



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 23, 2024 – 06:18 PM EDT

PDB ID : 5ESU
Title : Crystal Structure of M. tuberculosis MenD bound to Mg²⁺ and Covalent Intermediate II (a ThDP + de-carboxylated 2-oxoglutarate + Isochorismate adduct)
Authors : Johnston, J.M.; Jirgis, E.N.M.; Bashiri, G.; Bulloch, E.M.M.; Baker, E.N.
Deposited on : 2015-11-17
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

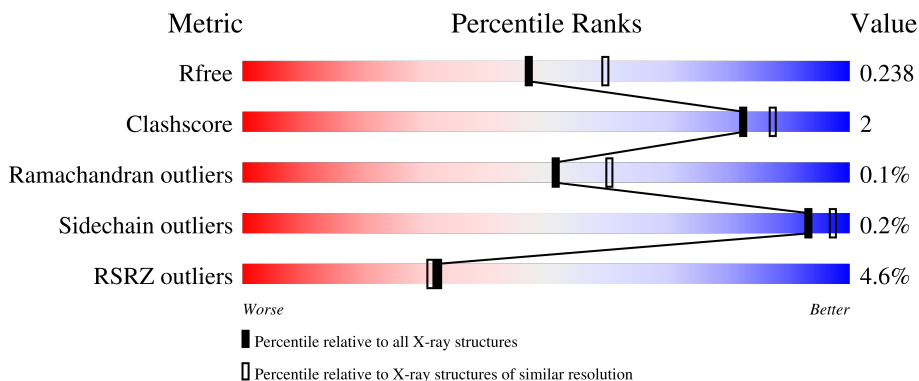
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

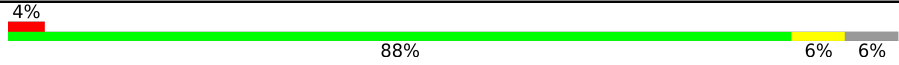


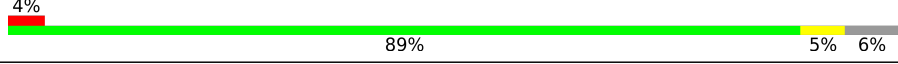
The reported resolution of this entry is 2.20 Å.

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	574	 4% 88% 6% 6%
1	B	574	 4% 87% 6% 7%
1	C	574	 5% 86% 7% 6%
1	D	574	 4% 89% 5% 6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16576 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	538	Total 3952	C 2465	N 733	O 743	S 11	0	3	0
1	B	535	Total 3935	C 2454	N 732	O 738	S 11	0	1	0
1	C	537	Total 3952	C 2467	N 735	O 741	S 9	0	2	0
1	D	542	Total 4022	C 2505	N 751	O 756	S 10	0	5	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WK11
A	-18	GLY	-	expression tag	UNP P9WK11
A	-17	SER	-	expression tag	UNP P9WK11
A	-16	SER	-	expression tag	UNP P9WK11
A	-15	HIS	-	expression tag	UNP P9WK11
A	-14	HIS	-	expression tag	UNP P9WK11
A	-13	HIS	-	expression tag	UNP P9WK11
A	-12	HIS	-	expression tag	UNP P9WK11
A	-11	HIS	-	expression tag	UNP P9WK11
A	-10	HIS	-	expression tag	UNP P9WK11
A	-9	SER	-	expression tag	UNP P9WK11
A	-8	SER	-	expression tag	UNP P9WK11
A	-7	GLY	-	expression tag	UNP P9WK11
A	-6	LEU	-	expression tag	UNP P9WK11
A	-5	VAL	-	expression tag	UNP P9WK11
A	-4	PRO	-	expression tag	UNP P9WK11
A	-3	ARG	-	expression tag	UNP P9WK11
A	-2	GLY	-	expression tag	UNP P9WK11
A	-1	SER	-	expression tag	UNP P9WK11
A	0	HIS	-	expression tag	UNP P9WK11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P9WK11
B	-18	GLY	-	expression tag	UNP P9WK11
B	-17	SER	-	expression tag	UNP P9WK11
B	-16	SER	-	expression tag	UNP P9WK11
B	-15	HIS	-	expression tag	UNP P9WK11
B	-14	HIS	-	expression tag	UNP P9WK11
B	-13	HIS	-	expression tag	UNP P9WK11
B	-12	HIS	-	expression tag	UNP P9WK11
B	-11	HIS	-	expression tag	UNP P9WK11
B	-10	HIS	-	expression tag	UNP P9WK11
B	-9	SER	-	expression tag	UNP P9WK11
B	-8	SER	-	expression tag	UNP P9WK11
B	-7	GLY	-	expression tag	UNP P9WK11
B	-6	LEU	-	expression tag	UNP P9WK11
B	-5	VAL	-	expression tag	UNP P9WK11
B	-4	PRO	-	expression tag	UNP P9WK11
B	-3	ARG	-	expression tag	UNP P9WK11
B	-2	GLY	-	expression tag	UNP P9WK11
B	-1	SER	-	expression tag	UNP P9WK11
B	0	HIS	-	expression tag	UNP P9WK11
C	-19	MET	-	initiating methionine	UNP P9WK11
C	-18	GLY	-	expression tag	UNP P9WK11
C	-17	SER	-	expression tag	UNP P9WK11
C	-16	SER	-	expression tag	UNP P9WK11
C	-15	HIS	-	expression tag	UNP P9WK11
C	-14	HIS	-	expression tag	UNP P9WK11
C	-13	HIS	-	expression tag	UNP P9WK11
C	-12	HIS	-	expression tag	UNP P9WK11
C	-11	HIS	-	expression tag	UNP P9WK11
C	-10	HIS	-	expression tag	UNP P9WK11
C	-9	SER	-	expression tag	UNP P9WK11
C	-8	SER	-	expression tag	UNP P9WK11
C	-7	GLY	-	expression tag	UNP P9WK11
C	-6	LEU	-	expression tag	UNP P9WK11
C	-5	VAL	-	expression tag	UNP P9WK11
C	-4	PRO	-	expression tag	UNP P9WK11
C	-3	ARG	-	expression tag	UNP P9WK11
C	-2	GLY	-	expression tag	UNP P9WK11
C	-1	SER	-	expression tag	UNP P9WK11
C	0	HIS	-	expression tag	UNP P9WK11
D	-19	MET	-	initiating methionine	UNP P9WK11
D	-18	GLY	-	expression tag	UNP P9WK11

