



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2025 – 11:11 am BST

PDB ID : 9QR1 / pdb_00009qr1
Title : Methyl-coenzyme M reductase of ANME-2d Candidatus Methanoperedens sp.
BLZ2 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	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
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Percentile relative to all X-ray structures

Percentile relative to X-ray structures of similar resolution

Metric

Whole archive
(#Entries)

Similar resolution
(#Entries, resolution range(Å))

 R_{free}

Clashscore

Ramachandran outliers

Sidechain outliers

RSRZ outliers

164625

180529

177936

177891

164620

1026 (1.02-0.94)

1154 (1.02-0.94)

1094 (1.02-0.94)

1095 (1.02-0.94)

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.

Quality of chain

97%

98%

97%

98%

98%

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Mol	Chain	Length	Quality of chain
3	F	249	<div><div>%</div><div><div></div><div>98%</div><div>.</div></div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 43033 atoms, of which 19676 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	560	Total	C	H	N	O	S	0	37	0
			8845	2838	4361	762	851	33			
1	D	560	Total	C	H	N	O	S	0	26	0
			8697	2796	4269	755	843	34			

- 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	32	0
			6768	2103	3448	564	630	23			
2	E	433	Total	C	H	N	O	S	0	47	0
			6920	2145	3534	574	644	23			

- Molecule 3 is a protein called coenzyme-B sulfoethylthiotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total	C	H	N	O	S	0	9	0
			4007	1266	1983	363	382	13			
3	F	248	Total	C	H	N	O	S	0	8	0
			3971	1251	1962	364	382	12			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



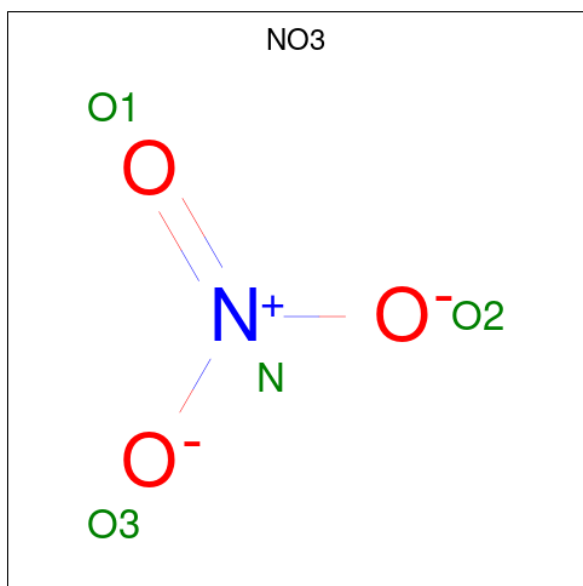
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	1
			7	2	3	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	1
			7	2	3	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	1
			10	2	6	2		
5	B	1	Total	C	H	O	0	1
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			9	2	5	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		

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

- Molecule 6 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



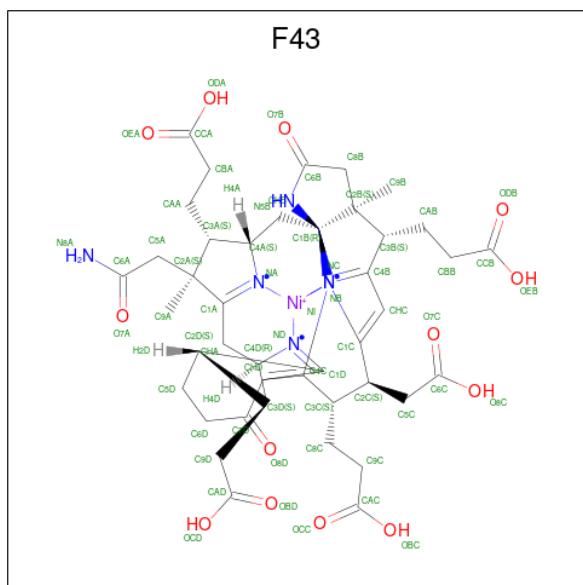
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		

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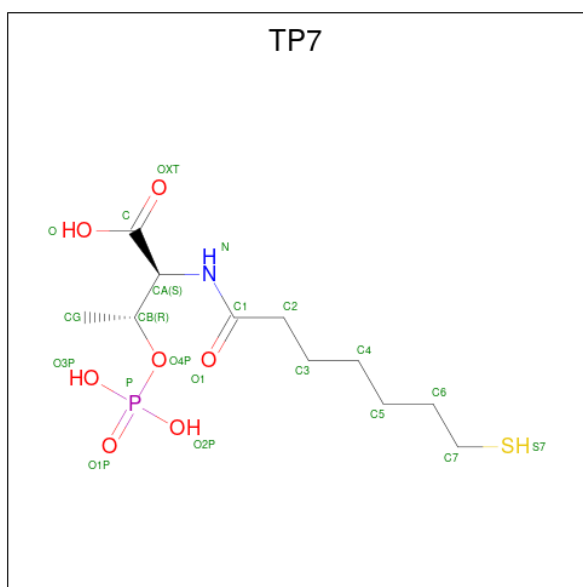
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is FACTOR 430 (CCD ID: F43) (formula: $\text{C}_{42}\text{H}_{51}\text{N}_6\text{NiO}_{13}$) (labeled as "Ligand of Interest" by depositor).



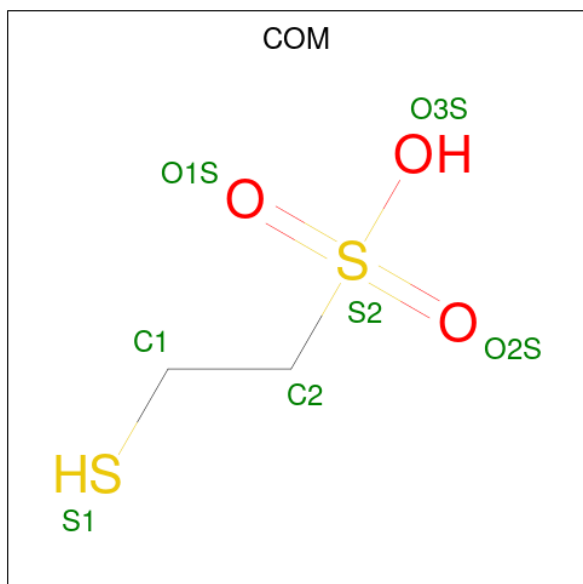
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 62	C 42	N 6	Ni 1	O 13	0	0
7	D	1	Total 62	C 42	N 6	Ni 1	O 13	0	0

- 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	0
			21	11	1	7	1	1		
8	D	1	Total	C	N	O	P	S	0	0
			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	0
			7	2	3	2		

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

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	K	0	0
			1	1		
10	E	1	Total	K	0	0
			1	1		

- Molecule 11 is water.

