



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2026 – 10:22 am BST

PDB ID : 5N2A / pdb_00005n2a
Title : METHYL-COENZYME M REDUCTASE III FROM METHANOTORRIS
FORMICICUS TRIGONAL FORM
Authors : Wagner, T.; Wegner, C.E.; Ermler, U.; Shima, S.
Deposited on : 2017-02-07
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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

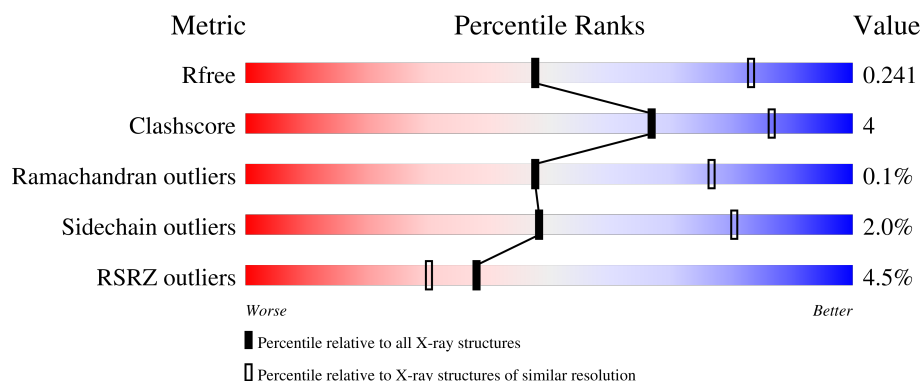
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	552	2% 87% 12% ..
2	B	444	4% 90% 10% ..
3	C	260	10% 85% 13% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9806 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4277	2721	718	816	22			

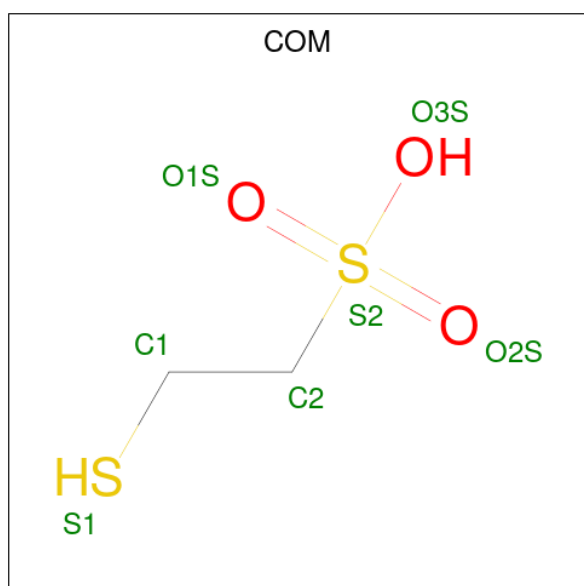
- Molecule 2 is a protein called Methyl-coenzyme M reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	443	Total	C	N	O	S	0	0	0
			3324	2123	551	630	20			

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

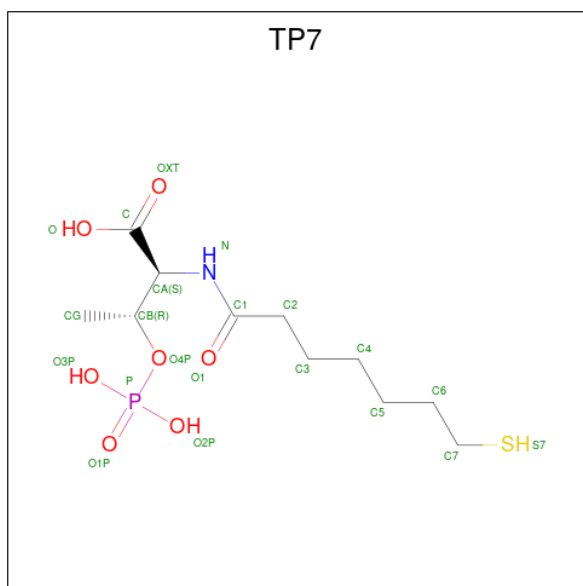
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	258	Total	C	N	O	S	0	0	0
			2113	1331	376	396	10			

- Molecule 4 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: C₂H₆O₃S₂).



