Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 03:22 PM EDT

PDB ID	:	5ICR
Title	:	2.25 Angstrom Resolution Crystal Structure of Fatty-Acid-CoA Ligase (FadD32) from Mycobacterium smegmatis in complex with Inhibitor 5'-O-[(11-phenoxyundecanoyl)sulfamoyl]adenosine.
Authors	:	Minasov, G.; Shuvalova, L.; Hung, D.; Fisher, S.L.; Edelstein, J.; Kiryukhina, O.; Dubrovska, I.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2016-02-23
Resolution	:	2.25 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:

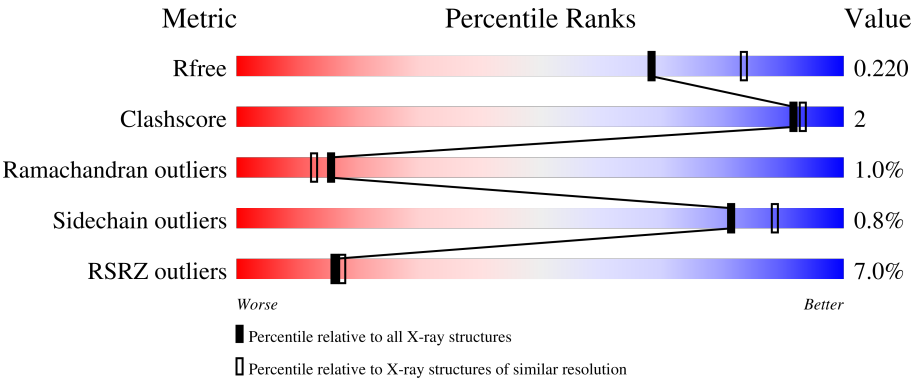
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	650	5% 89% • • 7%
1	B	650	7% 90% • 6%
1	C	650	6% 91% • 5%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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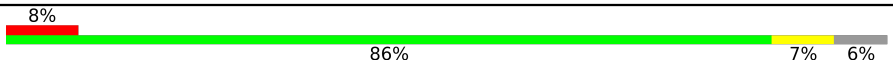
Mol	Chain	Length	Quality of chain
1	D	650	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20342 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 Acyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	14	0
			4782	3012	851	911	8			
1	B	609	Total	C	N	O	S	0	1	0
			4680	2957	829	887	7			
1	C	618	Total	C	N	O	S	0	4	0
			4768	3003	849	908	8			
1	D	609	Total	C	N	O	S	0	8	0
			4732	2989	839	897	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0R618
A	-18	GLY	-	expression tag	UNP A0R618
A	-17	SER	-	expression tag	UNP A0R618
A	-16	SER	-	expression tag	UNP A0R618
A	-15	HIS	-	expression tag	UNP A0R618
A	-14	HIS	-	expression tag	UNP A0R618
A	-13	HIS	-	expression tag	UNP A0R618
A	-12	HIS	-	expression tag	UNP A0R618
A	-11	HIS	-	expression tag	UNP A0R618
A	-10	HIS	-	expression tag	UNP A0R618
A	-9	SER	-	expression tag	UNP A0R618
A	-8	SER	-	expression tag	UNP A0R618
A	-7	GLY	-	expression tag	UNP A0R618
A	-6	LEU	-	expression tag	UNP A0R618
A	-5	VAL	-	expression tag	UNP A0R618
A	-4	PRO	-	expression tag	UNP A0R618
A	-3	ARG	-	expression tag	UNP A0R618
A	-2	GLY	-	expression tag	UNP A0R618
A	-1	SER	-	expression tag	UNP A0R618
A	0	HIS	-	expression tag	UNP A0R618
B	-19	MET	-	initiating methionine	UNP A0R618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0R618
B	-17	SER	-	expression tag	UNP A0R618
B	-16	SER	-	expression tag	UNP A0R618
B	-15	HIS	-	expression tag	UNP A0R618
B	-14	HIS	-	expression tag	UNP A0R618
B	-13	HIS	-	expression tag	UNP A0R618
B	-12	HIS	-	expression tag	UNP A0R618
B	-11	HIS	-	expression tag	UNP A0R618
B	-10	HIS	-	expression tag	UNP A0R618
B	-9	SER	-	expression tag	UNP A0R618
B	-8	SER	-	expression tag	UNP A0R618
B	-7	GLY	-	expression tag	UNP A0R618
B	-6	LEU	-	expression tag	UNP A0R618
B	-5	VAL	-	expression tag	UNP A0R618
B	-4	PRO	-	expression tag	UNP A0R618
B	-3	ARG	-	expression tag	UNP A0R618
B	-2	GLY	-	expression tag	UNP A0R618
B	-1	SER	-	expression tag	UNP A0R618
B	0	HIS	-	expression tag	UNP A0R618
C	-19	MET	-	initiating methionine	UNP A0R618
C	-18	GLY	-	expression tag	UNP A0R618
C	-17	SER	-	expression tag	UNP A0R618
C	-16	SER	-	expression tag	UNP A0R618
C	-15	HIS	-	expression tag	UNP A0R618
C	-14	HIS	-	expression tag	UNP A0R618
C	-13	HIS	-	expression tag	UNP A0R618
C	-12	HIS	-	expression tag	UNP A0R618
C	-11	HIS	-	expression tag	UNP A0R618
C	-10	HIS	-	expression tag	UNP A0R618
C	-9	SER	-	expression tag	UNP A0R618
C	-8	SER	-	expression tag	UNP A0R618
C	-7	GLY	-	expression tag	UNP A0R618
C	-6	LEU	-	expression tag	UNP A0R618
C	-5	VAL	-	expression tag	UNP A0R618
C	-4	PRO	-	expression tag	UNP A0R618
C	-3	ARG	-	expression tag	UNP A0R618
C	-2	GLY	-	expression tag	UNP A0R618
C	-1	SER	-	expression tag	UNP A0R618
C	0	HIS	-	expression tag	UNP A0R618
D	-19	MET	-	initiating methionine	UNP A0R618
D	-18	GLY	-	expression tag	UNP A0R618
D	-17	SER	-	expression tag	UNP A0R618