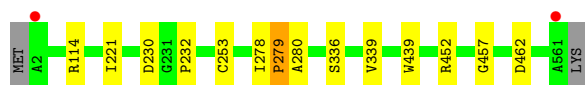
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	736	Total	O	0	90
			736	736		
11	B	604	Total	O	0	69
			604	604		
11	C	419	Total	O	0	67
			419	419		
11	D	693	Total	O	0	85
			693	693		
11	E	582	Total	O	0	75
			582	582		
11	F	385	Total	O	0	24
			385	385		

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:  97%



- Molecule 1: Methyl-coenzyme M reductase subunit alpha

Chain D:  98%



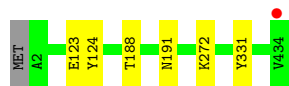
- Molecule 2: Methyl-coenzyme M reductase subunit beta

Chain B:  97%



- Molecule 2: Methyl-coenzyme M reductase subunit beta

Chain E:  98%

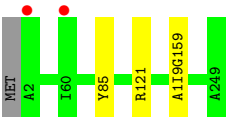


- Molecule 3: coenzyme-B sulfoethylthiotransferase

Chain C:  98%



- Molecule 3: coenzyme-B sulfoethylthiotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.58Å 189.30Å 84.11Å 90.00° 114.27° 90.00°	Depositor
Resolution (Å)	41.78 – 0.98 41.78 – 0.98	Depositor EDS
% Data completeness (in resolution range)	84.4 (41.78-0.98) 85.4 (41.78-0.98)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 0.98Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.102 , 0.118 0.125 , 0.133	Depositor DCC
R_{free} test set	67067 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	6.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o, F_c correlation	0.99	EDS
Total number of atoms	43033	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 2.92% 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: CSO, AGM, A1I9G, NA, SMC, GL3, F43, COM, MHS, NO3, EDO, K, TP7, DYA, TRX

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	0.50	0/4677	0.75	4/6322 (0.1%)
1	D	0.49	2/4548 (0.0%)	0.72	0/6147
2	B	0.51	0/3479	0.71	1/4705 (0.0%)
2	E	0.52	2/3603 (0.1%)	0.69	0/4871
3	C	0.48	0/2081	0.72	0/2808
3	F	0.45	0/2064	0.68	0/2785
All	All	0.50	4/20452 (0.0%)	0.72	5/27638 (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
1	D	0	1
2	B	0	1
2	E	0	1
3	C	0	2
3	F	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	176[A]	ILE	C-O	7.06	1.30	1.24
1	D	176[B]	ILE	C-O	7.06	1.30	1.24
2	E	123[A]	GLU	C-O	5.51	1.30	1.24
2	E	123[B]	GLU	C-O	5.51	1.30	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280[A]	ALA	N-CA-C	5.45	117.22	111.28
1	A	280[B]	ALA	N-CA-C	5.45	117.22	111.28
2	B	423	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	279[A]	PRO	N-CA-C	5.39	118.77	111.22
1	A	279[B]	PRO	N-CA-C	5.39	118.77	111.22

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	452	ARG	Sidechain
2	B	331	TYR	Sidechain
3	C	121	ARG	Sidechain
3	C	235	ARG	Sidechain
1	D	452	ARG	Sidechain
2	E	331	TYR	Sidechain
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	4484	4361	4296	5	0
1	D	4428	4269	4265	5	0
2	B	3320	3448	3399	9	0
2	E	3386	3534	3416	3	0
3	C	2024	1983	1983	1	0
3	F	2009	1962	1954	1	0
4	A	1	0	0	0	0
5	A	20	24	30	0	0
5	B	24	35	35	0	0
5	C	8	12	12	0	0
5	D	16	24	24	0	0
5	E	8	12	12	0	0
5	F	8	12	12	0	0
6	A	4	0	0	0	0
6	B	8	0	0	0	0
6	D	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	4	0	0	0	0
7	A	62	0	43	1	0
7	D	62	0	43	1	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	4	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
11	A	736	0	0	0	0
11	B	604	0	0	0	0
11	C	419	0	0	0	0
11	D	693	0	0	0	0
11	E	582	0	0	0	0
11	F	385	0	0	0	0
All	All	23357	19676	19570	22	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 1.