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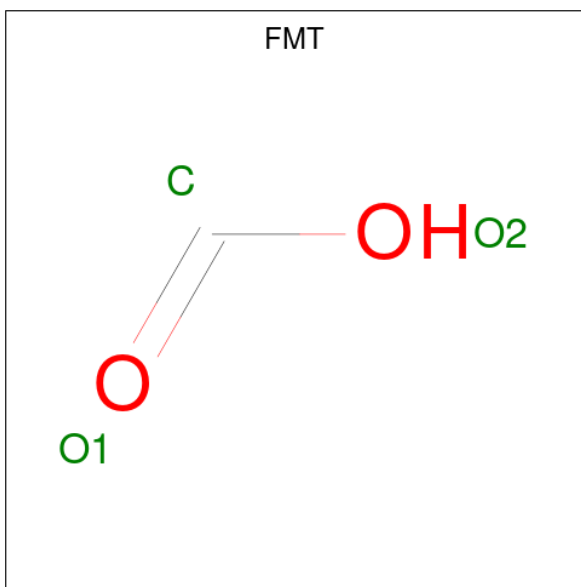
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP P9WK11
D	-16	SER	-	expression tag	UNP P9WK11
D	-15	HIS	-	expression tag	UNP P9WK11
D	-14	HIS	-	expression tag	UNP P9WK11
D	-13	HIS	-	expression tag	UNP P9WK11
D	-12	HIS	-	expression tag	UNP P9WK11
D	-11	HIS	-	expression tag	UNP P9WK11
D	-10	HIS	-	expression tag	UNP P9WK11
D	-9	SER	-	expression tag	UNP P9WK11
D	-8	SER	-	expression tag	UNP P9WK11
D	-7	GLY	-	expression tag	UNP P9WK11
D	-6	LEU	-	expression tag	UNP P9WK11
D	-5	VAL	-	expression tag	UNP P9WK11
D	-4	PRO	-	expression tag	UNP P9WK11
D	-3	ARG	-	expression tag	UNP P9WK11
D	-2	GLY	-	expression tag	UNP P9WK11
D	-1	SER	-	expression tag	UNP P9WK11
D	0	HIS	-	expression tag	UNP P9WK11

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

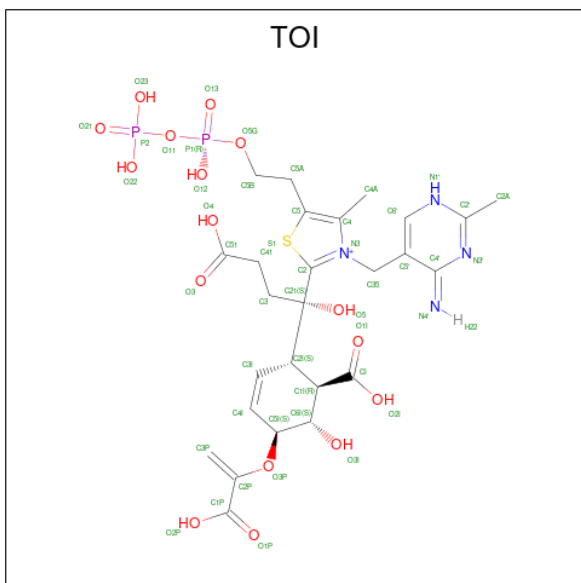
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



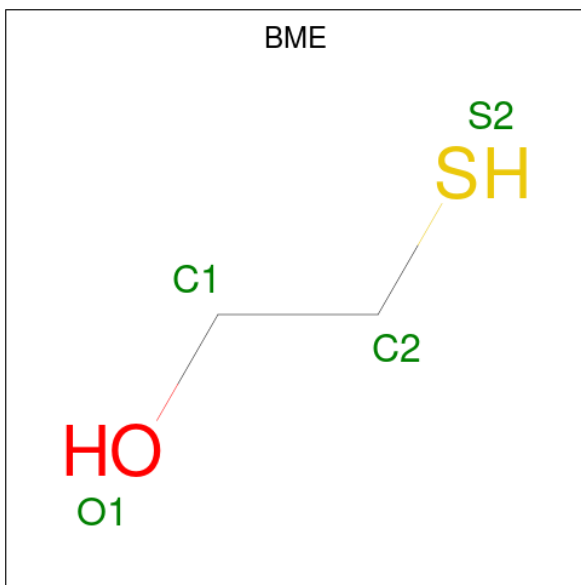
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0

- Molecule 4 is (1 {R},2 {S},5 {S},6 {S})-2-[(1 {S})-1-[3-[(4-azanylidene-2-methyl-1 {H})-pyrimidin-5-yl)methyl]-4-methyl-5-[2-[oxidanyl (phosphonoxy)phosphoryl]oxyethyl]-1,3-thiazol-3-ium-2-yl]-1,4-bis(oxidanyl)-4-oxidanylidene-butyl]-6-oxidanyl-5-(3-oxid anyl-3-oxidanylid ene-prop-1-en-2-yl)oxy-cyclohex-3-ene-1-carboxylic acid (three-letter code: TOI) (formula: $C_{26}H_{35}N_4O_{16}P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	C	1	Total	C	N	O	P	S	0	0
			49	26	4	16	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			49	26	4	16	2	1		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