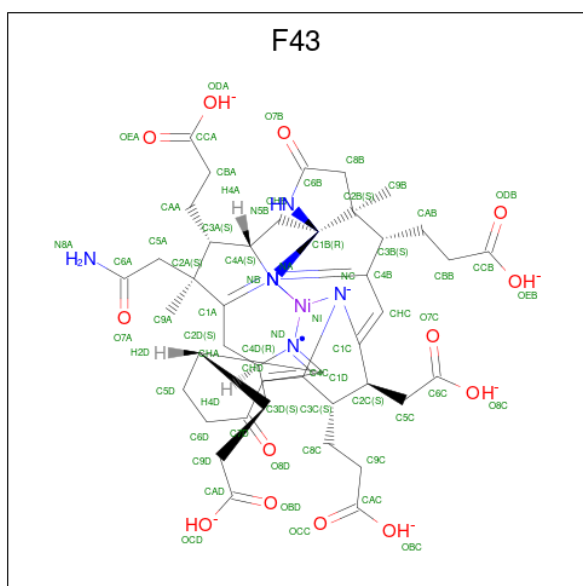
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 5 is Coenzyme B (CCD ID: TP7) (formula: $\text{C}_{11}\text{H}_{22}\text{NO}_7\text{PS}$).



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

- Molecule 6 is FACTOR 430 (CCD ID: F43) (formula: $\text{C}_{42}\text{H}_{51}\text{N}_6\text{NiO}_{13}$).



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

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

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

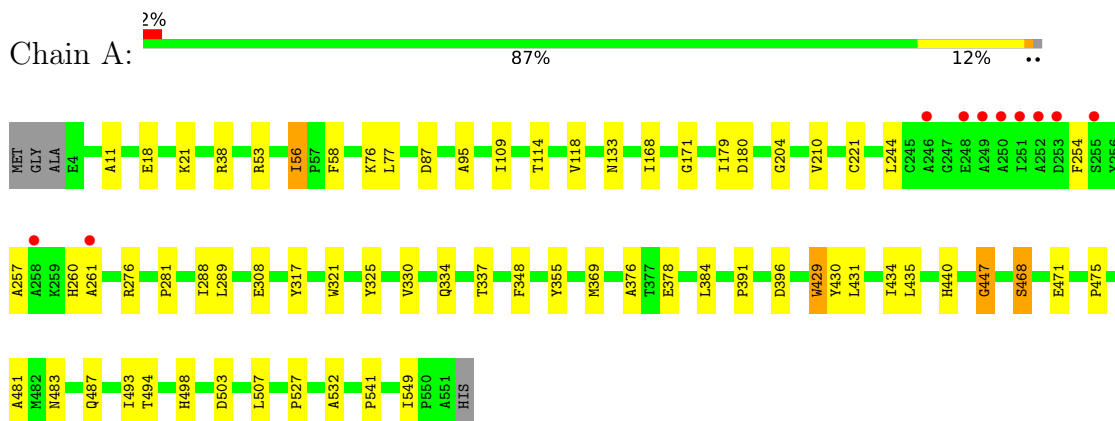
- Molecule 8 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Br	0	0
			1	1		

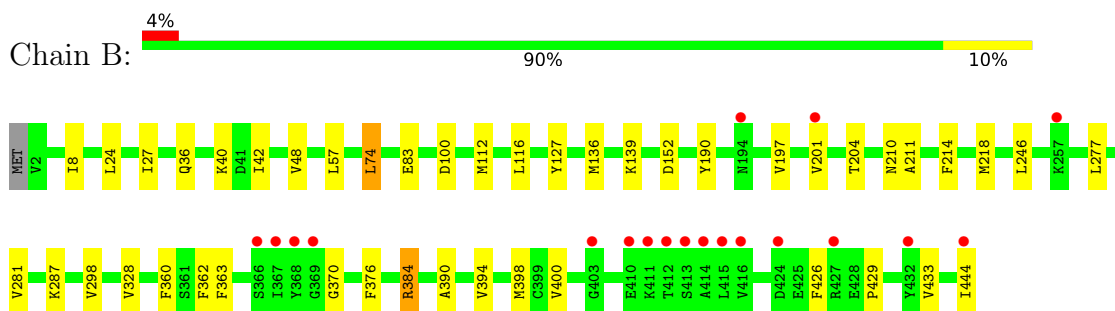
3 Residue-property plots [i](#)

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.

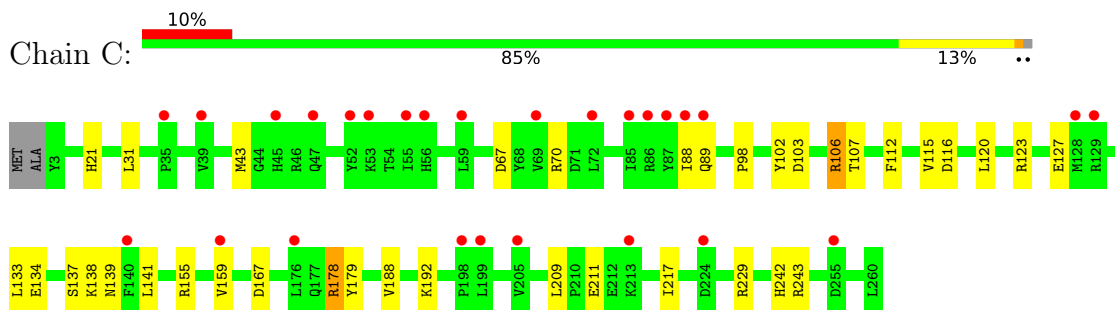
- Molecule 1: Methyl-coenzyme M reductase subunit alpha