All (22) 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[A]:TYR:CE1	2:B:188:THR:HG21	2.13	0.84
2:E:124[B]:TYR:CE1	2:E:188:THR:HG21	2.21	0.74
1:D:339:VAL:HB	7:D:607:F43:H9A1	1.86	0.58
1:A:339:VAL:HB	7:A:607:F43:H9A1	1.88	0.55
1:A:253:CYS:HB2	3:F:85:TYR:CE1	2.44	0.53
1:A:114:ARG:HB2	1:A:221[B]:ILE:HG13	1.90	0.53
3:C:85:TYR:CE1	1:D:253:CYS:HB2	2.46	0.50
2:E:124[B]:TYR:CD1	2:E:124[B]:TYR:N	2.79	0.50
2:B:299[B]:LYS:HB2	2:B:299[B]:LYS:HE2	1.36	0.47
1:A:278:ILE:HB	1:A:279[A]:PRO:HD2	1.98	0.45
1:D:118[A]:VAL:HG21	1:D:238:MET:HE2	1.98	0.44
1:D:230:ASP:CG	1:D:232:PRO:HD2	2.42	0.44
1:A:230:ASP:CG	1:A:232:PRO:HD2	2.43	0.43
1:D:118[A]:VAL:CG2	1:D:238:MET:HE2	2.49	0.42
2:B:191[B]:ASN:OD1	2:B:191[B]:ASN:C	2.63	0.42
2:B:107:LYS:HB3	2:B:108[B]:GLN:NE2	2.36	0.41
2:B:124[A]:TYR:CZ	2:B:188:THR:HG21	2.54	0.41
2:E:191[B]:ASN:OD1	2:E:191[B]:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193[B]:MET:HE3	2:B:193[B]:MET:HB3	1.91	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	590/563 (105%)	570 (97%)	19 (3%)	1 (0%)	44	15
1	D	577/563 (102%)	558 (97%)	18 (3%)	1 (0%)	44	15
2	B	465/434 (107%)	455 (98%)	10 (2%)	0	100	100
2	E	481/434 (111%)	470 (98%)	11 (2%)	0	100	100
3	C	254/249 (102%)	247 (97%)	7 (3%)	0	100	100
3	F	253/249 (102%)	247 (98%)	6 (2%)	0	100	100
All	All	2620/2492 (105%)	2547 (97%)	71 (3%)	2 (0%)	48	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	SER
1	D	336	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	468/434 (108%)	468 (100%)	0	100	100
1	D	455/434 (105%)	454 (100%)	1 (0%)	92	72
2	B	366/334 (110%)	363 (99%)	3 (1%)	79	47
2	E	381/334 (114%)	379 (100%)	2 (0%)	86	63
3	C	217/209 (104%)	217 (100%)	0	100	100
3	F	216/209 (103%)	216 (100%)	0	100	100
All	All	2103/1954 (108%)	2097 (100%)	6 (0%)	92	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	11	ARG
2	B	123[A]	GLU
2	B	123[B]	GLU
1	D	433	GLN
2	E	272[A]	LYS
2	E	272[B]	LYS

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	62	GLN
1	A	158	GLN
1	A	217	GLN
1	A	328	GLN
2	B	104	ASN
1	D	6	GLN
1	D	328	GLN
1	D	461	GLN
1	D	468	ASN
1	D	489	ASN
3	F	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	GL3	A	457	1	2,3,4	3.20	1 (50%)	1,2,4	0.27	0
1	DYA	A	462	1	7,7,8	1.26	1 (14%)	5,8,10	2.31	2 (40%)
3	A1I9G	F	159	3	5,11,12	0.61	0	8,14,16	1.84	2 (25%)
1	CSO	A	51	1	3,6,7	1.12	0	0,6,8	-	-
1	SMC	A	464	1	5,6,7	0.69	0	2,6,8	1.19	0
1	MHS	A	268	1	7,11,12	0.77	0	6,14,16	0.78	0
1	SMC	D	464	1	5,6,7	0.73	0	2,6,8	1.25	0
1	MHS	D	268	1	7,11,12	0.78	0	6,14,16	0.59	0
1	TRX	D	439	1	14,16,17	0.65	0	15,22,24	0.89	0
1	AGM	D	282	1	10,11,12	0.72	0	6,13,15	0.68	0
1	DYA	D	462	1	7,7,8	1.15	0	5,8,10	1.93	1 (20%)
1	GL3	D	457	1	2,3,4	3.16	1 (50%)	1,2,4	0.33	0
1	CSO	D	51[B]	1	3,6,7	1.08	0	0,6,8	-	-
1	TRX	A	439	1	14,16,17	0.67	0	15,22,24	1.03	1 (6%)
1	AGM	A	282	1	10,11,12	0.58	0	6,13,15	0.76	0
3	A1I9G	C	159	3	5,11,12	0.73	0	8,14,16	1.81	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GL3	A	457	1	-	0/1/1/2	-
1	DYA	A	462	1	-	3/4/6/8	-
3	A1I9G	F	159	3	-	2/6/10/12	0/1/1/1
1	CSO	A	51	1	-	0/1/5/7	-
1	SMC	A	464	1	-	1/3/5/7	-
1	MHS	A	268	1	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	D	464	1	-	1/3/5/7	-
1	MHS	D	268	1	-	0/5/6/8	0/1/1/1
1	TRX	D	439	1	-	0/4/6/8	0/2/2/2
1	AGM	D	282	1	-	1/10/11/13	-
1	DYA	D	462	1	-	3/4/6/8	-
1	GL3	D	457	1	-	0/1/1/2	-
1	CSO	D	51[B]	1	-	0/1/5/7	-
1	TRX	A	439	1	-	0/4/6/8	0/2/2/2
1	AGM	A	282	1	-	2/10/11/13	-
3	A1I9G	C	159	3	-	2/6/10/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	GL3	C-S	-4.52	1.65	1.80
1	D	457	GL3	C-S	-4.46	1.65	1.80
1	A	462	DYA	OD1-CG	-2.06	1.25	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	159	A1I9G	CB-CG-ND1	4.19	127.76	120.16
1	A	462	DYA	O-C-CA	-3.90	120.43	125.39
3	F	159	A1I9G	CB-CG-ND1	3.87	127.19	120.16
1	D	462	DYA	O-C-CA	-3.20	121.32	125.39
1	A	439	TRX	CH2-CZ2-CE2	-2.22	116.94	119.29
1	A	462	DYA	OD2-CG-CB	-2.22	116.83	123.89
3	F	159	A1I9G	CD2-CG-CB	-2.09	126.03	129.25

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	462	DYA	O-C-CA-CB
1	A	462	DYA	CA-CB-CG-OD1
1	A	464	SMC	CA-CB-SG-CS
3	C	159	A1I9G	O-C-CA-CB
1	D	462	DYA	O-C-CA-CB
1	D	462	DYA	CA-CB-CG-OD1
1	D	464	SMC	CA-CB-SG-CS

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Mol	Chain	Res	Type	Atoms
3	F	159	A1I9G	O-C-CA-CB
1	A	462	DYA	CA-CB-CG-OD2
1	D	462	DYA	CA-CB-CG-OD2
3	F	159	A1I9G	CF-CB-CG-CD2
3	C	159	A1I9G	CF-CB-CG-CD2
1	A	282	AGM	NE1-CD-CG-CB
1	D	282	AGM	NE1-CD-CG-CB
1	A	282	AGM	CE2-CD-NE1-CZ