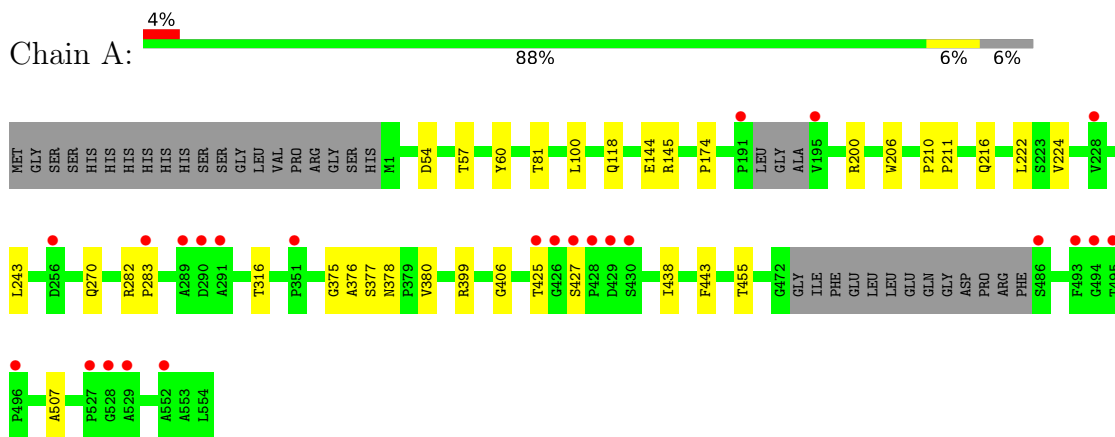
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	170	Total	O	0	0
			170	170		
6	B	145	Total	O	0	0
			145	145		
6	C	87	Total	O	0	0
			87	87		
6	D	198	Total	O	0	0
			198	198		

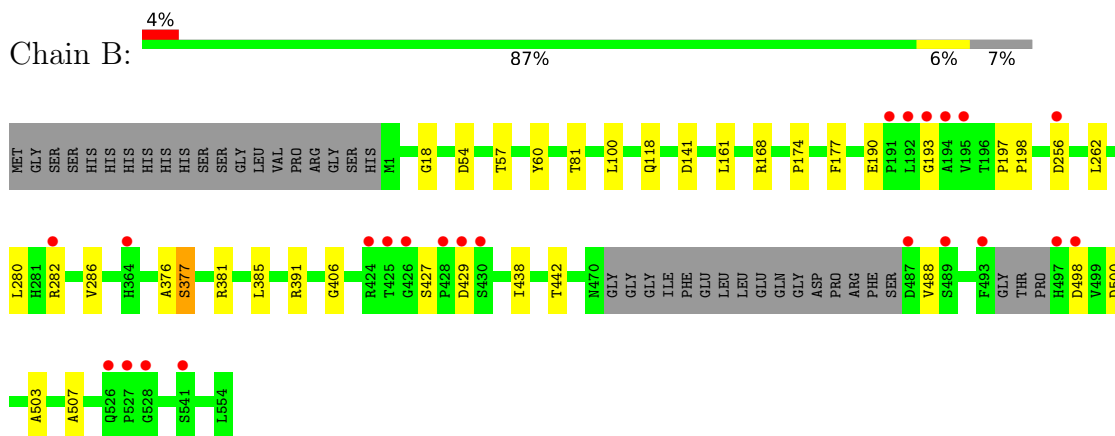
3 Residue-property plots [i](#)

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.

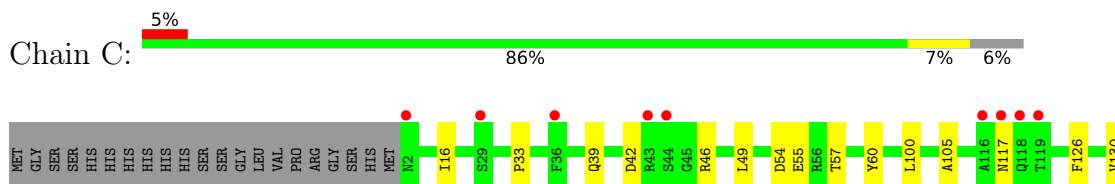
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

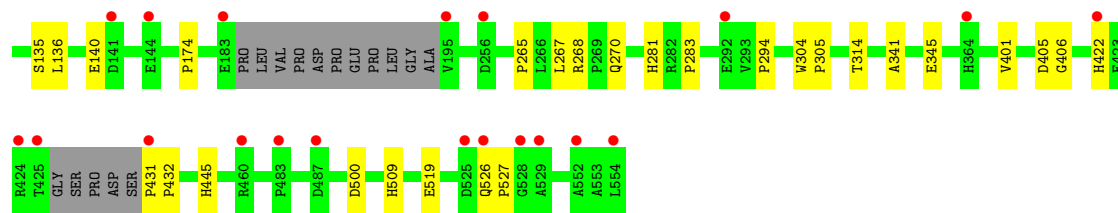


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

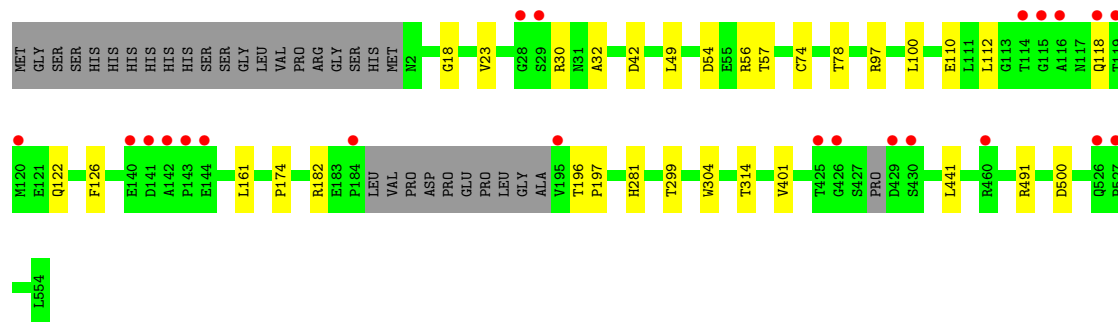
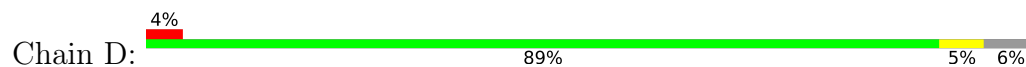