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.70Å 127.70Å 160.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.85 – 2.80 39.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.85-2.80) 99.8 (39.85-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.198 , 0.221 0.218 , 0.241	Depositor DCC
R_{free} test set	1901 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9806	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COM, MHS, TRX, TP7, BR, F43, MGN, K, AGM, GL3

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	0.68	0/4319	1.25	10/5844 (0.2%)
2	B	0.73	0/3382	1.27	8/4590 (0.2%)
3	C	0.70	0/2161	1.19	1/2919 (0.0%)
All	All	0.70	0/9862	1.24	19/13353 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	LEU	CA-C-N	6.29	128.99	120.38
2	B	57	LEU	C-N-CA	6.29	128.99	120.38
1	A	221	CYS	N-CA-C	5.91	113.62	108.78
2	B	298	VAL	N-CA-C	-5.83	104.65	111.00
3	C	167	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	254	PHE	CA-CB-CG	5.36	119.16	113.80
2	B	360	PHE	CA-CB-CG	5.35	119.15	113.80
2	B	100	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	348	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	435	LEU	CA-C-N	5.26	127.33	120.28
1	A	435	LEU	C-N-CA	5.26	127.33	120.28
1	A	396	ASP	CA-CB-CG	5.26	117.86	112.60
2	B	277	LEU	CA-C-N	5.26	127.33	120.28
2	B	277	LEU	C-N-CA	5.26	127.33	120.28
2	B	127	TYR	N-CA-C	5.21	118.90	112.54
1	A	483	ASN	N-CA-C	5.20	117.96	109.59
1	A	483	ASN	CA-C-N	5.06	128.34	120.34
1	A	483	ASN	C-N-CA	5.06	128.34	120.34
1	A	58	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4277	0	4141	32	0
2	B	3324	0	3372	19	0
3	C	2113	0	2073	22	0
4	A	7	0	6	1	0
5	A	21	0	19	0	0
6	A	62	0	43	3	0
7	A	1	0	0	0	0
8	C	1	0	0	0	0
All	All	9806	0	9654	71	0