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 35 ligands modelled in this entry, 3 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	B	508	-	3,3,3	0.63	0	2,2,2	0.25	0
7	F43	A	607	9,1	61,71,71	2.14	4 (6%)	64,118,118	1.07	5 (7%)
5	EDO	D	603	-	3,3,3	0.55	0	2,2,2	0.15	0
5	EDO	B	503[A]	-	3,3,3	0.22	0	2,2,2	0.44	0
6	NO3	A	605	-	1,3,3	0.54	0	0,3,3	-	-
5	EDO	D	606	-	3,3,3	0.43	0	2,2,2	0.46	0
8	TP7	A	609	-	19,20,20	0.76	1 (5%)	24,26,26	0.73	0
5	EDO	B	504[A]	-	3,3,3	0.09	0	2,2,2	0.60	0
5	EDO	A	604	-	3,3,3	0.10	0	2,2,2	0.15	0
6	NO3	E	504	10	1,3,3	0.17	0	0,3,3	-	-
5	EDO	E	503	-	3,3,3	0.10	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	TP7	D	608	-	19,20,20	0.84	0	24,26,26	0.63	0
5	EDO	B	502	-	3,3,3	0.48	0	2,2,2	0.32	0
5	EDO	D	602	-	3,3,3	0.54	0	2,2,2	0.32	0
5	EDO	B	505	-	3,3,3	0.51	0	2,2,2	0.39	0
5	EDO	B	506	10	3,3,3	0.88	0	2,2,2	0.45	0
5	EDO	C	301	-	3,3,3	0.05	0	2,2,2	0.17	0
5	EDO	F	302	-	3,3,3	0.49	0	2,2,2	0.46	0
6	NO3	D	605	-	1,3,3	0.48	0	0,3,3	-	-
5	EDO	C	302	-	3,3,3	0.39	0	2,2,2	0.31	0
7	F43	D	607	1,9	61,71,71	2.15	6 (9%)	64,118,118	1.20	7 (10%)
6	NO3	B	507	10	1,3,3	0.28	0	0,3,3	-	-
5	EDO	E	502	-	3,3,3	0.51	0	2,2,2	0.20	0
9	COM	A	610	7	6,6,6	0.55	0	7,8,8	0.63	0
5	EDO	D	601	-	3,3,3	0.46	0	2,2,2	0.26	0
5	EDO	A	608	-	3,3,3	0.42	0	2,2,2	0.45	0
5	EDO	A	603[B]	-	3,3,3	0.48	0	2,2,2	0.40	0
5	EDO	A	602	-	3,3,3	0.54	0	2,2,2	0.38	0
5	EDO	A	606[A]	-	3,3,3	0.54	0	2,2,2	0.32	0
6	NO3	B	509	-	1,3,3	1.77	0	0,3,3	-	-
9	COM	D	604	7	6,6,6	0.63	0	7,8,8	0.79	0
5	EDO	F	301	-	3,3,3	0.50	0	2,2,2	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	508	-	-	0/1/1/1	-
7	F43	A	607	9,1	-	7/28/185/185	-
5	EDO	D	603	-	-	1/1/1/1	-
5	EDO	B	503[A]	-	-	1/1/1/1	-
5	EDO	D	606	-	-	0/1/1/1	-
8	TP7	A	609	-	-	0/24/24/24	-
5	EDO	B	504[A]	-	-	1/1/1/1	-
5	EDO	A	604	-	-	0/1/1/1	-
5	EDO	E	503	-	-	0/1/1/1	-
8	TP7	D	608	-	-	0/24/24/24	-
5	EDO	B	502	-	-	0/1/1/1	-
5	EDO	D	602	-	-	0/1/1/1	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	B	506	10	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	301	-	-	0/1/1/1	-
5	EDO	F	302	-	-	0/1/1/1	-
5	EDO	C	302	-	-	0/1/1/1	-
7	F43	D	607	1,9	-	8/28/185/185	-
5	EDO	E	502	-	-	0/1/1/1	-
9	COM	A	610	7	-	0/4/4/4	-
5	EDO	D	601	-	-	0/1/1/1	-
5	EDO	A	608	-	-	0/1/1/1	-
5	EDO	A	603[B]	-	-	1/1/1/1	-
5	EDO	A	602	-	-	0/1/1/1	-
5	EDO	A	606[A]	-	-	0/1/1/1	-
9	COM	D	604	7	-	0/4/4/4	-
5	EDO	F	301	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	607	F43	NI-NA	9.90	2.10	1.89
7	D	607	F43	NI-NB	9.37	2.09	1.89
7	D	607	F43	NI-NA	8.91	2.08	1.89
7	A	607	F43	NI-NB	8.67	2.08	1.89
7	A	607	F43	NI-ND	7.65	2.06	1.89
7	D	607	F43	NI-ND	7.55	2.05	1.89
7	D	607	F43	CHD-C1D	-3.22	1.39	1.43
7	A	607	F43	CHD-C1D	-2.60	1.40	1.43
7	D	607	F43	OBD-CAD	2.32	1.29	1.22
8	A	609	TP7	P-O4P	2.14	1.63	1.59
7	D	607	F43	CHC-C4B	2.14	1.45	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	607	F43	C2B-C1B-NB	2.84	106.09	101.84
7	D	607	F43	C2B-C1B-NB	2.63	105.78	101.84
7	D	607	F43	C4A-NA-C1A	-2.43	106.02	108.97
7	D	607	F43	OBD-CAD-C9D	-2.42	115.04	122.80
7	D	607	F43	C3D-C4D-ND	2.42	106.10	102.34
7	D	607	F43	OCC-CAC-C9C	-2.41	115.33	123.08
7	D	607	F43	O8D-C7D-C6D	-2.38	116.96	120.86
7	A	607	F43	O8D-C7D-C6D	-2.25	117.17	120.86
7	D	607	F43	CAB-C3B-C2B	-2.19	114.46	119.09
7	A	607	F43	C3B-C4B-CHC	-2.09	118.81	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	607	F43	OCC-CAC-C9C	-2.06	116.47	123.08
7	A	607	F43	CAB-C3B-C2B	-2.05	114.76	119.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	607	F43	C3A-CAA-CBA-CCA
5	B	503[A]	EDO	O1-C1-C2-O2
5	D	603	EDO	O1-C1-C2-O2
7	A	607	F43	CAB-CBB-CCB-ODB
7	D	607	F43	CAB-CBB-CCB-ODB
7	A	607	F43	CAB-CBB-CCB-OEB
7	D	607	F43	CAB-CBB-CCB-OEB
7	A	607	F43	C3A-CAA-CBA-CCA
7	A	607	F43	CAA-CBA-CCA-ODA
7	D	607	F43	CAA-CBA-CCA-ODA
7	A	607	F43	CAA-CBA-CCA-OEA
7	D	607	F43	C3D-C9D-CAD-OC'D
7	D	607	F43	CAA-CBA-CCA-OEA
5	A	603[B]	EDO	O1-C1-C2-O2
5	B	504[A]	EDO	O1-C1-C2-O2
7	A	607	F43	C2C-C5C-C6C-O8C
7	A	607	F43	C2D-C3D-C9D-CAD
7	D	607	F43	C2D-C3D-C9D-CAD
7	D	607	F43	C3D-C9D-CAD-OB'D