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase





- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.45Å 139.82Å 183.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 2.20 19.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.85-2.20) 98.9 (19.85-2.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.19Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.194 , 0.237 0.195 , 0.238	Depositor DCC
R_{free} test set	6638 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.430	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16576	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: MG, TOI, FMT, BME

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	0.21	0/4045	0.41	0/5545
1	B	0.21	0/4018	0.41	0/5503
1	C	0.22	0/4039	0.43	0/5530
1	D	0.22	0/4113	0.42	0/5627
All	All	0.22	0/16215	0.42	0/22205

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3952	0	3979	21	0
1	B	3935	0	3978	23	0
1	C	3952	0	3975	25	0
1	D	4022	0	4050	22	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	1	0	0
3	B	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	49	0	0	1	0
4	D	49	0	0	2	0
5	C	4	0	5	1	0
5	D	4	0	5	0	0
6	A	170	0	0	0	0
6	B	145	0	0	0	0
6	C	87	0	0	0	0
6	D	198	0	0	1	0
All	All	16576	0	15994	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (79) 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)
1:B:280:LEU:O	1:B:381:ARG:NH1	2.30	0.64
1:A:377:SER:OG	1:A:378:ASN:N	2.29	0.63
1:A:81:THR:HG23	1:D:401:VAL:HG11	1.83	0.61
1:C:33:PRO:HB3	1:C:105:ALA:HB2	1.84	0.59
1:B:81:THR:HG23	1:C:401:VAL:HG11	1.85	0.58
1:A:145:ARG:NH1	1:B:141:ASP:OD2	2.36	0.58
1:B:427:SER:OG	1:B:429:ASP:OD2	2.23	0.56
1:D:122:GLN:HE22	1:D:126:PHE:HD2	1.52	0.56
1:D:30:ARG:NH2	1:D:110:GLU:OE1	2.38	0.56
1:D:97:ARG:NH1	6:D:705:HOH:O	2.38	0.56
1:B:190:GLU:HB2	1:B:193:GLY:HA2	1.87	0.55
1:B:500:ASP:OD1	1:B:503:ALA:N	2.39	0.55
1:B:488:VAL:HG21	1:C:39:GLN:HB2	1.89	0.54
1:C:140:GLU:OE1	1:D:182:ARG:NH1	2.34	0.54
1:C:341:ALA:O	1:C:345:GLU:HG2	2.08	0.53
1:B:280:LEU:HD11	1:B:381:ARG:HG2	1.90	0.53
1:C:42:ASP:HB2	1:C:49:LEU:HG	1.91	0.52
1:D:118:GLN:N	1:D:118:GLN:OE1	2.42	0.52
1:D:304:TRP:CG	1:D:314:THR:HG21	2.45	0.51
1:B:168:ARG:NH2	1:D:299:THR:O	2.43	0.51
1:A:144:GLU:H	1:A:144:GLU:CD	2.13	0.51
1:C:55:GLU:HG2	5:C:603:BME:H21	1.91	0.51
1:B:118:GLN:OE1	4:C:601:TOI:O5	2.29	0.50
1:B:54:ASP:HB3	1:B:57:THR:HG22	1.95	0.49
1:A:375:GLY:O	1:A:380:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ILE:HG23	1:B:442:THR:HB	1.94	0.48
1:A:118:GLN:OE1	4:D:602:TOI:O5	2.31	0.48
1:C:267:LEU:O	1:C:268:ARG:HD2	2.13	0.48
1:A:60:TYR:CG	1:A:406:GLY:HA3	2.49	0.48
1:A:438:ILE:HD11	1:A:443:PHE:HD1	1.79	0.47
1:A:507:ALA:HA	1:D:500:ASP:HB3	1.96	0.47
1:C:54:ASP:HB3	1:C:57:THR:HG22	1.96	0.47
1:B:18:GLY:HA3	1:B:161:LEU:HD13	1.97	0.47
1:B:60:TYR:CG	1:B:406:GLY:HA3	2.49	0.47
1:D:18:GLY:HA3	1:D:161:LEU:HD13	1.96	0.47
1:C:135:SER:HB3	1:D:112:LEU:HB3	1.97	0.47
1:A:54:ASP:OD1	1:D:56:ARG:NH2	2.43	0.47
1:A:200:ARG:HG2	1:A:206:TRP:HA	1.98	0.46
1:D:32:ALA:HA	1:D:78:THR:HG22	1.97	0.46
1:A:224:VAL:HG12	1:A:270[B]:GLN:HB2	1.98	0.45
1:C:265:PRO:HG3	1:C:283:PRO:HB3	1.98	0.45
1:D:30:ARG:HH22	1:D:110:GLU:CD	2.20	0.45
1:D:100:LEU:O	1:D:174:PRO:HA	2.17	0.45
1:C:267:LEU:C	1:C:268:ARG:HD2	2.38	0.45
1:B:256:ASP:HB2	1:B:391:ARG:NH1	2.32	0.44
1:D:42:ASP:HB2	1:D:49:LEU:HG	1.99	0.44
1:C:431:PRO:HA	1:C:432:PRO:HD3	1.87	0.44
1:C:526:GLN:HA	1:C:527:PRO:HD3	1.78	0.44
1:A:376:ALA:O	1:A:399:ARG:NH1	2.50	0.44
1:D:23:VAL:HG22	1:D:74:CYS:HB2	1.99	0.44
1:A:455:THR:HG21	1:D:491:ARG:HG2	2.00	0.44
1:B:498:ASP:O	1:C:509:HIS:NE2	2.45	0.44
1:B:376:ALA:O	1:B:377:SER:OG	2.24	0.44
1:C:16:ILE:HD13	1:C:46:ARG:HB3	2.00	0.44
1:A:222:LEU:HD22	1:A:243:LEU:HD11	1.99	0.43
1:B:377:SER:O	1:B:381:ARG:HG3	2.19	0.43
1:C:270:GLN:O	1:C:294:PRO:HD2	2.18	0.43
1:C:405:ASP:HB3	1:C:445:HIS:CE1	2.54	0.43
1:A:54:ASP:HB3	1:A:57:THR:HG22	2.00	0.43
1:D:304:TRP:CD2	1:D:314:THR:HG21	2.54	0.43
1:A:425:THR:O	1:A:427:SER:N	2.47	0.43
1:D:54:ASP:HB3	1:D:57:THR:HG22	2.00	0.43
1:D:196:THR:HA	1:D:197:PRO:HD2	1.82	0.42
1:C:60:TYR:CG	1:C:406:GLY:HA3	2.54	0.42
1:A:282:ARG:N	1:A:283:PRO:HD2	2.34	0.42
1:B:100:LEU:O	1:B:174:PRO:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LEU:HD12	1:C:136:LEU:HA	1.92	0.42
1:C:422:HIS:ND1	1:C:432:PRO:HD3	2.34	0.41
1:D:441:LEU:HB2	4:D:602:TOI:P1	2.60	0.41
1:B:282:ARG:O	1:B:286:VAL:HG23	2.21	0.41
1:B:507:ALA:HA	1:C:500:ASP:HB3	2.01	0.41
1:C:126:PHE:O	1:C:130:VAL:HG22	2.20	0.41
1:A:100:LEU:O	1:A:174:PRO:HA	2.21	0.41
1:B:197:PRO:HA	1:B:198:PRO:HD3	1.75	0.41
1:C:304:TRP:CG	1:C:314:THR:HG21	2.56	0.41
1:A:210:PRO:HA	1:A:211:PRO:HD3	1.98	0.40
1:B:262:LEU:HD11	1:B:385:LEU:HD11	2.03	0.40
1:C:100:LEU:O	1:C:174:PRO:HA	2.21	0.40
1:A:216:GLN:HB3	1:A:316:THR:HG23	2.04	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	535/574 (93%)	517 (97%)	18 (3%)	0	100	100
1	B	529/574 (92%)	516 (98%)	12 (2%)	1 (0%)	47	55
1	C	533/574 (93%)	518 (97%)	14 (3%)	1 (0%)	47	55
1	D	541/574 (94%)	527 (97%)	13 (2%)	1 (0%)	47	55
All	All	2138/2296 (93%)	2078 (97%)	57 (3%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	377	SER
1	D	281	HIS