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

All (71) 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)
3:C:89:GLN:HB2	3:C:155:ARG:O	1.84	0.76
1:A:308:GLU:HG3	1:A:527:PRO:HD2	1.73	0.70
3:C:103:ASP:O	3:C:107:THR:HG23	1.92	0.69
2:B:328:VAL:HG21	2:B:394:VAL:HA	1.75	0.67
3:C:137:SER:HA	3:C:141:LEU:HB2	1.80	0.64
2:B:204:THR:HG21	2:B:211:ALA:HB2	1.78	0.64
1:A:257:ALA:HA	1:A:261:ALA:HB3	1.83	0.60
1:A:434:ILE:HD11	3:C:242:HIS:HB2	1.83	0.59
2:B:48:VAL:HB	2:B:112:MET:HB3	1.86	0.58
3:C:178:ARG:HA	3:C:192:LYS:HB2	1.87	0.57
3:C:67:ASP:HB3	3:C:70:ARG:HB3	1.88	0.55
2:B:42:ILE:HG12	2:B:426:PHE:HE2	1.74	0.53
2:B:400:VAL:HG12	3:C:70:ARG:HG3	1.90	0.52
3:C:102:TYR:O	3:C:106:ARG:HG2	2.10	0.52
1:A:38:ARG:HH11	1:A:38:ARG:HA	1.74	0.52
1:A:429:TRX:HD1	1:A:430:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:PHE:HB2	2:B:429:PRO:HG3	1.92	0.51
2:B:246:LEU:HD22	2:B:433:VAL:HG21	1.94	0.50
1:A:21:LYS:HA	1:A:391:PRO:HD2	1.94	0.50
3:C:31:LEU:HD13	3:C:209:LEU:HD11	1.94	0.50
2:B:42:ILE:HD12	2:B:218:MET:HE2	1.94	0.49
1:A:308:GLU:CG	1:A:527:PRO:HD2	2.40	0.49
1:A:38:ARG:HG2	1:A:87:ASP:HB2	1.96	0.48
1:A:369:MET:HG2	3:C:243:ARG:HG3	1.96	0.48
3:C:112:PHE:HB2	3:C:115:VAL:HG11	1.95	0.48
1:A:281:PRO:HB2	1:A:321:TRP:HB2	1.94	0.48
2:B:390:ALA:O	2:B:394:VAL:HG23	2.14	0.48
3:C:179:TYR:HD2	3:C:188:VAL:HG11	1.78	0.47
2:B:201:VAL:HG21	2:B:398:MET:HB2	1.95	0.47
2:B:74:LEU:HD11	2:B:152:ASP:HB3	1.97	0.47
3:C:21:HIS:HB3	3:C:107:THR:HG21	1.97	0.47
1:A:384:LEU:HD23	1:A:440:HIS:CE1	2.50	0.47
1:A:471:GLU:HG3	1:A:494:THR:HG23	1.96	0.47
2:B:197:VAL:HG23	2:B:376:PHE:O	2.15	0.47
1:A:288:ILE:HG13	1:A:507:LEU:HD23	1.97	0.46
1:A:77:LEU:HG	1:A:532:ALA:HB2	1.98	0.46
1:A:330:VAL:HB	6:A:603:F43:H9A1	1.96	0.46
1:A:114:THR:O	1:A:118:VAL:HG23	2.17	0.44
1:A:447:GL3:HA1	2:B:362:PHE:HB2	1.99	0.44
1:A:334:GLN:HA	1:A:337:THR:OG1	2.17	0.44
6:A:603:F43:H9A3	6:A:603:F43:HAA1	1.78	0.44
1:A:171:GLY:HA3	1:A:204:GLY:O	2.17	0.44
1:A:376:ALA:HB3	1:A:431:LEU:HD23	1.99	0.44
3:C:116:ASP:HB3	3:C:127:GLU:HB2	2.00	0.44
1:A:168:ILE:HD13	1:A:179:ILE:HD13	2.01	0.43
2:B:36:GLN:HE21	2:B:40:LYS:HD2	1.84	0.43
2:B:210:ASN:HB3	2:B:429:PRO:HD2	2.00	0.43
1:A:133:ASN:OD1	1:A:180:ASP:HB2	2.19	0.43
1:A:429:TRX:HE3	1:A:493:ILE:HD11	2.00	0.43
1:A:498:HIS:HB3	1:A:503:ASP:HB2	2.01	0.43
3:C:179:TYR:HD2	3:C:188:VAL:CG1	2.32	0.43
3:C:98:PRO:HB3	3:C:217:ILE:HD12	2.00	0.42
3:C:138:LYS:HG3	3:C:139:ASN:H	1.84	0.42
2:B:24:LEU:O	2:B:27:ILE:HG13	2.19	0.42
1:A:56:ILE:H	1:A:56:ILE:HG13	1.72	0.42
1:A:355:TYR:CE1	1:A:378:GLU:HG2	2.54	0.42
2:B:363:PHE:HB3	2:B:370:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:HB1	1:A:541:PRO:HG3	2.03	0.41
1:A:317:TYR:HB3	1:A:487:GLN:HE21	1.84	0.41
4:A:601:COM:H22	6:A:603:F43:C6B	2.50	0.41
3:C:21:HIS:HB3	3:C:107:THR:CG2	2.50	0.41
1:A:109:ILE:HG12	1:A:210:VAL:HG22	2.01	0.41
3:C:120:LEU:HD13	3:C:123:ARG:HG3	2.03	0.41
3:C:88:ILE:HG22	3:C:133:LEU:HD11	2.02	0.41
1:A:11:ALA:HB2	1:A:76:LYS:HE3	2.03	0.41
1:A:321:TRP:O	1:A:325:TYR:HB2	2.21	0.41
1:A:475:PRO:O	1:A:481:ALA:HA	2.21	0.40
2:B:136:MET:HA	2:B:139:LYS:HD2	2.03	0.40
2:B:190:TYR:HE2	2:B:384:ARG:HB2	1.86	0.40
3:C:43:MET:HE1	3:C:134:GLU:HA	2.02	0.40
3:C:123:ARG:HD3	3:C:159:VAL:HG21	2.03	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	541/552 (98%)	513 (95%)	27 (5%)	1 (0%)	43	72
2	B	441/444 (99%)	430 (98%)	11 (2%)	0	100	100
3	C	256/260 (98%)	245 (96%)	11 (4%)	0	100	100
All	All	1238/1256 (99%)	1188 (96%)	49 (4%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/438 (100%)	428 (98%)	8 (2%)	51	82
2	B	350/351 (100%)	342 (98%)	8 (2%)	44	78
3	C	228/229 (100%)	224 (98%)	4 (2%)	51	82
All	All	1014/1018 (100%)	994 (98%)	20 (2%)	48	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	53	ARG
1	A	56	ILE
1	A	244	LEU
1	A	276	ARG
1	A	289	LEU
1	A	468	SER
1	A	549	ILE
2	B	8	ILE
2	B	74	LEU
2	B	83	GLU
2	B	116	LEU
2	B	281	VAL
2	B	287	LYS
2	B	384	ARG
2	B	444	ILE
3	C	106	ARG
3	C	178	ARG
3	C	211	GLU
3	C	229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS