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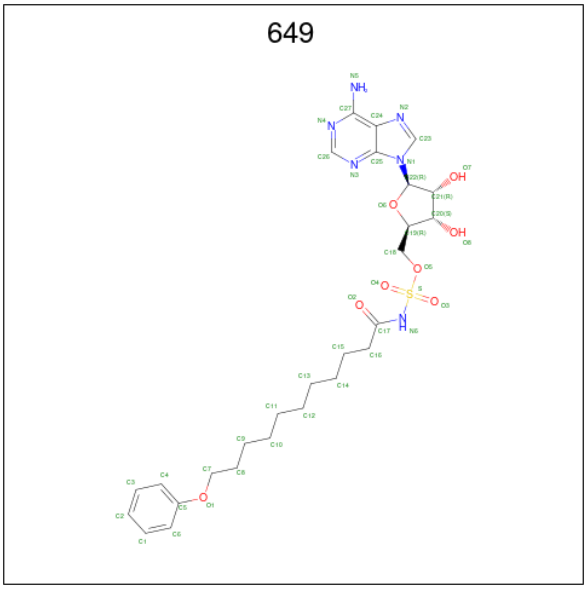
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0R618
D	-15	HIS	-	expression tag	UNP A0R618
D	-14	HIS	-	expression tag	UNP A0R618
D	-13	HIS	-	expression tag	UNP A0R618
D	-12	HIS	-	expression tag	UNP A0R618
D	-11	HIS	-	expression tag	UNP A0R618
D	-10	HIS	-	expression tag	UNP A0R618
D	-9	SER	-	expression tag	UNP A0R618
D	-8	SER	-	expression tag	UNP A0R618
D	-7	GLY	-	expression tag	UNP A0R618
D	-6	LEU	-	expression tag	UNP A0R618
D	-5	VAL	-	expression tag	UNP A0R618
D	-4	PRO	-	expression tag	UNP A0R618
D	-3	ARG	-	expression tag	UNP A0R618
D	-2	GLY	-	expression tag	UNP A0R618
D	-1	SER	-	expression tag	UNP A0R618
D	0	HIS	-	expression tag	UNP A0R618

- Molecule 2 is 5'-O-[(11-phenoxyundecanoyl)sulfamoyl]adenosine (three-letter code: 649) (formula: $C_{27}H_{38}N_6O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			42	27	6	8	1		
2	B	1	Total	C	N	O	S	0	0
			42	27	6	8	1		

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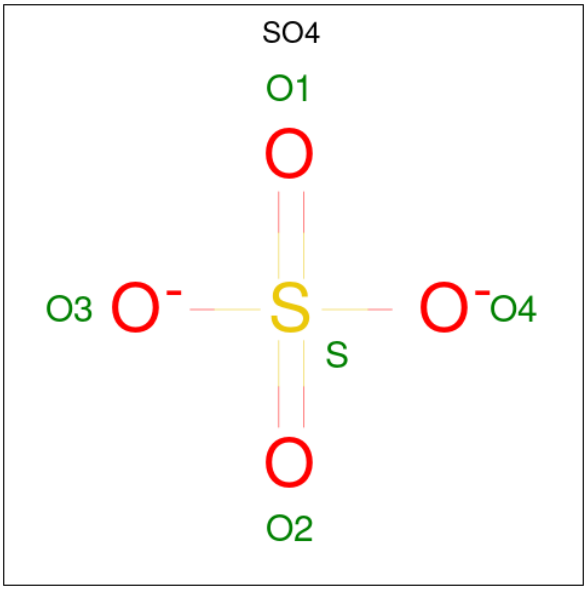
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O S 42 27 6 8 1	0	0
2	D	1	Total C N O S 42 27 6 8 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