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Mol	Chain	Res	Type
1	C	281	HIS

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	416/445 (94%)	416 (100%)	0	100	100
1	B	414/445 (93%)	413 (100%)	1 (0%)	93	97
1	C	412/445 (93%)	409 (99%)	3 (1%)	84	91
1	D	423/445 (95%)	423 (100%)	0	100	100
All	All	1665/1780 (94%)	1661 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	177	PHE
1	C	117	ASN
1	C	305	PRO
1	C	519	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	422	HIS
1	C	117	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	BME	D	603	1	3,3,3	0.85	0	1,2,2	1.41	0
4	TOI	C	601	2	43,51,51	1.18	4 (9%)	49,77,77	1.56	8 (16%)
3	FMT	B	601	-	2,2,2	0.70	0	1,1,1	0.24	0
4	TOI	D	602	2	43,51,51	1.19	5 (11%)	49,77,77	1.58	9 (18%)
3	FMT	A	602	2	2,2,2	0.73	0	1,1,1	0.28	0
5	BME	C	603	1	3,3,3	0.76	0	1,2,2	0.88	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	BME	D	603	1	-	0/1/1/1	-
4	TOI	C	601	2	-	7/37/64/64	0/3/3/3
4	TOI	D	602	2	-	7/37/64/64	0/3/3/3
5	BME	C	603	1	-	0/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	TOI	C5A-C5	2.98	1.52	1.50
4	C	601	TOI	O3P-C2P	2.96	1.46	1.36
4	D	602	TOI	O3P-C2P	2.92	1.46	1.36
4	D	602	TOI	C5A-C5	2.87	1.52	1.50
4	D	602	TOI	C35-C5'	2.46	1.52	1.50
4	C	601	TOI	C6'-C5'	2.30	1.39	1.36
4	D	602	TOI	C6'-C5'	2.24	1.39	1.36
4	C	601	TOI	C35-C5'	2.19	1.52	1.50
4	D	602	TOI	O3P-C5I	-2.02	1.43	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	TOI	C1I-C2I-C3I	4.25	114.08	107.16
4	C	601	TOI	C1I-C2I-C3I	4.06	113.78	107.16
4	C	601	TOI	C6I-C5I-C4I	-3.84	105.81	111.89
4	D	602	TOI	C5A-C5-C4	-3.47	124.65	127.43
4	D	602	TOI	C2I-C1I-C6I	3.45	117.82	110.48
4	D	602	TOI	O2P-C1P-C2P	3.37	119.65	113.91
4	C	601	TOI	O2P-C1P-C2P	3.27	119.48	113.91
4	C	601	TOI	C5A-C5-C4	-3.25	124.82	127.43
4	D	602	TOI	C6I-C5I-C4I	-2.91	107.28	111.89
4	D	602	TOI	C6I-C1I-CI	-2.82	105.65	110.45
4	C	601	TOI	C2I-C1I-C6I	2.81	116.46	110.48
4	C	601	TOI	C6I-C1I-CI	-2.37	106.42	110.45
4	C	601	TOI	P1-O11-P2	-2.28	124.99	132.83
4	D	602	TOI	O1P-C1P-C2P	-2.23	118.43	121.79
4	C	601	TOI	O1P-C1P-C2P	-2.17	118.52	121.79
4	D	602	TOI	C4A-C4-N3	2.06	125.28	122.69
4	D	602	TOI	P1-O11-P2	-2.03	125.86	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	TOI	C2-C21-C2I-C3I
4	C	601	TOI	O5-C21-C3-C41
4	C	601	TOI	C2-C21-C3-C41
4	D	602	TOI	C2-C21-C2I-C3I
4	D	602	TOI	O5-C21-C3-C41
4	D	602	TOI	C2-C21-C3-C41
4	D	602	TOI	P1-O11-P2-O22