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Mol	Chain	Res	Type
1	A	195	GLN
1	A	233	GLN
1	A	265	GLN
1	A	305	GLN
1	A	436	HIS
1	A	495	GLN
2	B	36	GLN
2	B	166	GLN
2	B	259	ASN
2	B	405	GLN
3	C	124	GLN
3	C	177	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	MGN	A	402	1	6,9,10	0.62	0	5,12,14	0.62	0
1	AGM	A	274	1	10,11,12	0.49	0	6,13,15	0.59	0
1	GL3	A	447	1	2,3,4	3.35	1 (50%)	1,2,4	0.09	0
1	TRX	A	429	1	15,16,17	1.90	2 (13%)	19,22,24	1.67	3 (15%)
1	MHS	A	260	1	10,11,12	1.21	0	6,14,16	3.22	2 (33%)

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	MGN	A	402	1	-	0/7/9/12	-
1	AGM	A	274	1	-	3/10/11/13	-
1	GL3	A	447	1	-	1/1/1/2	-
1	TRX	A	429	1	-	0/5/6/8	0/2/2/2
1	MHS	A	260	1	-	0/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	429	TRX	CD2-CE2	5.79	1.48	1.41
1	A	447	GL3	C-S	-4.74	1.64	1.80
1	A	429	TRX	CD2-CG	2.92	1.48	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	MHS	ND1-CE1-NE2	-6.80	108.95	112.93
1	A	429	TRX	CZ2-CE2-CD2	-4.51	118.75	122.45
1	A	260	MHS	CD2-NE2-CE1	2.47	108.23	105.22
1	A	429	TRX	CE3-CD2-CE2	2.29	121.29	118.83
1	A	429	TRX	CZ3-CE3-CD2	-2.07	117.58	120.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	274	AGM	CE2-CD-CG-CB
1	A	274	AGM	NE1-CD-CG-CB
1	A	447	GL3	S-C-CA-N
1	A	274	AGM	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	447	GL3	1	0
1	A	429	TRX	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	TP7	A	602	-	19,20,20	0.63	0	24,26,26	0.70	0
4	COM	A	601	-	6,6,6	1.36	2 (33%)	7,8,8	3.16	4 (57%)
6	F43	A	603	1	61,71,71	2.02	6 (9%)	64,118,118	1.24	8 (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
5	TP7	A	602	-	-	1/24/24/24	-
4	COM	A	601	-	-	0/4/4/4	-
6	F43	A	603	1	-	9/28/185/185	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	F43	NI-NA	7.73	2.06	1.89
6	A	603	F43	NI-NB	7.15	2.04	1.89
6	A	603	F43	NI-ND	6.85	2.04	1.89
6	A	603	F43	CHD-C1D	-6.03	1.35	1.43
6	A	603	F43	CHC-C4B	2.77	1.47	1.39
4	A	601	COM	O1S-S2	2.20	1.51	1.45
6	A	603	F43	C4D-ND	-2.17	1.45	1.49
4	A	601	COM	O2S-S2	2.06	1.51	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	COM	O2S-S2-C2	5.25	113.23	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	COM	O2S-S2-O1S	-4.30	99.08	113.95
4	A	601	COM	O1S-S2-C2	4.27	112.06	106.92
6	A	603	F43	C4D-ND-C1D	2.70	112.07	108.51
6	A	603	F43	ODA-CCA-CBA	2.32	121.48	114.03
6	A	603	F43	OEA-CCA-CBA	-2.30	115.69	123.08
6	A	603	F43	O8D-C7D-C6D	-2.27	117.15	120.86
6	A	603	F43	C9D-C3D-C4D	-2.25	108.74	114.67
4	A	601	COM	O3S-S2-C2	2.23	109.38	105.77
6	A	603	F43	C2B-C1B-NB	2.20	105.13	101.84
6	A	603	F43	O7B-C6B-C8B	-2.04	124.10	126.59
6	A	603	F43	OCD-CAD-C9D	2.02	120.54	114.07

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	F43	C2A-C3A-CAA-CBA
6	A	603	F43	C4A-C3A-CAA-CBA
6	A	603	F43	C4B-C3B-CAB-CBB
6	A	603	F43	CAB-CBB-CCB-OEB
6	A	603	F43	CAB-CBB-CCB-ODB
6	A	603	F43	C3D-C9D-CAD-OB
6	A	603	F43	C3D-C9D-CAD-OCD
6	A	603	F43	C2D-C3D-C9D-CAD
5	A	602	TP7	C3-C4-C5-C6
6	A	603	F43	CAA-CBA-CCA-ODA

