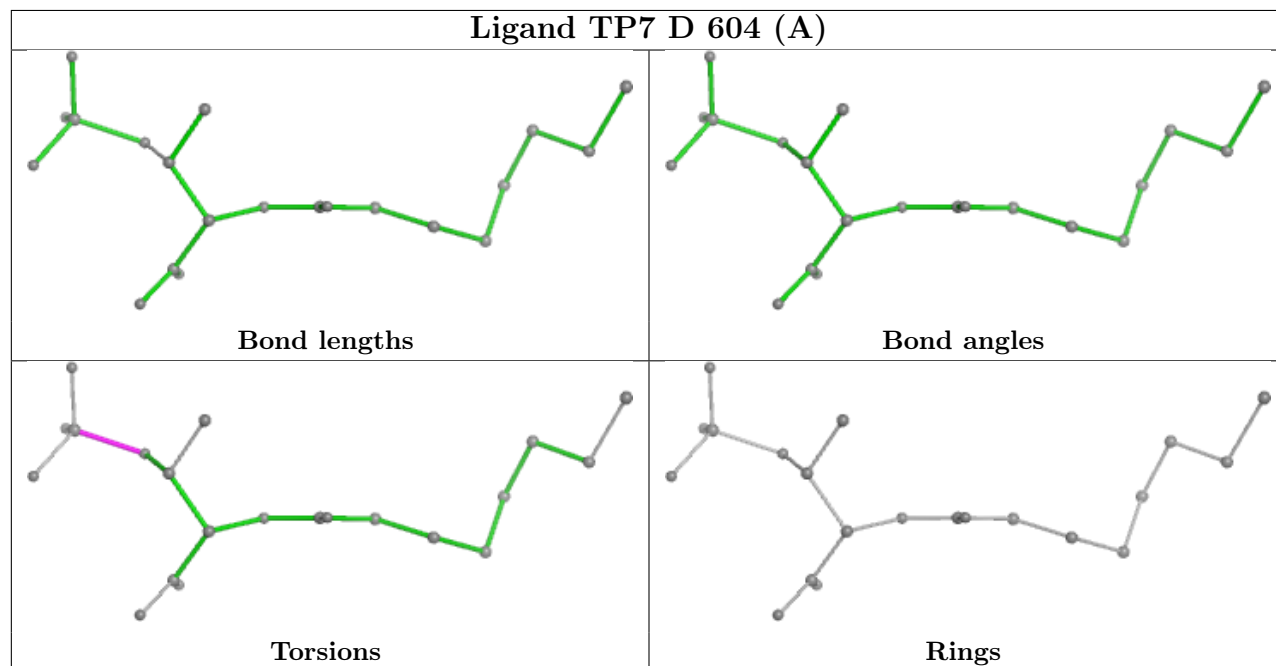
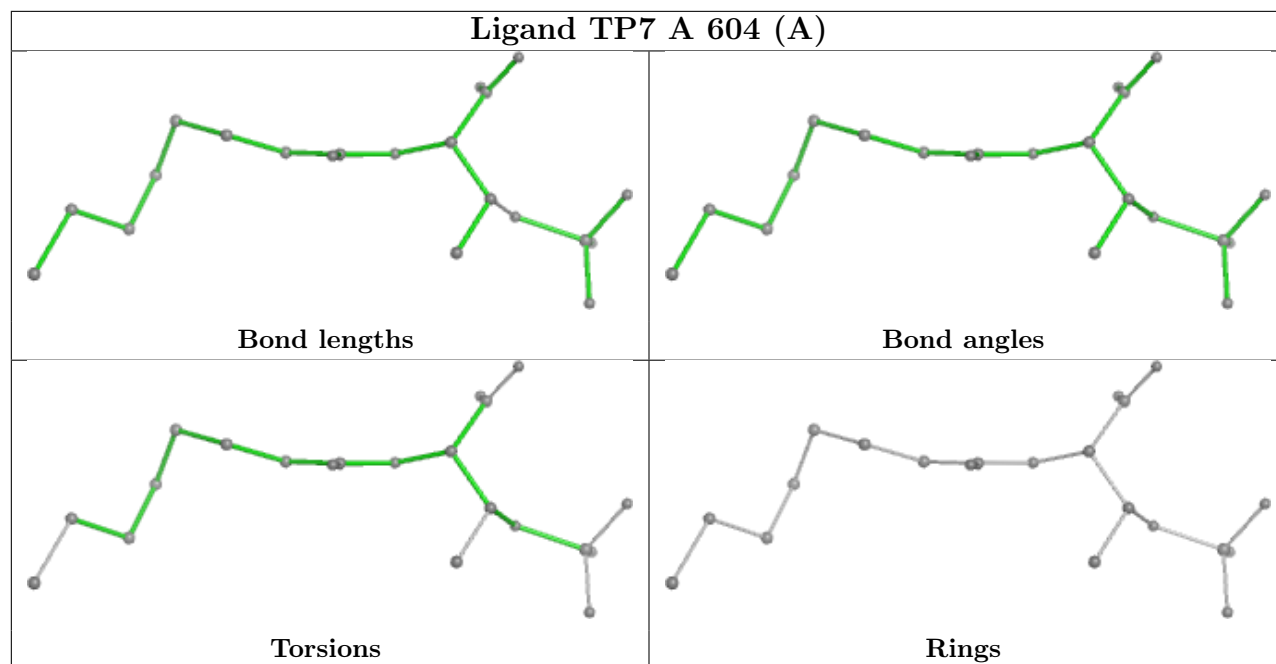
Rings