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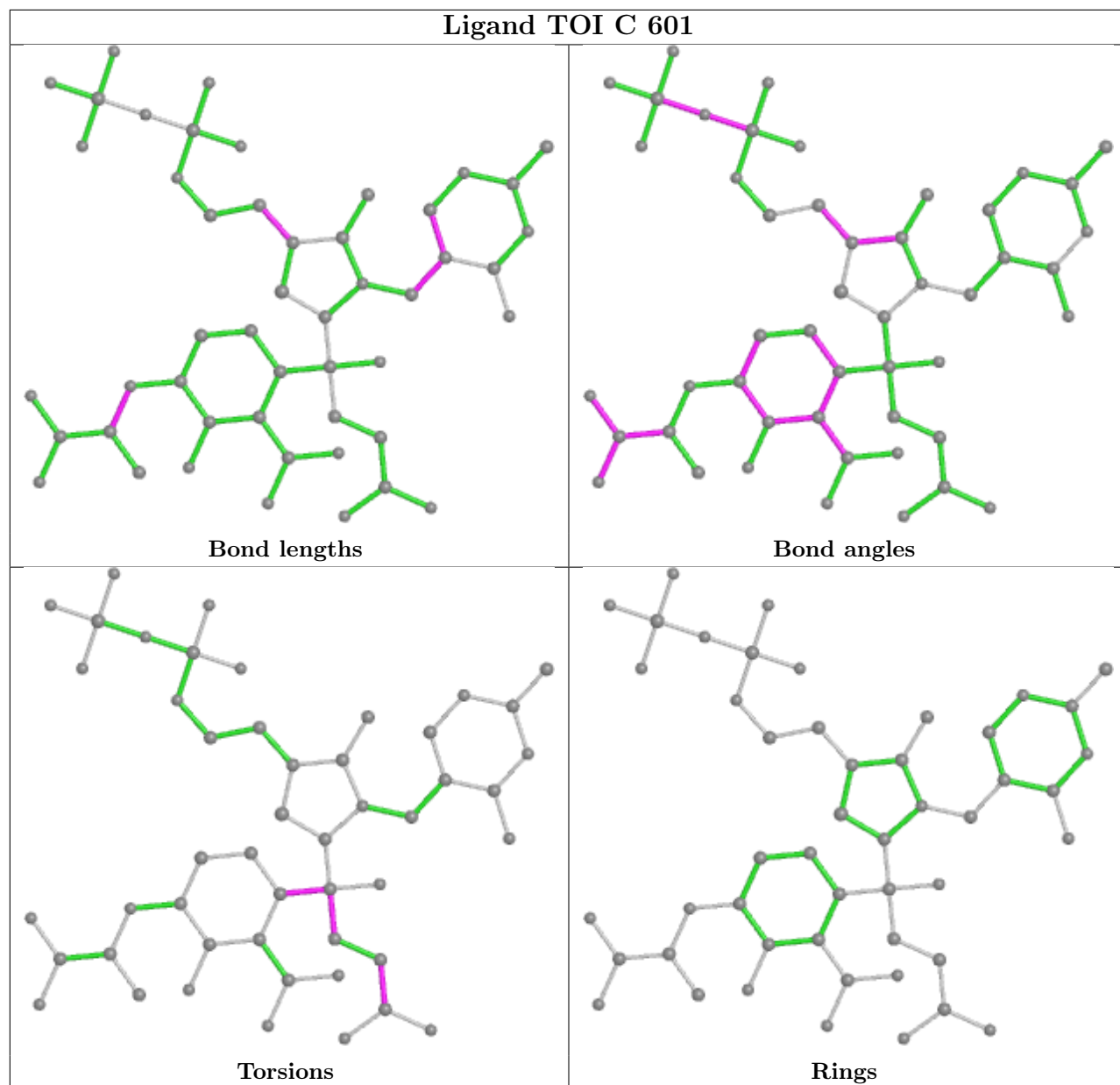
Mol	Chain	Res	Type	Atoms
4	C	601	TOI	C2I-C21-C3-C41
4	D	602	TOI	C2I-C21-C3-C41
4	C	601	TOI	C3-C21-C2I-C3I
4	D	602	TOI	C3-C41-C51-O4
4	D	602	TOI	C3-C41-C51-O3
4	C	601	TOI	C3-C41-C51-O4
4	C	601	TOI	C3-C41-C51-O3