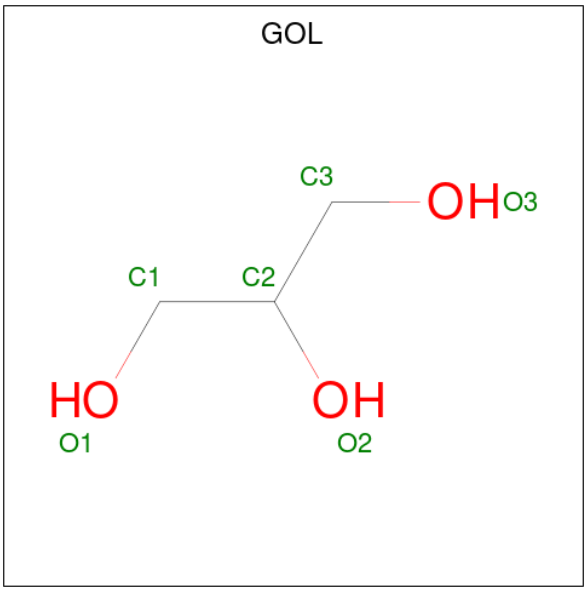


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

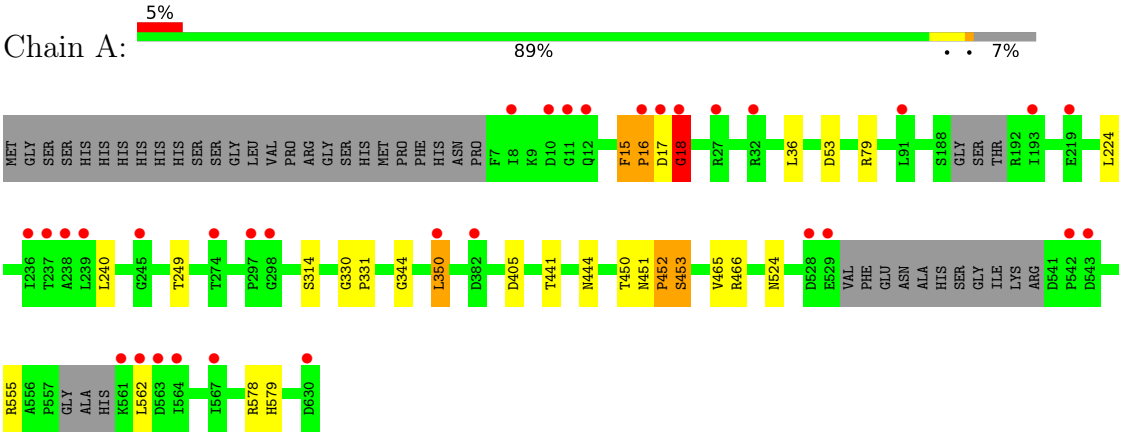
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	369	Total O 388 388	0	22
6	B	241	Total O 252 252	0	13
6	C	283	Total O 294 294	0	12
6	D	232	Total O 246 246	0	15

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.

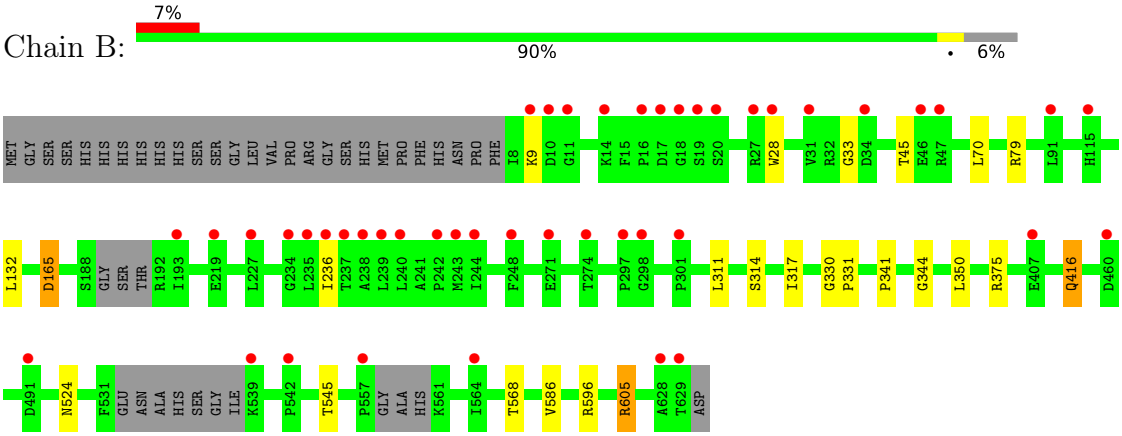
• Molecule 1: Acyl-CoA synthase

Chain A:



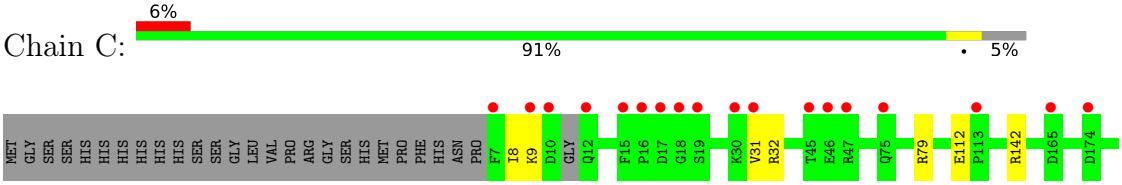
• Molecule 1: Acyl-CoA synthase

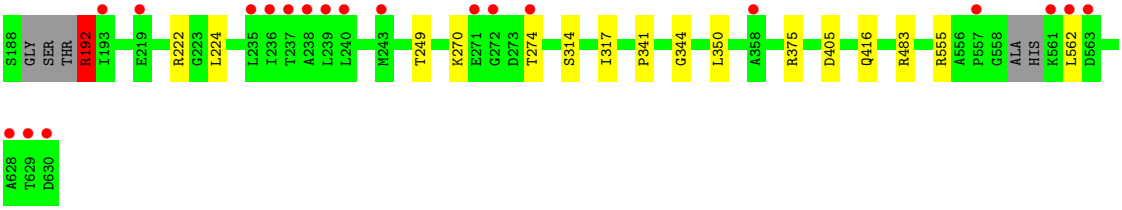
Chain B:



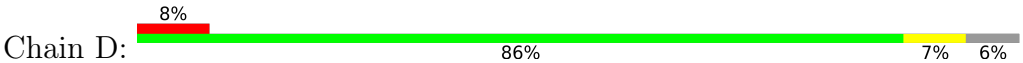
• Molecule 1: Acyl-CoA synthase

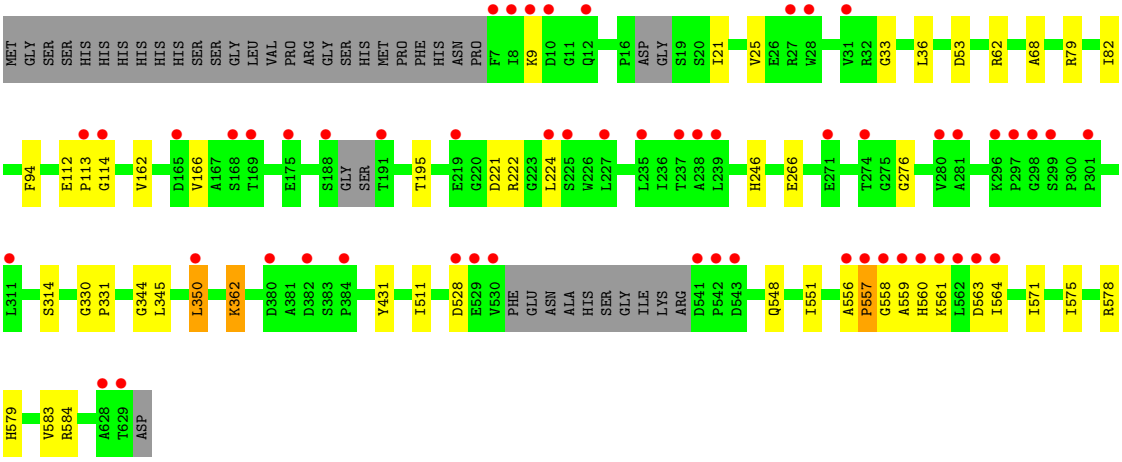
Chain C:





• Molecule 1: Acyl-CoA synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.29Å 153.56Å 201.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.25 29.86 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.86-2.25) 100.0 (29.86-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.173 , 0.219 0.178 , 0.220	Depositor DCC
R_{free} test set	6648 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20342	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 649, CL, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.58	0/4894	0.79	2/6665 (0.0%)
1	B	0.55	0/4790	0.79	4/6529 (0.1%)
1	C	0.54	0/4877	0.76	2/6642 (0.0%)
1	D	0.54	0/4844	0.75	0/6601
All	All	0.55	0/19405	0.77	8/26437 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	605	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	B	605	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	605	ARG	CG-CD-NE	6.99	126.48	111.80
1	C	192	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	B	605	ARG	CD-NE-CZ	5.26	130.96	123.60
1	A	405	ASP	N-CA-C	-5.23	96.88	111.00
1	A	18	GLY	N-CA-C	5.22	126.15	113.10
1	C	405	ASP	N-CA-C	-5.16	97.07	111.00

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	4782	0	4662	14	0
1	B	4680	0	4593	11	0
1	C	4768	0	4668	12	0
1	D	4732	0	4637	25	0
2	A	42	0	0	0	0
2	B	42	0	0	0	0
2	C	42	0	0	0	0
2	D	42	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	1	0	0	0	0
5	C	6	0	8	0	0
6	A	388	0	0	0	0
6	B	252	0	0	1	0
6	C	294	0	0	3	0
6	D	246	0	0	0	0
All	All	20342	0	18568	62	0

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

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:ILE:HD11	1:D:571:ILE:HD11	1.63	0.80
1:D:362[A]:LYS:HB2	1:D:362[A]:LYS:NZ	2.00	0.75
1:D:362[A]:LYS:HB2	1:D:362[A]:LYS:HZ3	1.55	0.69
1:C:317:ILE:HD13	1:C:341:PRO:HB3	1.76	0.68
1:A:555:ARG:NH1	1:A:562:LEU:O	2.27	0.66
1:D:36:LEU:HD11	1:D:53:ASP:HB3	1.80	0.63
1:D:564:ILE:HD12	1:D:564:ILE:H	1.64	0.63
1:C:555:ARG:NH1	1:C:562:LEU:O	2.33	0.61
1:C:31:VAL:HG23	1:C:32:ARG:HG3	1.86	0.56
1:B:28[A]:TRP:NE1	6:B:801[A]:HOH:O	1.98	0.55
1:A:15:PHE:O	1:A:16:PRO:C	2.46	0.54
1:D:68:ALA:HB3	1:D:166:VAL:HG12	1.90	0.54
1:B:375:ARG:NE	1:B:416:GLN:OE1	2.41	0.53
1:C:483:ARG:NH2	6:C:801:HOH:O	2.39	0.53
1:B:165:ASP:OD1	1:B:165:ASP:N	2.36	0.53
1:A:444:ASN:ND2	1:A:466[B]:ARG:HG3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:HD13	1:B:341:PRO:HB3	1.92	0.51
1:A:240:LEU:HD12	1:A:240:LEU:C	2.31	0.50
1:D:564:ILE:HD12	1:D:564:ILE:N	2.26	0.50
1:C:222:ARG:NH2	1:C:270:LYS:HD3	2.28	0.49
1:D:578:ARG:HG3	1:D:579:HIS:CD2	2.48	0.48
1:A:452[B]:PRO:O	1:A:453[B]:SER:HB3	2.13	0.48
1:A:16:PRO:HA	1:A:18:GLY:N	2.28	0.48
1:D:551:ILE:HD11	1:D:575:ILE:CD1	2.43	0.48
1:D:557:PRO:HA	1:D:559:ALA:N	2.29	0.48
1:D:222:ARG:HB3	1:D:246:HIS:CD2	2.50	0.46
1:A:466[A]:ARG:O	1:A:466[A]:ARG:HG3	2.15	0.46
1:C:344:GLY:HA3	1:C:350:LEU:O	2.16	0.46
1:B:344:GLY:HA3	1:B:350:LEU:O	2.16	0.45
1:B:524:ASN:OD1	1:B:545:THR:HG22	2.16	0.45
1:C:375[B]:ARG:NE	1:C:416:GLN:HG2	2.32	0.45
1:D:221:ASP:HA	1:D:276:GLY:O	2.16	0.45
1:B:70:LEU:HD11	1:B:132:LEU:HD11	1.99	0.45
1:B:311:LEU:HD12	1:B:311:LEU:N	2.31	0.45
1:C:192:ARG:HH21	1:C:192:ARG:HG3	1.81	0.45
1:D:224:LEU:HD22	1:D:266:GLU:HB3	1.98	0.45
1:D:330:GLY:N	1:D:331:PRO:CD	2.80	0.44
1:C:224:LEU:HA	1:C:249:THR:O	2.17	0.44
1:D:62:ARG:NH1	1:D:162:VAL:O	2.50	0.44
1:A:450:THR:O	1:A:453[B]:SER:HB2	2.16	0.44
1:B:568:THR:HG23	1:B:586:VAL:HB	2.00	0.44
1:C:142:ARG:NH2	6:C:806:HOH:O	2.51	0.44
1:B:236:ILE:HB	1:B:350:LEU:HD22	2.00	0.44
1:A:330:GLY:N	1:A:331:PRO:CD	2.81	0.43
1:A:36:LEU:HD11	1:A:53:ASP:HB3	2.01	0.43
1:D:556:ALA:O	1:D:558:GLY:HA3	2.20	0.42
1:B:330:GLY:N	1:B:331:PRO:CD	2.83	0.42
1:D:82:ILE:HD11	1:D:94:PHE:HA	2.00	0.42
1:A:441:THR:O	1:A:465:VAL:HA	2.19	0.42
1:D:548:GLN:HB3	1:D:584:ARG:HG3	2.02	0.42
1:A:224:LEU:HA	1:A:249:THR:O	2.20	0.42
1:C:112:GLU:O	1:C:112:GLU:HG3	2.20	0.41
1:D:345:LEU:HD23	1:D:345:LEU:N	2.35	0.41
1:C:375[B]:ARG:NH2	6:C:803:HOH:O	2.46	0.41
1:D:564:ILE:H	1:D:564:ILE:CD1	2.33	0.41
1:D:195:THR:HB	1:D:431:TYR:CD1	2.56	0.41
1:D:21:ILE:O	1:D:25:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:GLY:HA3	1:D:350:LEU:O	2.21	0.41
1:A:578:ARG:HG3	1:A:579:HIS:CD2	2.56	0.40
1:D:112:GLU:HB3	1:D:113:PRO:HD2	2.04	0.40
1:A:344:GLY:HA3	1:A:350:LEU:O	2.21	0.40
1:D:551:ILE:HD12	1:D:583:VAL:HG21	2.02	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	613/650 (94%)	593 (97%)	10 (2%)	10 (2%)	9 5
1	B	602/650 (93%)	580 (96%)	18 (3%)	4 (1%)	22 21
1	C	614/650 (94%)	598 (97%)	13 (2%)	3 (0%)	29 29
1	D	609/650 (94%)	582 (96%)	19 (3%)	8 (1%)	12 8
All	All	2438/2600 (94%)	2353 (96%)	60 (2%)	25 (1%)	15 13