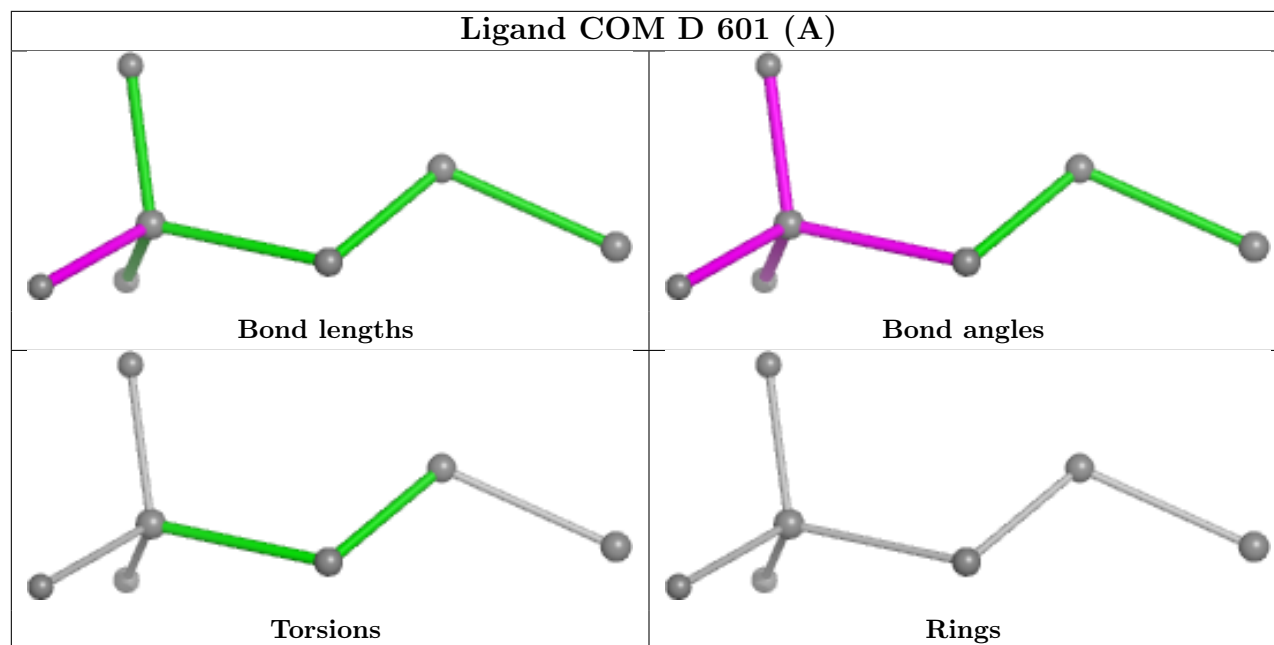
Ligand SHT A 608 (C)



Ligand SHT D 610 (C)