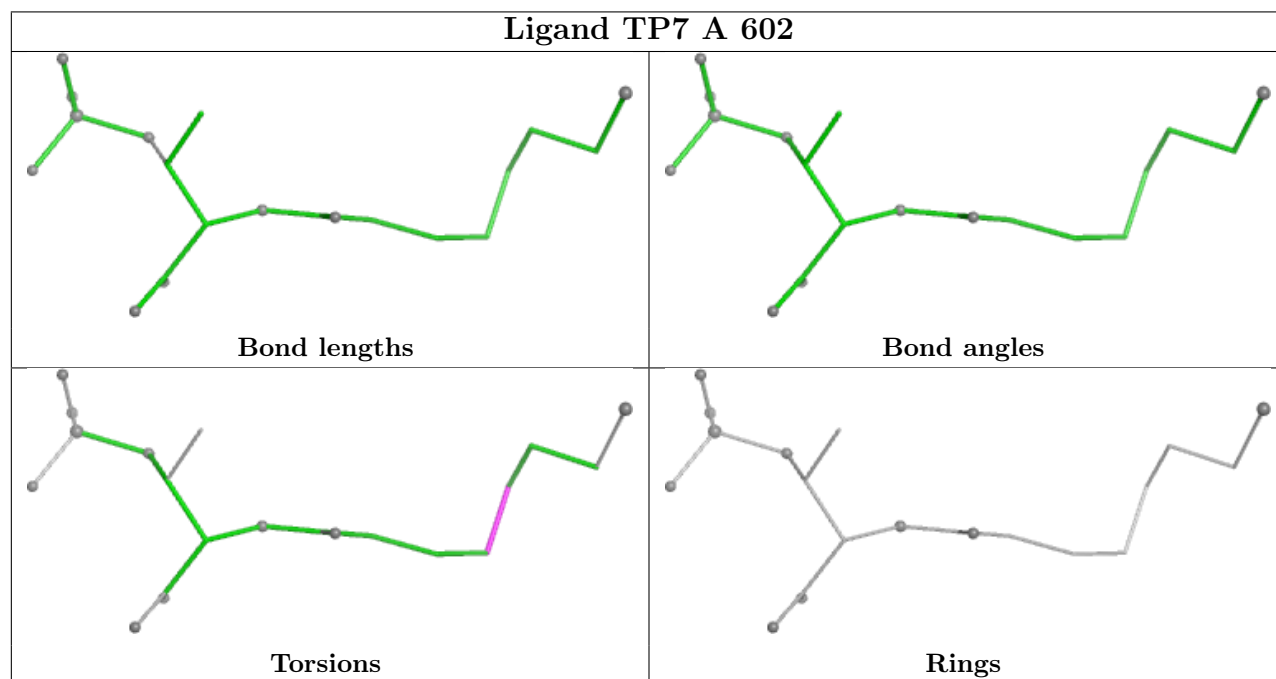
There are no ring outliers.