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	A	16	PRO
1	A	17	ASP
1	B	33	GLY
1	D	33	GLY
1	A	15	PHE
1	C	9	LYS
1	D	314	SER
1	D	561	LYS
1	D	563	ASP

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Mol	Chain	Res	Type
1	A	314	SER
1	B	45	THR
1	B	314	SER
1	C	314	SER
1	D	114	GLY
1	D	560	HIS
1	A	350	LEU
1	A	453[A]	SER
1	A	453[B]	SER
1	B	9	LYS
1	D	350	LEU
1	C	8	ILE
1	D	557	PRO
1	A	452[A]	PRO
1	A	452[B]	PRO

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	497/518 (96%)	494 (99%)	3 (1%)	86	91
1	B	486/518 (94%)	481 (99%)	5 (1%)	76	84
1	C	495/518 (96%)	492 (99%)	3 (1%)	86	91
1	D	491/518 (95%)	486 (99%)	5 (1%)	76	84
All	All	1969/2072 (95%)	1953 (99%)	16 (1%)	81	88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	451	ASN
1	A	524	ASN
1	B	79	ARG
1	B	165	ASP
1	B	416	GLN

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Mol	Chain	Res	Type
1	B	596	ARG
1	B	605	ARG
1	C	79	ARG
1	C	192	ARG
1	C	274	THR
1	D	9	LYS
1	D	79	ARG
1	D	362[A]	LYS
1	D	362[B]	LYS
1	D	528	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#\|Z\| > 2$
2	649	C	701	-	42,45,45	1.81	6 (14%)	45,61,61	1.35	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	703	-	4,4,4	0.37	0	6,6,6	0.09	0
2	649	D	701	-	42,45,45	1.57	5 (11%)	45,61,61	1.35	5 (11%)
3	SO4	A	703	-	4,4,4	0.47	0	6,6,6	0.07	0
2	649	A	701	-	42,45,45	1.69	5 (11%)	45,61,61	1.56	4 (8%)
3	SO4	D	702	-	4,4,4	0.34	0	6,6,6	0.11	0
5	GOL	C	703	-	5,5,5	0.31	0	5,5,5	0.13	0
2	649	B	701	-	42,45,45	1.82	7 (16%)	45,61,61	1.44	4 (8%)
3	SO4	A	702	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	C	702	-	4,4,4	0.35	0	6,6,6	0.11	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
2	649	C	701	-	-	3/24/45/45	0/4/4/4
2	649	D	701	-	-	5/24/45/45	0/4/4/4
2	649	A	701	-	-	1/24/45/45	0/4/4/4
5	GOL	C	703	-	-	0/4/4/4	-
2	649	B	701	-	-	3/24/45/45	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	649	O3-S	7.57	1.48	1.42
2	A	701	649	O3-S	7.35	1.48	1.42
2	B	701	649	O4-S	6.34	1.47	1.42
2	C	701	649	O4-S	5.94	1.47	1.42
2	B	701	649	O3-S	5.93	1.47	1.42
2	D	701	649	O4-S	5.54	1.47	1.42
2	D	701	649	O3-S	5.52	1.47	1.42