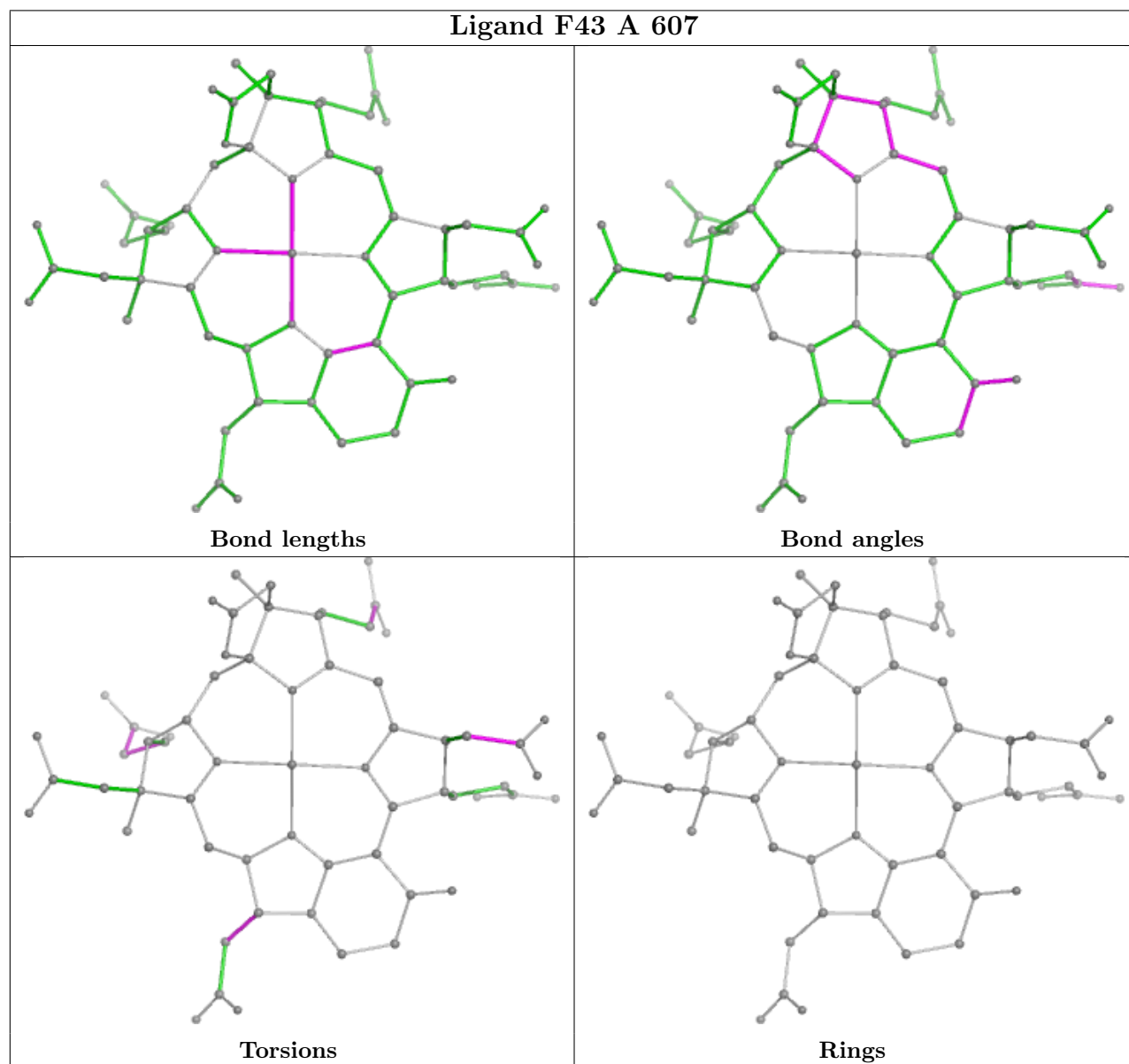
There are no ring outliers.

2 monomers are involved in 2 short contacts:

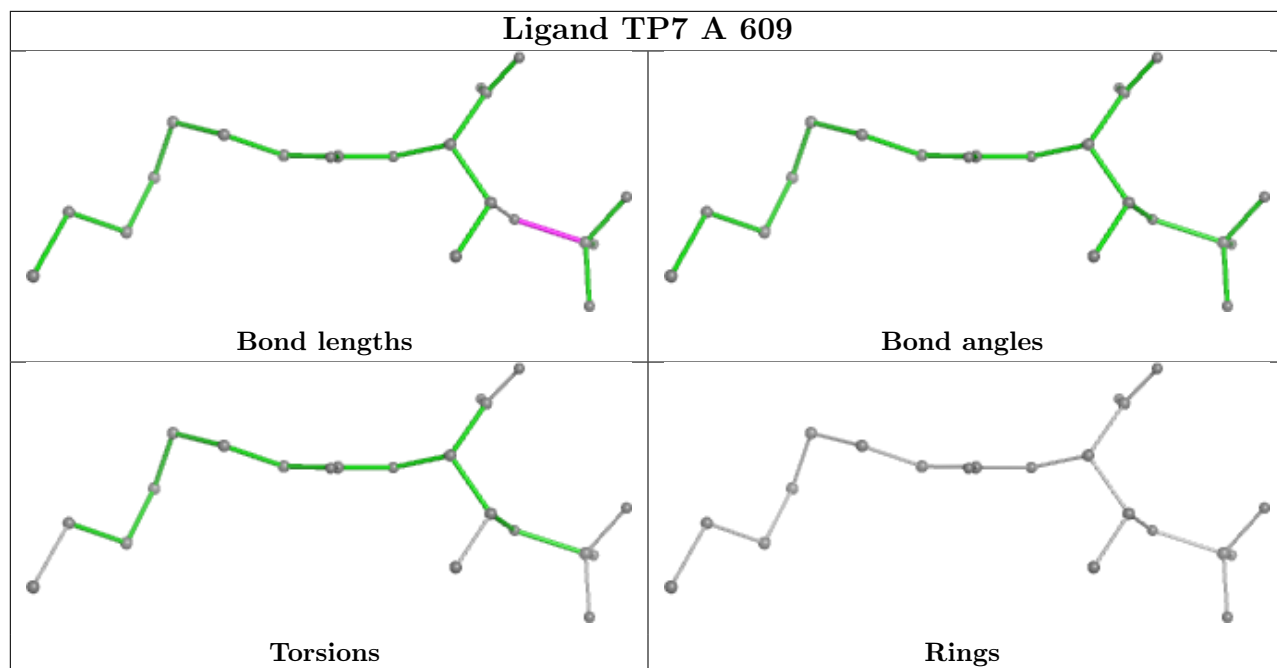
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	607	F43	1	0
7	D	607	F43	1	0

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

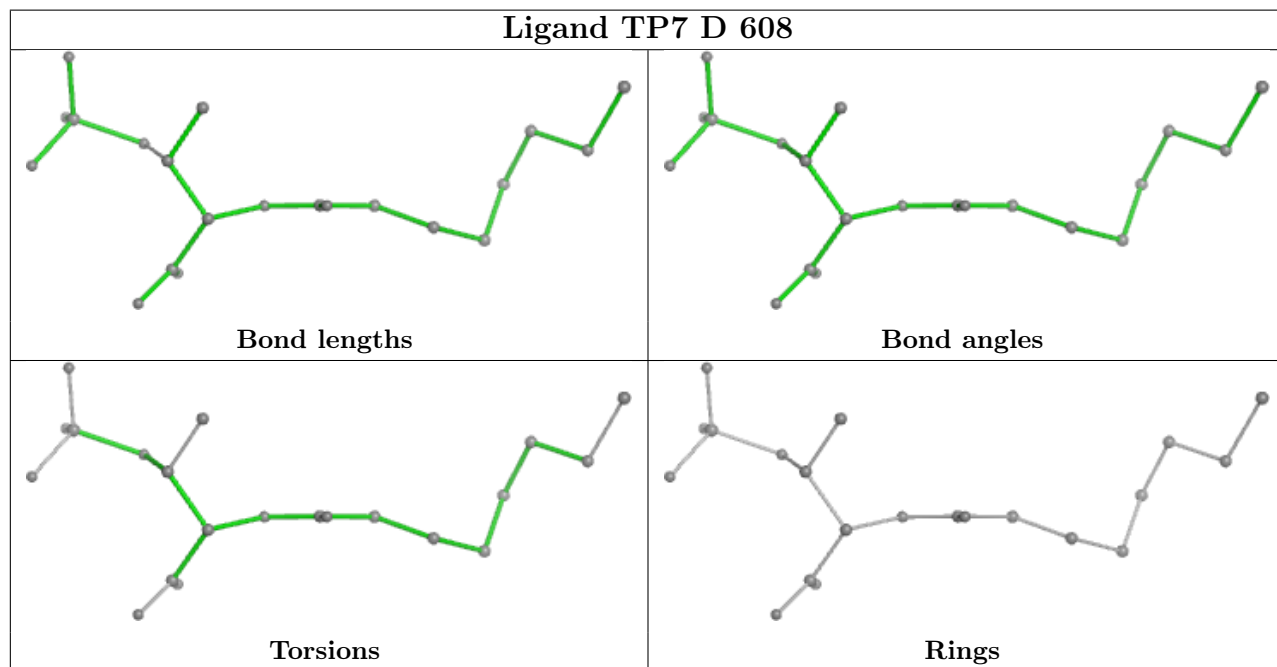
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