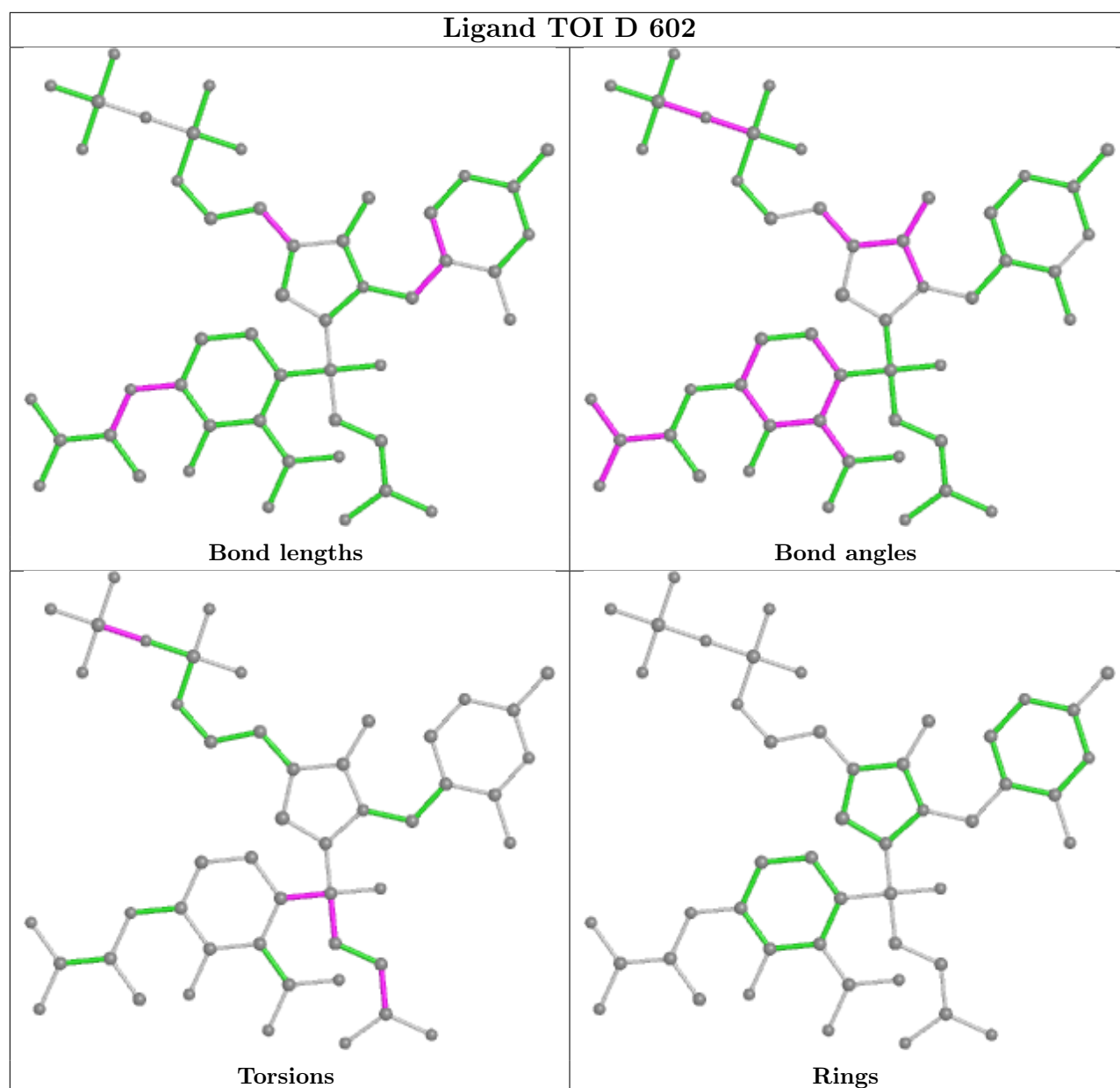
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	TOI	1	0
4	D	602	TOI	2	0
5	C	603	BME	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.





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	538/574 (93%)	-0.11	24 (4%) 33 32	25, 43, 80, 110	0
1	B	535/574 (93%)	-0.17	23 (4%) 35 33	28, 42, 81, 118	0
1	C	537/574 (93%)	0.01	29 (5%) 25 24	32, 52, 82, 105	0
1	D	542/574 (94%)	-0.24	22 (4%) 37 35	24, 40, 71, 98	0
All	All	2152/2296 (93%)	-0.13	98 (4%) 32 31	24, 44, 79, 118	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	LEU	7.5
1	B	426	GLY	7.1
1	A	428	PRO	5.8
1	C	29	SER	5.4
1	C	195	VAL	5.4
1	C	118	GLN	5.0
1	B	493	PHE	4.8
1	A	527	PRO	4.6
1	B	193	GLY	4.6
1	B	429	ASP	4.6
1	A	494	GLY	4.5
1	C	117	ASN	4.4
1	B	428	PRO	4.4
1	C	116	ALA	4.4
1	C	425	THR	4.2
1	B	528	GLY	4.2
1	C	528	GLY	4.1
1	B	194	ALA	4.1
1	D	195	VAL	4.1
1	A	289	ALA	4.0
1	D	429	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	184	PRO	3.8
1	A	291	ALA	3.8
1	A	426	GLY	3.6
1	B	527	PRO	3.6
1	A	495	THR	3.5
1	B	191	PRO	3.5
1	C	36	PHE	3.4
1	A	496	PRO	3.4
1	D	141	ASP	3.2
1	A	486	SER	3.2
1	C	554	LEU	3.2
1	C	364	HIS	3.1
1	B	425	THR	3.1
1	A	430	SER	3.1
1	D	119	THR	3.0
1	D	426	GLY	3.0
1	A	427	SER	3.0
1	C	552	ALA	3.0
1	C	460	ARG	3.0
1	C	422	HIS	2.9
1	D	118	GLN	2.9
1	D	116	ALA	2.8
1	C	529	ALA	2.8
1	A	429	ASP	2.8
1	A	195	VAL	2.8
1	B	282	ARG	2.7
1	B	256	ASP	2.7
1	D	120	MET	2.7
1	C	141	ASP	2.7
1	C	526	GLN	2.6
1	C	119	THR	2.6
1	D	430	SER	2.6
1	A	425	THR	2.6
1	B	430	SER	2.6
1	C	483	PRO	2.6
1	D	526	GLN	2.6
1	B	497	HIS	2.6
1	C	183	GLU	2.5
1	B	489	SER	2.5
1	D	425	THR	2.5
1	A	493	PHE	2.5
1	C	2	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	191	PRO	2.5
1	B	487	ASP	2.4
1	A	529	ALA	2.4
1	D	144	GLU	2.4
1	B	526	GLN	2.4
1	C	43	ARG	2.4
1	C	256	ASP	2.4
1	B	498	ASP	2.3
1	C	487	ASP	2.3
1	D	29	SER	2.3
1	D	143	PRO	2.3
1	D	114	THR	2.3
1	B	364	HIS	2.3
1	D	527	PRO	2.3
1	B	424	ARG	2.3
1	B	195	VAL	2.3
1	C	292	GLU	2.3
1	C	431	PRO	2.2
1	A	256	ASP	2.2
1	A	283	PRO	2.2
1	B	541	SER	2.2
1	A	351	PRO	2.2
1	C	525	ASP	2.2
1	C	144	GLU	2.1
1	D	460	ARG	2.1
1	C	424	ARG	2.1
1	A	528	GLY	2.1
1	A	290	ASP	2.1
1	D	115	GLY	2.1
1	D	142	ALA	2.1
1	A	228	VAL	2.1
1	D	28	GLY	2.0
1	D	140	GLU	2.0
1	C	44	SER	2.0
1	A	552	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