2	A	701	649	O4-S	5.21	1.46	1.42
2	B	701	649	S-N6	-4.80	1.51	1.59
2	D	701	649	S-N6	-3.80	1.53	1.59
2	C	701	649	S-N6	-3.52	1.53	1.59
2	A	701	649	S-N6	-3.45	1.53	1.59
2	B	701	649	O5-S	-3.02	1.53	1.59
2	B	701	649	C17-N6	-2.98	1.33	1.38
2	C	701	649	O5-S	-2.78	1.53	1.59
2	C	701	649	C17-N6	-2.62	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	649	C17-N6	-2.50	1.34	1.38
2	A	701	649	O5-S	-2.49	1.54	1.59
2	D	701	649	O5-S	-2.43	1.54	1.59
2	B	701	649	C26-N3	2.38	1.35	1.32
2	A	701	649	C17-N6	-2.36	1.34	1.38
2	C	701	649	C26-N3	2.15	1.35	1.32
2	B	701	649	O6-C22	2.11	1.44	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	649	O3-S-O4	-6.17	111.14	120.76
2	B	701	649	O3-S-O4	-5.69	111.89	120.76
2	C	701	649	O3-S-O4	-4.92	113.09	120.76
2	A	701	649	N3-C26-N4	-4.55	121.56	128.68
2	D	701	649	N3-C26-N4	-4.49	121.66	128.68
2	D	701	649	O3-S-O4	-4.16	114.27	120.76
2	B	701	649	N3-C26-N4	-3.89	122.60	128.68
2	C	701	649	N3-C26-N4	-3.81	122.72	128.68
2	A	701	649	C7-O1-C5	3.03	125.86	117.93
2	C	701	649	O1-C7-C8	2.96	119.33	108.33
2	A	701	649	O1-C7-C8	2.70	118.38	108.33
2	B	701	649	O1-C7-C8	2.69	118.33	108.33
2	D	701	649	O1-C7-C8	2.62	118.09	108.33
2	D	701	649	C7-O1-C5	2.32	123.98	117.93
2	C	701	649	C7-O1-C5	2.21	123.70	117.93
2	C	701	649	O5-S-N6	2.18	111.67	105.60
2	B	701	649	C9-C8-C7	-2.07	104.34	113.49
2	D	701	649	C17-N6-S	-2.01	121.04	124.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	649	C4-C5-O1-C7
2	D	701	649	O1-C7-C8-C9
2	B	701	649	C6-C5-O1-C7
2	B	701	649	O1-C7-C8-C9
2	D	701	649	C4-C5-O1-C7
2	C	701	649	O1-C7-C8-C9
2	D	701	649	C6-C5-O1-C7
2	C	701	649	C4-C5-O1-C7

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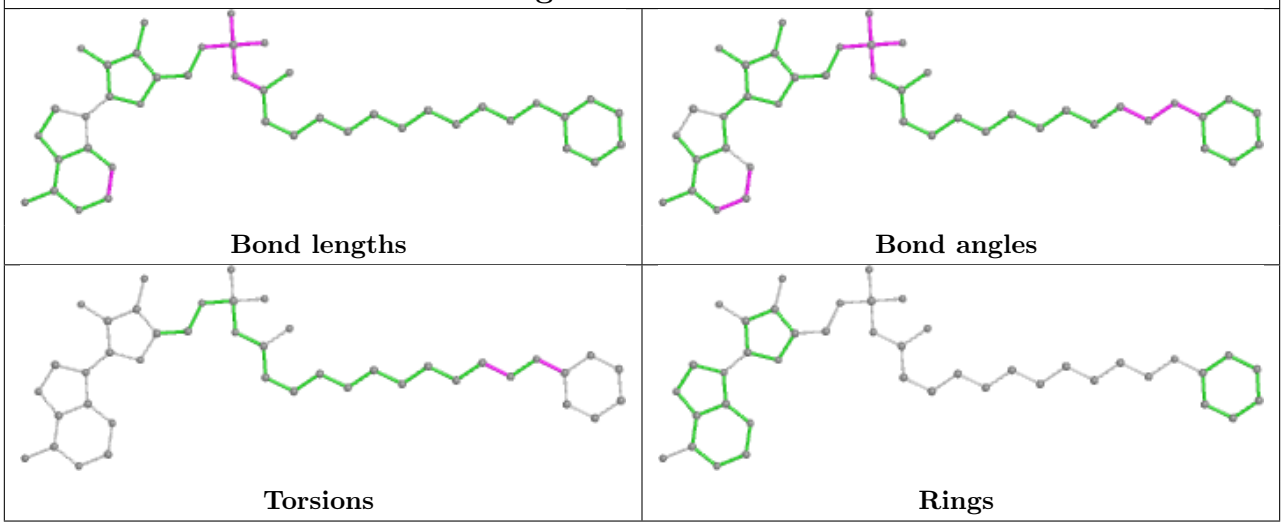
Mol	Chain	Res	Type	Atoms
2	C	701	649	C6-C5-O1-C7
2	D	701	649	C10-C11-C12-C13
2	D	701	649	C11-C12-C13-C14
2	A	701	649	C11-C12-C13-C14

There are no ring outliers.

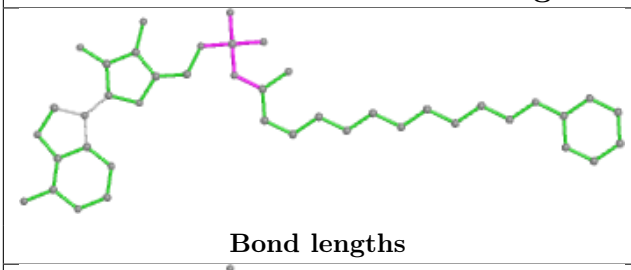
No monomer is involved in short contacts.

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 then 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.