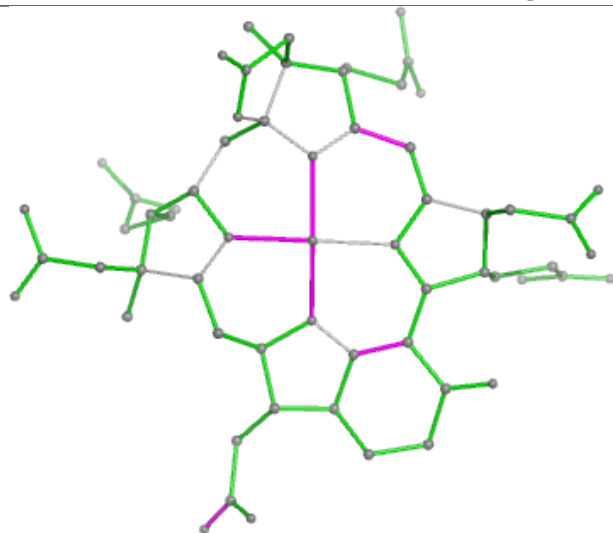
Ligand TP7 A 609



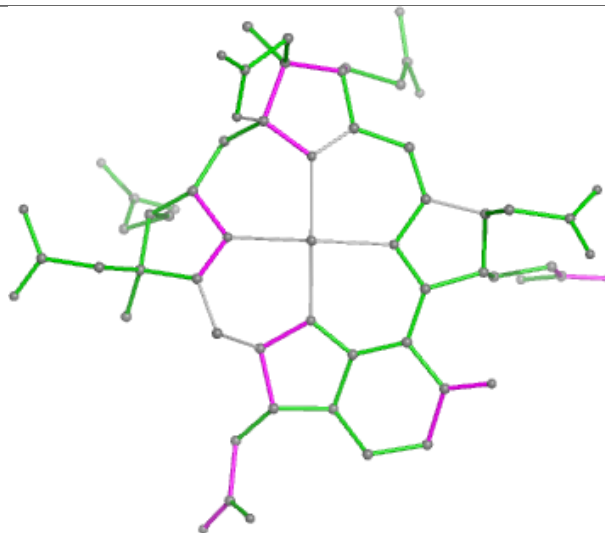
Ligand TP7 D 608



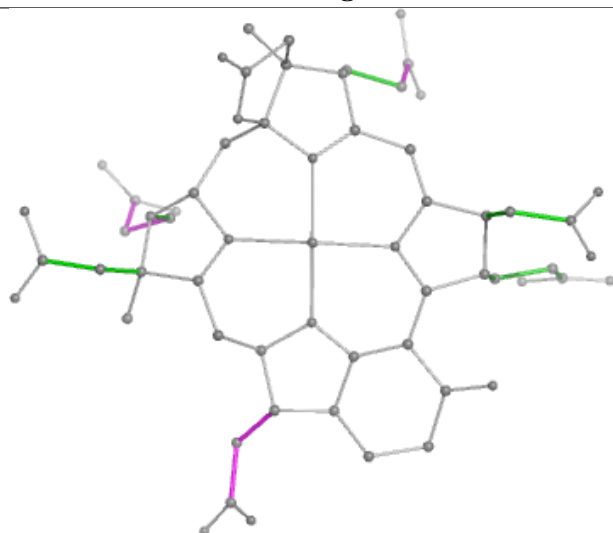
Ligand F43 D 607



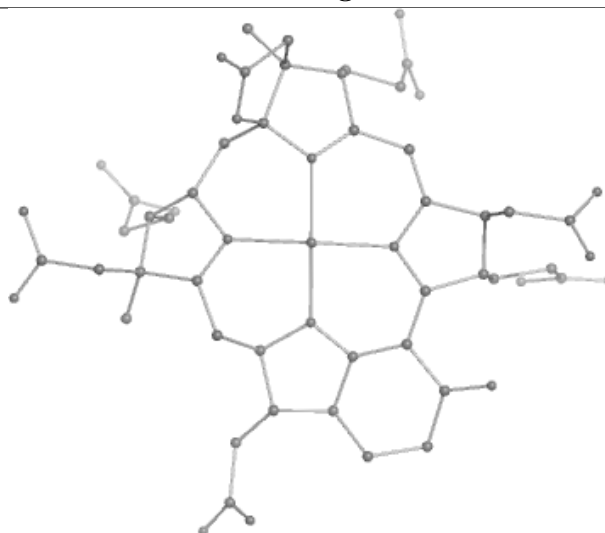
Bond lengths



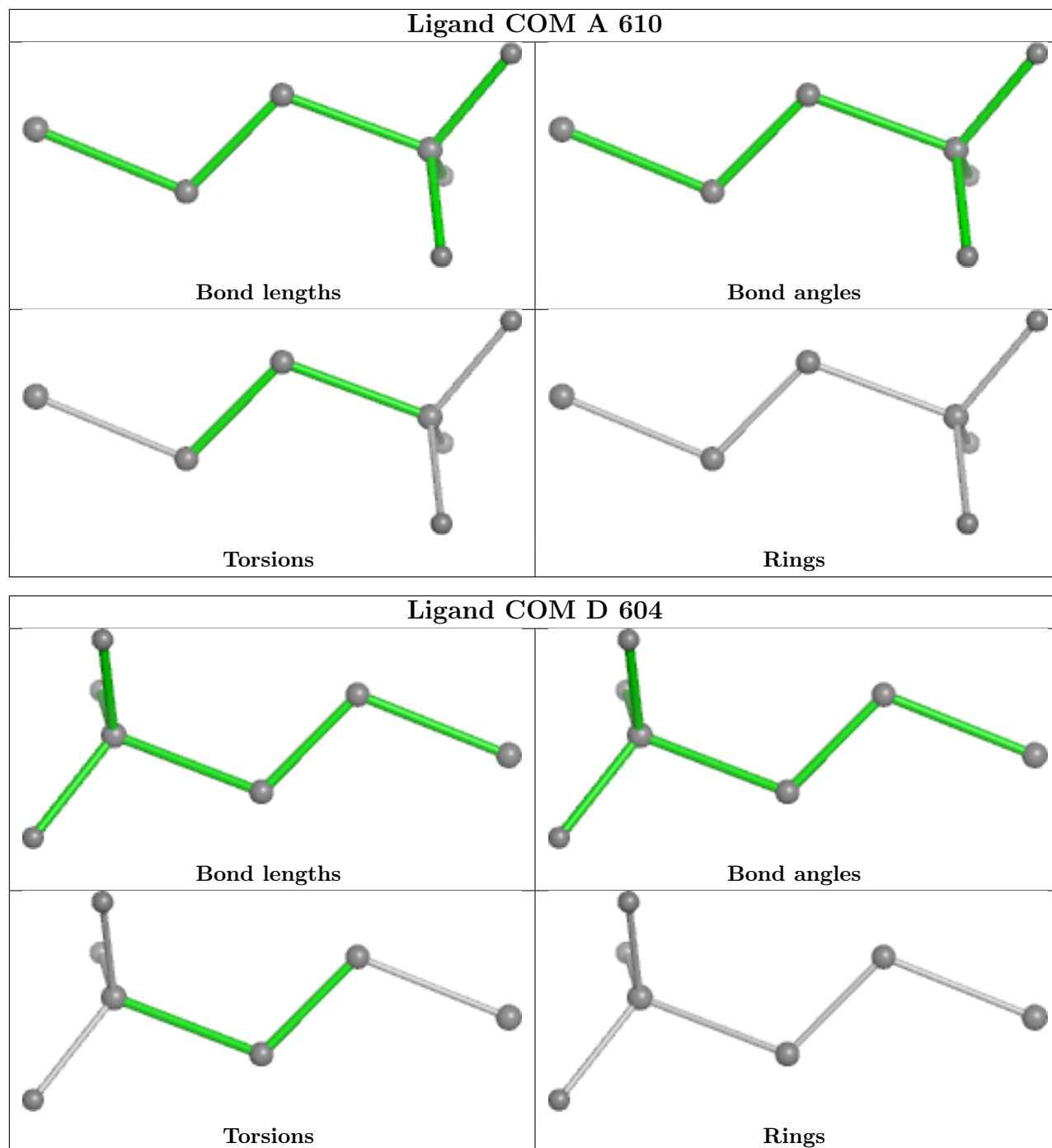
Bond angles



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(Å ²)	Q<0.9
1	A	553/563 (98%)	-0.78	2 (0%) 89 89	4, 8, 16, 28	26 (4%)
1	D	553/563 (98%)	-0.74	3 (0%) 87 89	4, 8, 18, 33	18 (3%)
2	B	433/434 (99%)	-0.75	0 100 100	3, 8, 16, 24	26 (6%)
2	E	433/434 (99%)	-0.73	1 (0%) 92 90	3, 8, 15, 25	34 (7%)
3	C	247/249 (99%)	-0.73	1 (0%) 89 89	5, 8, 16, 32	9 (3%)
3	F	247/249 (99%)	-0.59	2 (0%) 82 85	6, 10, 21, 34	7 (2%)
All	All	2466/2492 (98%)	-0.74	9 (0%) 89 89	3, 8, 17, 34	120 (4%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	2	ALA	4.7
1	A	2	ALA	3.2
1	A	561	ALA	2.9
3	F	60	ILE	2.9
2	E	434	VAL	2.7
1	D	561	ALA	2.7
3	F	2	ALA	2.5
1	D	2	ALA	2.4
1	D	23	LYS	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(\AA^2)	Q<0.9
1	MHS	A	268	11/12	0.98	0.05	5,6,10,14	0
1	MHS	D	268	11/12	0.98	0.05	5,6,10,15	0
1	AGM	A	282	12/13	0.99	0.03	5,5,6,7	0
1	TRX	A	439	15/16	0.99	0.04	4,5,5,5	0
1	DYA	A	462	8/9	0.99	0.03	4,5,6,6	0
1	SMC	A	464	7/8	0.99	0.04	5,5,7,7	0
3	A1I9G	C	159	11/12	0.99	0.04	5,5,6,6	0
1	CSO	D	51[B]	7/8	0.99	0.05	7,7,10,16	7
1	CSO	A	51	7/8	0.99	0.05	8,8,9,15	0
1	AGM	D	282	12/13	0.99	0.04	5,5,6,7	0
1	TRX	D	439	15/16	0.99	0.04	5,5,5,6	0
1	DYA	D	462	8/9	0.99	0.03	4,5,6,6	0
3	A1I9G	F	159	11/12	0.99	0.05	6,6,7,7	0
1	GL3	A	457	4/5	1.00	0.03	4,4,4,4	0
1	SMC	D	464	7/8	1.00	0.03	5,5,7,7	0