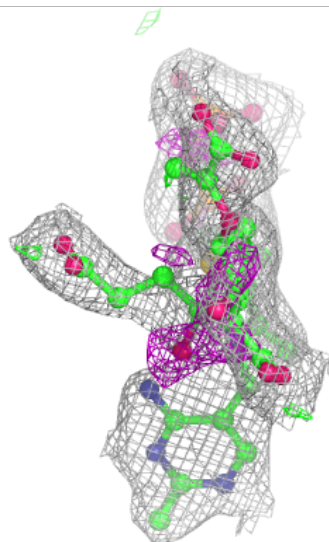
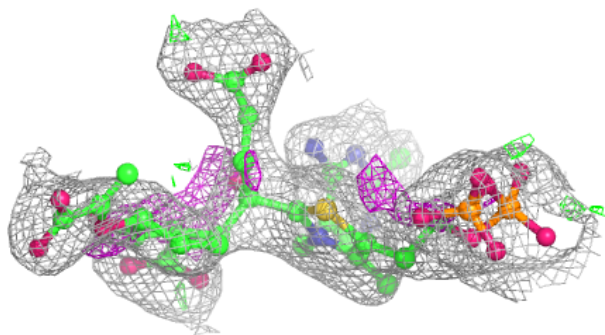
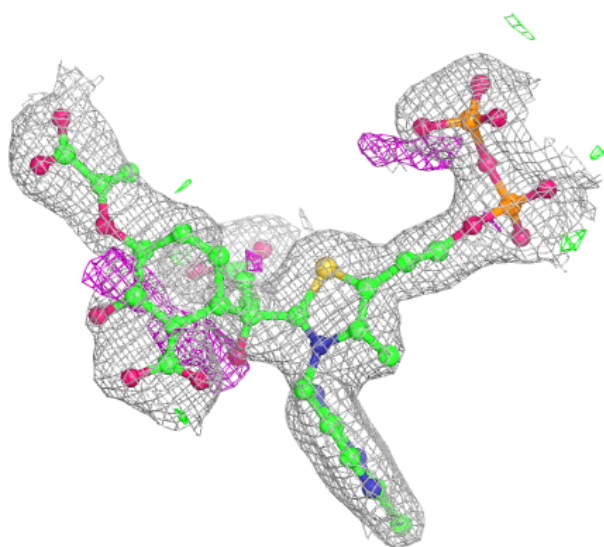
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FMT	B	601	3/3	0.86	0.13	44,44,56,57	0
5	BME	D	603	4/4	0.89	0.15	53,58,65,73	0
5	BME	C	603	4/4	0.90	0.14	60,60,62,69	0
3	FMT	A	602	3/3	0.91	0.09	53,53,55,63	0
4	TOI	C	601	49/49	0.93	0.14	41,52,67,70	0
2	MG	A	601	1/1	0.96	0.10	56,56,56,56	0
4	TOI	D	602	49/49	0.97	0.11	26,35,52,59	0
2	MG	D	601	1/1	0.97	0.11	33,33,33,33	0
2	MG	C	602	1/1	0.97	0.08	42,42,42,42	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.

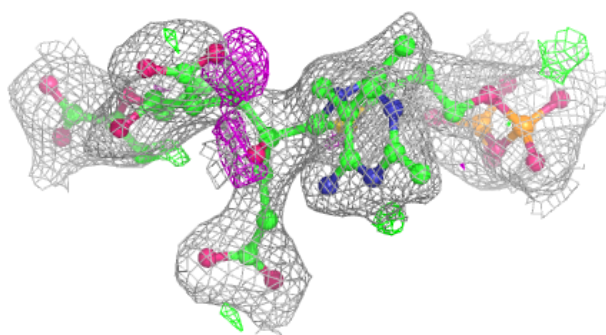
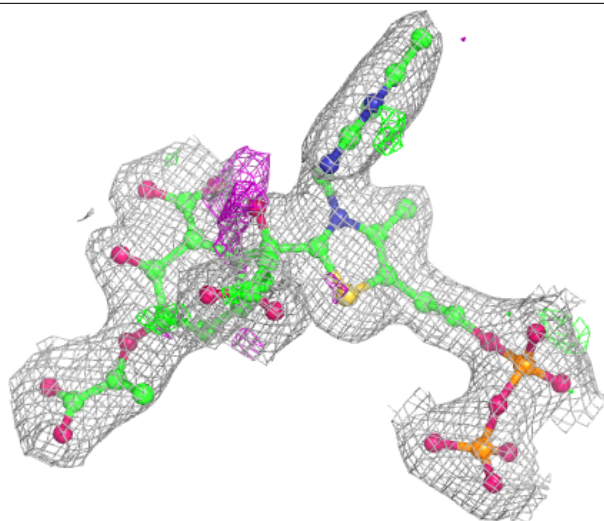
Electron density around TOI C 601:

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



Electron density around TOI D 602:

$2mF_o-DF_c$ (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.