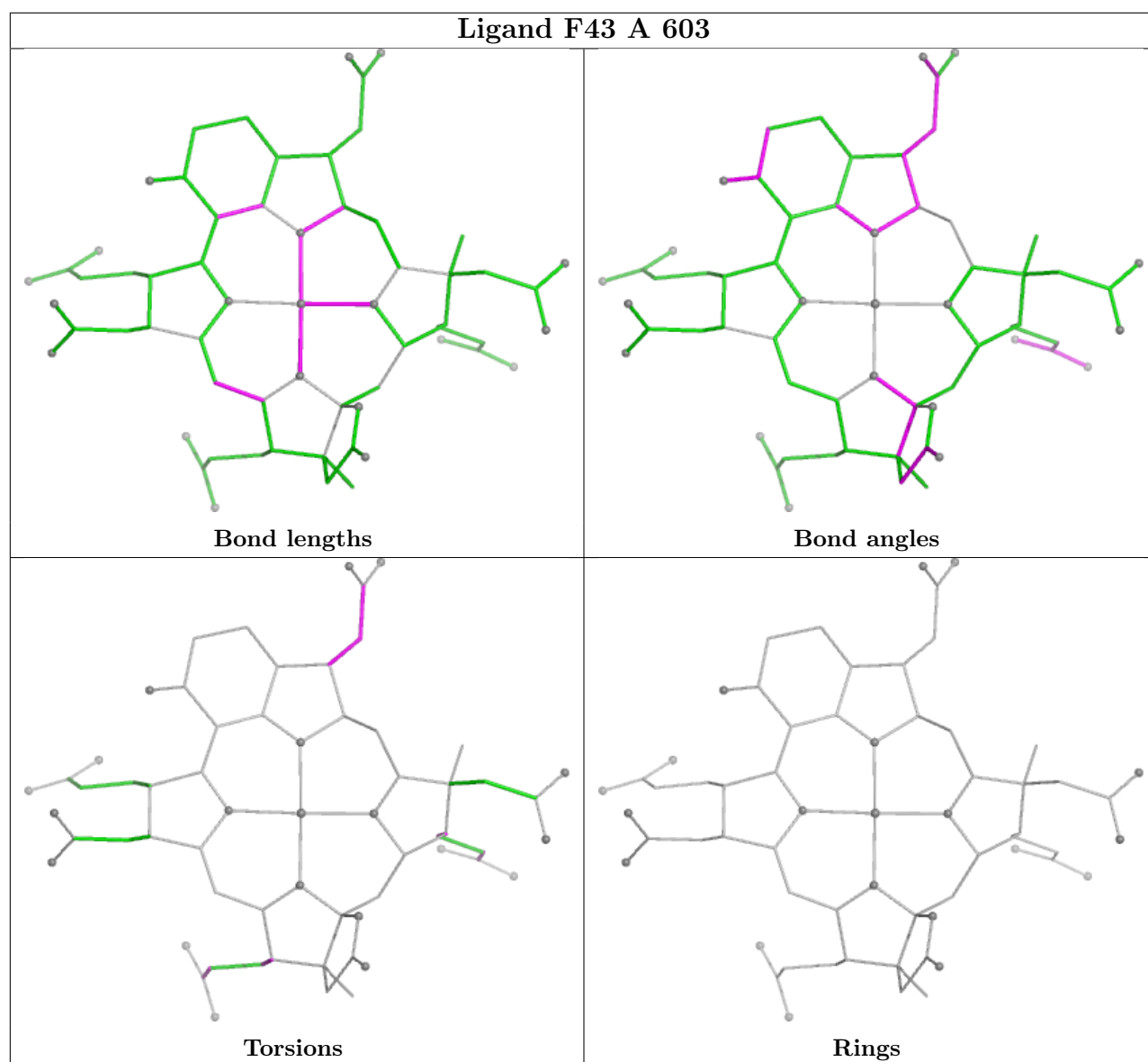
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	COM	1	0
6	A	603	F43	3	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/552 (98%)	-0.08	10 (1%) 67 58	30, 48, 83, 102	0
2	B	443/444 (99%)	0.18	19 (4%) 40 31	37, 55, 84, 94	0
3	C	258/260 (99%)	0.74	27 (10%) 11 8	35, 76, 121, 132	0
All	All	1244/1256 (99%)	0.18	56 (4%) 38 30	30, 54, 101, 132	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	415	LEU	4.4
2	B	416	VAL	4.1
3	C	55	ILE	3.7
3	C	59	LEU	3.6
1	A	249	ALA	3.3
2	B	414	ALA	3.3
1	A	252	ALA	3.1
1	A	251	ILE	3.1
2	B	403	GLY	3.0
3	C	140	PHE	3.0
3	C	159	VAL	3.0
3	C	89	GLN	3.0
1	A	246	ALA	3.0
2	B	368	TYR	3.0
1	A	248	GLU	3.0
1	A	255	SER	2.9
1	A	250	ALA	2.9
3	C	45	HIS	2.8
3	C	85	ILE	2.8
3	C	213	LYS	2.8
3	C	129	ARG	2.8
2	B	424	ASP	2.7
1	A	261	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	86	ARG	2.6
1	A	253	ASP	2.6
2	B	412	THR	2.6
3	C	88	ILE	2.6
3	C	205	VAL	2.6
2	B	413	SER	2.5
3	C	199	LEU	2.4
3	C	72	LEU	2.4
2	B	366	SER	2.4
3	C	198	PRO	2.4
2	B	201	VAL	2.4
2	B	411	LYS	2.4
2	B	369	GLY	2.4
3	C	69	VAL	2.4
3	C	224	ASP	2.3
3	C	128	MET	2.3
3	C	47	GLN	2.3
3	C	87	TYR	2.3
3	C	56	HIS	2.2
2	B	444	ILE	2.2
2	B	427	ARG	2.2
3	C	39	VAL	2.2
3	C	52	TYR	2.2
1	A	258	ALA	2.2
2	B	432	TYR	2.1
3	C	35	PRO	2.1
3	C	255	ASP	2.1
2	B	410	GLU	2.1
2	B	194	ASN	2.0
2	B	367	ILE	2.0
3	C	176	LEU	2.0
2	B	257	LYS	2.0
3	C	53	LYS	2.0

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

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
1	MHS	A	260	11/12	0.81	0.19	70,72,74,74	0
1	AGM	A	274	12/13	0.94	0.09	43,45,47,47	0
1	MGN	A	402	10/11	0.94	0.09	40,42,46,47	0
1	TRX	A	429	15/16	0.95	0.09	39,42,44,45	0
1	GL3	A	447	4/5	0.96	0.07	40,40,44,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