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	557/566 (98%)	-0.69	3 (0%) 87 89	3, 8, 16, 30	20 (3%)
2	B	433/434 (99%)	-0.74	2 (0%) 87 89	3, 7, 14, 22	30 (6%)
2	E	433/434 (99%)	-0.68	0 100 100	3, 8, 15, 23	26 (6%)
3	C	247/249 (99%)	-0.68	1 (0%) 89 89	5, 8, 15, 24	12 (4%)
3	F	247/249 (99%)	-0.42	3 (1%) 76 81	6, 11, 19, 28	9 (3%)
4	D	557/566 (98%)	-0.77	1 (0%) 92 90	3, 7, 15, 26	22 (3%)
All	All	2474/2498 (99%)	-0.69	10 (0%) 89 89	3, 8, 16, 30	119 (4%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	7.5
3	F	2	ALA	5.9
3	C	2	ALA	4.1
3	F	60	ILE	3.4
4	D	565	ALA	3.4
1	A	565	ALA	3.3
1	A	3	GLU	2.6
2	B	94[A]	SER	2.6
2	B	95[A]	GLY	2.5
3	F	61	GLY	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(\AA^2)	Q<0.9
4	MHS	D	272	11/12	0.98	0.06	4,5,10,12	0
1	MHS	A	272	11/12	0.99	0.05	5,6,10,12	0
1	AGM	A	286	12/13	0.99	0.04	3,4,5,6	0
1	TRX	A	443	15/16	0.99	0.04	4,5,5,6	0
1	DYA	A	466	8/9	0.99	0.03	4,5,6,6	0
1	CSO	A	55	7/8	0.99	0.05	7,7,8,13	0
4	AGM	D	286	12/13	0.99	0.04	4,4,5,6	0
4	TRX	D	443	15/16	0.99	0.03	4,4,5,5	0
4	DYA	D	466	8/9	0.99	0.03	4,5,6,6	0
3	A1I9G	C	159	11/12	0.99	0.04	5,5,6,6	0
3	A1I9G	F	159	11/12	0.99	0.04	6,6,7,7	0
1	SMC	A	468	7/8	1.00	0.04	4,4,6,6	0
4	SMC	D	468	7/8	1.00	0.03	4,4,6,7	0
1	GL3	A	461	4/5	1.00	0.03	4,4,4,4	0
4	GL3	D	461	4/5	1.00	0.04	4,4,4,5	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(\AA^2)	Q<0.9
7	EDO	E	502	4/4	0.75	0.17	23,32,43,44	0
7	EDO	B	507	4/4	0.80	0.15	26,31,36,43	0
7	EDO	D	611	4/4	0.81	0.17	18,24,29,29	10
7	EDO	B	504	4/4	0.82	0.17	14,20,24,29	0
7	EDO	B	506	4/4	0.83	0.12	28,34,35,36	0
7	EDO	D	607	4/4	0.85	0.12	29,35,36,37	0
7	EDO	D	609	4/4	0.85	0.13	26,32,32,33	0
7	EDO	B	503	4/4	0.88	0.12	21,26,28,30	0
7	EDO	B	505	4/4	0.91	0.12	12,21,25,27	0
7	EDO	A	605	4/4	0.92	0.10	20,24,26,27	0
7	EDO	D	608	4/4	0.93	0.10	21,25,28,29	0
7	EDO	D	605	4/4	0.93	0.09	20,24,26,27	0
7	EDO	B	501	4/4	0.94	0.09	16,22,25,27	0
7	EDO	D	606	4/4	0.95	0.08	14,17,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	606	4/4	0.96	0.07	16,20,23,23	0
7	EDO	E	501	4/4	0.96	0.08	13,16,16,17	0
7	EDO	B	502	4/4	0.96	0.07	12,14,15,15	0
7	EDO	C	301	4/4	0.97	0.06	12,14,16,16	0
10	SHT	A	608[C]	28/28	0.97	0.06	5,5,9,10	28
7	EDO	F	301	4/4	0.98	0.05	14,17,18,21	0
7	EDO	C	302	4/4	0.98	0.04	13,16,18,21	0
10	SHT	D	610[C]	28/28	0.98	0.06	4,5,8,8	28
7	EDO	D	602	4/4	0.99	0.04	8,10,12,12	0
7	EDO	A	603	4/4	0.99	0.04	7,9,11,11	0
9	COM	A	607[A]	7/7	0.99	0.07	3,4,6,6	7
9	COM	D	601[A]	7/7	0.99	0.06	5,6,8,8	7
6	F43	A	602	62/62	0.99	0.04	4,5,8,10	0
6	F43	D	603	62/62	0.99	0.05	5,6,10,11	0
8	TP7	A	604[A]	21/21	1.00	0.03	2,3,4,6	21
8	TP7	D	604[A]	21/21	1.00	0.03	3,4,5,6	21
5	K	A	601	1/1	1.00	0.04	8,8,8,8	0

6.5 Other polymers ⓘ

There are no such residues in this entry.