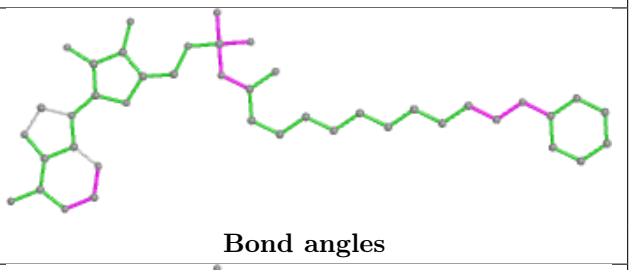
Ligand 649 C 701



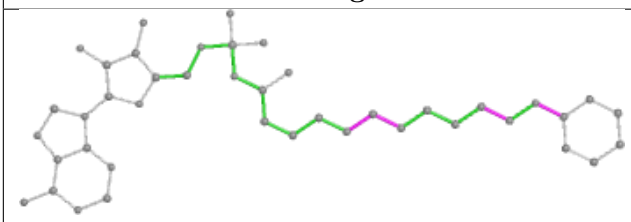
Ligand 649 D 701



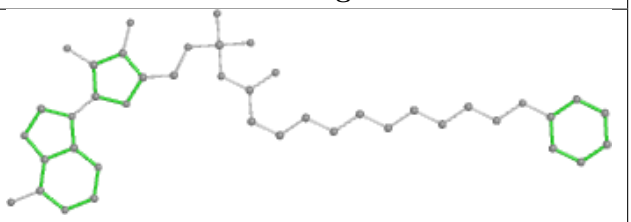
Bond lengths



Bond angles

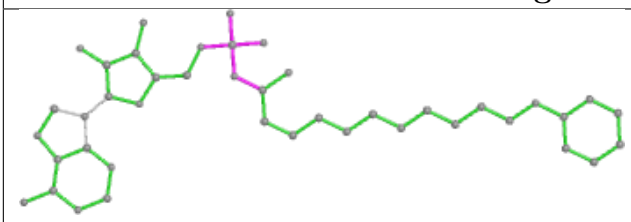


Torsions

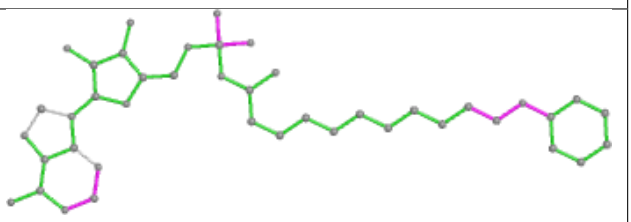


Rings

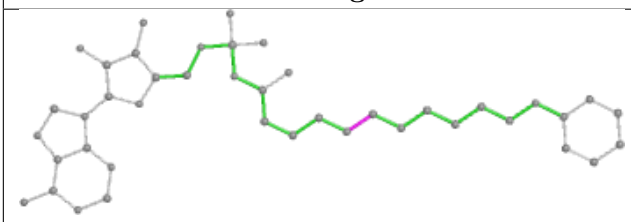
Ligand 649 A 701



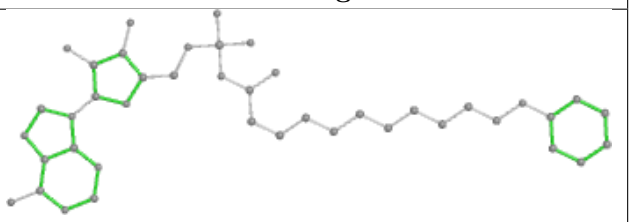
Bond lengths



Bond angles

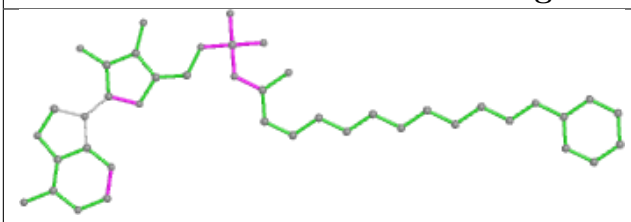


Torsions

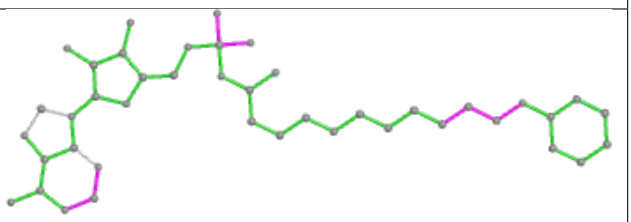


Rings

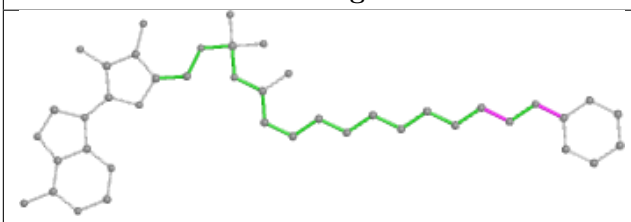
Ligand 649 B 701



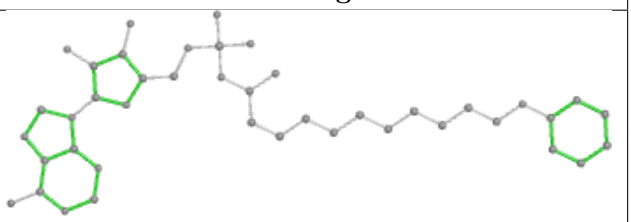
Bond lengths



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

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, 95^{th} 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	607/650 (93%)	-0.10	32 (5%)	26	29	20, 36, 74, 122	0
1	B	609/650 (93%)	0.02	45 (7%)	14	15	26, 45, 92, 133	0
1	C	618/650 (95%)	-0.04	38 (6%)	21	23	24, 45, 92, 124	0
1	D	609/650 (93%)	0.18	55 (9%)	9	10	26, 49, 93, 144	0
All	All	2443/2600 (93%)	0.02	170 (6%)	16	17	20, 44, 91, 144	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	ILE	7.7
1	D	559	ALA	6.9
1	A	8	ILE	5.6
1	A	630	ASP	5.6
1	D	562	LEU	5.5
1	C	9	LYS	5.3
1	A	17	ASP	5.3
1	D	560	HIS	5.2
1	C	193	ILE	5.0
1	D	191	THR	4.9
1	B	9	LYS	4.8
1	C	18	GLY	4.5
1	D	542	PRO	4.5
1	A	10	ASP	4.4
1	D	271	GLU	4.4
1	A	11	GLY	4.3
1	C	10	ASP	4.3
1	C	630	ASP	4.3
1	B	274	THR	4.3
1	A	16	PRO	4.2
1	D	31	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	28[A]	TRP	4.2
1	B	219	GLU	4.1
1	D	561	LYS	4.1
1	D	543	ASP	4.1
1	A	543	ASP	4.0
1	C	17	ASP	4.0
1	B	628	ALA	4.0
1	D	27	ARG	3.9
1	A	562	LEU	3.8
1	C	165	ASP	3.8
1	C	235	LEU	3.8
1	A	561	LYS	3.8
1	D	563	ASP	3.7
1	B	31	VAL	3.7
1	D	7	PHE	3.7
1	B	193	ILE	3.7
1	B	10	ASP	3.7
1	C	7	PHE	3.6
1	D	188	SER	3.6
1	D	530	VAL	3.6
1	D	219	GLU	3.5
1	B	115	HIS	3.5
1	B	239	LEU	3.5
1	C	236	ILE	3.5
1	B	28[A]	TRP	3.4
1	D	10	ASP	3.4
1	C	629	THR	3.4
1	B	557	PRO	3.4
1	A	542	PRO	3.4
1	B	47	ARG	3.4
1	B	301	PRO	3.4
1	D	274	THR	3.3
1	C	561	LYS	3.3
1	C	47	ARG	3.3
1	B	564	ILE	3.3
1	B	238	ALA	3.2
1	A	236	ILE	3.2
1	C	237	THR	3.2