1	GL3	D	457	4/5	1.00	0.03	4,4,4,4	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
5	EDO	B	503[A]	4/4	0.77	0.16	33,39,41,43	10
5	EDO	B	505	4/4	0.80	0.14	28,34,35,36	0
5	EDO	D	603	4/4	0.83	0.13	30,36,37,37	0
6	NO3	A	605	4/4	0.83	0.15	39,39,40,41	0
5	EDO	F	301	4/4	0.84	0.11	30,36,38,40	0
6	NO3	D	605	4/4	0.84	0.14	39,40,40,41	0
5	EDO	A	604	4/4	0.87	0.10	25,30,31,32	0
6	NO3	B	509	4/4	0.90	0.12	14,18,20,25	0
5	EDO	A	603[B]	4/4	0.90	0.14	18,20,24,24	7
5	EDO	D	602	4/4	0.92	0.10	20,27,31,34	0
4	NA	A	601	1/1	0.92	0.48	28,28,28,28	0
5	EDO	B	506	4/4	0.92	0.10	14,18,22,22	0
5	EDO	E	503	4/4	0.94	0.08	23,28,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	504[A]	4/4	0.95	0.10	7,18,22,22	10
5	EDO	C	301	4/4	0.95	0.08	19,23,24,24	0
5	EDO	A	602	4/4	0.95	0.08	17,24,27,31	0
5	EDO	B	502	4/4	0.96	0.07	17,20,23,23	0
5	EDO	E	502	4/4	0.97	0.06	15,21,24,27	0
6	NO3	B	507	4/4	0.97	0.06	10,13,15,18	0
5	EDO	B	508	4/4	0.97	0.06	17,20,24,26	0
5	EDO	D	606	4/4	0.97	0.06	10,12,14,14	0
5	EDO	C	302	4/4	0.98	0.05	12,16,20,24	0
5	EDO	F	302	4/4	0.98	0.05	14,17,20,25	0
6	NO3	E	504	4/4	0.98	0.05	10,13,13,18	0
5	EDO	A	606[A]	4/4	0.99	0.04	5,6,7,7	7
5	EDO	A	608	4/4	0.99	0.05	11,17,20,23	0
5	EDO	D	601	4/4	0.99	0.05	12,16,20,20	0
8	TP7	A	609	21/21	0.99	0.04	4,5,6,6	0
7	F43	D	607	62/62	1.00	0.03	4,5,8,12	0
7	F43	A	607	62/62	1.00	0.03	4,4,8,12	0
8	TP7	D	608	21/21	1.00	0.03	5,5,6,6	0
9	COM	A	610	7/7	1.00	0.02	4,5,5,6	0
9	COM	D	604	7/7	1.00	0.02	5,5,6,6	0
10	K	B	501	1/1	1.00	0.06	9,9,9,9	0
10	K	E	501	1/1	1.00	0.07	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.