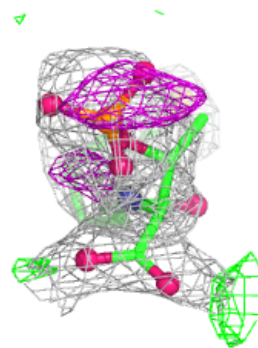
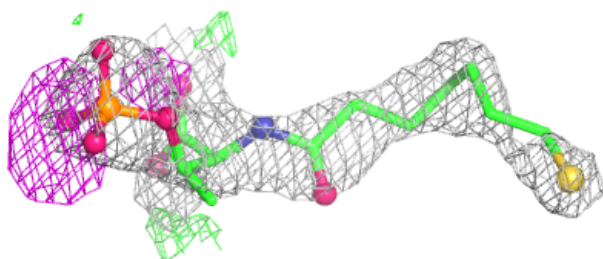
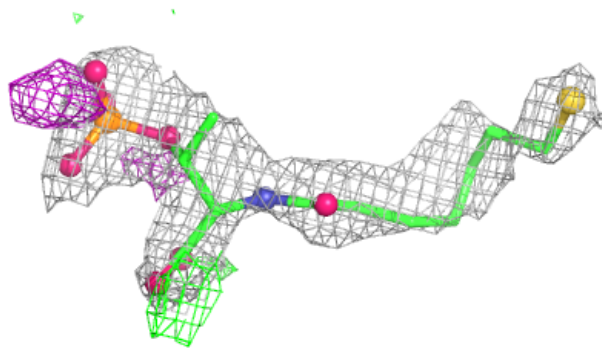
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	TP7	A	602	21/21	0.80	0.19	80,82,89,90	0
4	COM	A	601	7/7	0.91	0.17	70,77,81,82	0
8	BR	C	301	1/1	0.92	0.12	94,94,94,94	0
7	K	A	604	1/1	0.94	0.21	89,89,89,89	1
6	F43	A	603	62/62	0.94	0.11	55,59,67,72	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.

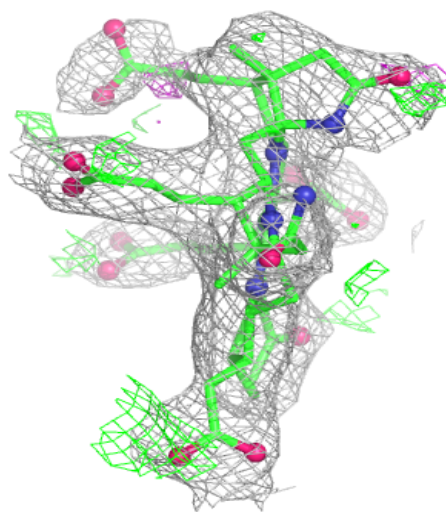
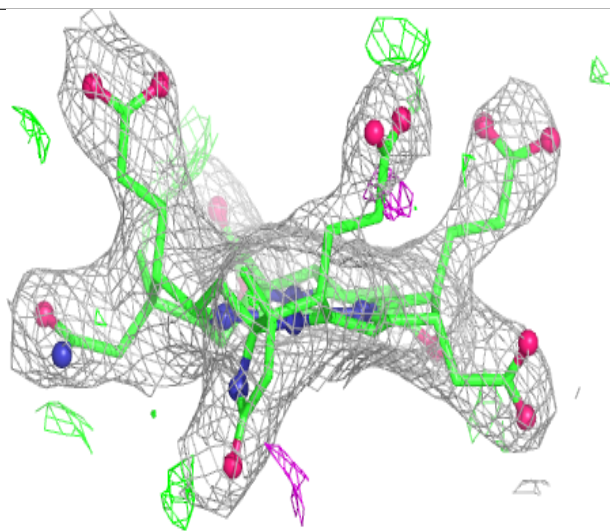
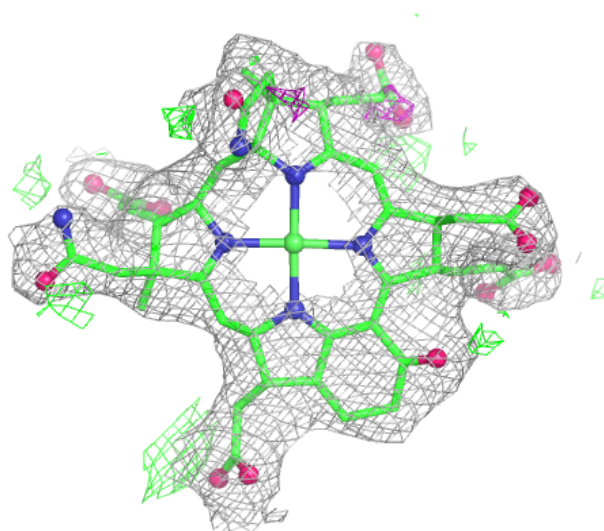
Electron density around TP7 A 602:

$2mF_o-DF_c$ (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.