1	C	239	LEU	3.2
1	D	558	GLY	3.2
1	A	219	GLU	3.2
1	D	238	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	16	PRO	3.1
1	C	271	GLU	3.1
1	B	17	ASP	3.1
1	C	46	GLU	3.1
1	D	299	SER	3.1
1	D	380	ASP	3.1
1	D	12	GLN	3.1
1	D	239	LEU	3.1
1	A	274	THR	3.1
1	D	557	PRO	3.1
1	A	18	GLY	3.0
1	C	238	ALA	3.0
1	B	235	LEU	3.0
1	B	271	GLU	3.0
1	D	564	ILE	2.9
1	D	297[A]	PRO	2.9
1	B	27	ARG	2.9
1	A	528	ASP	2.9
1	A	237	THR	2.9
1	C	240	LEU	2.8
1	C	563	ASP	2.8
1	D	556	ALA	2.8
1	B	234	GLY	2.8
1	D	298[A]	GLY	2.8
1	B	237	THR	2.8
1	D	280	VAL	2.8
1	A	563	ASP	2.7
1	D	629	THR	2.7
1	A	193	ILE	2.7
1	B	18	GLY	2.7
1	C	272	GLY	2.7
1	D	384	PRO	2.7
1	C	628	ALA	2.7
1	C	562	LEU	2.7
1	B	19	SER	2.7
1	C	15	PHE	2.7
1	A	382	ASP	2.7
1	B	491	ASP	2.7
1	B	244	ILE	2.7
1	B	297	PRO	2.6
1	C	16	PRO	2.6
1	A	567	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	529	GLU	2.6
1	B	242	PRO	2.6
1	A	298	GLY	2.6
1	B	298	GLY	2.6
1	D	168	SER	2.6
1	D	528	ASP	2.6
1	C	19	SER	2.6
1	D	235	LEU	2.6
1	D	301	PRO	2.5
1	D	350	LEU	2.5
1	B	11	GLY	2.5
1	D	225	SER	2.5
1	A	27	ARG	2.5
1	A	350	LEU	2.5
1	C	358	ALA	2.5
1	C	31	VAL	2.5
1	D	175	GLU	2.5
1	A	12	GLN	2.5
1	B	20	SER	2.4
1	B	240	LEU	2.4
1	A	297	PRO	2.4
1	B	46	GLU	2.4
1	B	14	LYS	2.4
1	C	557	PRO	2.4
1	A	238	ALA	2.4
1	C	45	THR	2.4
1	B	460	ASP	2.4
1	A	239	LEU	2.4
1	C	274	THR	2.4
1	D	296	LYS	2.3
1	B	539	LYS	2.3
1	D	224	LEU	2.3
1	D	382	ASP	2.3
1	B	542	PRO	2.3
1	C	113	PRO	2.3
1	D	628	ALA	2.3
1	A	564	ILE	2.3
1	B	243	MET	2.2
1	C	174	ASP	2.2
1	B	236	ILE	2.2
1	D	169	THR	2.2
1	D	165	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	114	GLY	2.2
1	D	311	LEU	2.2
1	C	75	GLN	2.2
1	A	91	LEU	2.2
1	D	529	GLU	2.2
1	A	32	ARG	2.1
1	B	407	GLU	2.1
1	B	91	LEU	2.1
1	B	248	PHE	2.1
1	B	34	ASP	2.1
1	D	9	LYS	2.1
1	D	541	ASP	2.1
1	B	227	LEU	2.1
1	C	12	GLN	2.1
1	A	245	GLY	2.1
1	C	243[A]	MET	2.1
1	D	113	PRO	2.1
1	D	281	ALA	2.0
1	C	219	GLU	2.0
1	C	30	LYS	2.0
1	B	629	THR	2.0
1	D	237	THR	2.0
1	D	227	LEU	2.0

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

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, 95^{th} 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.

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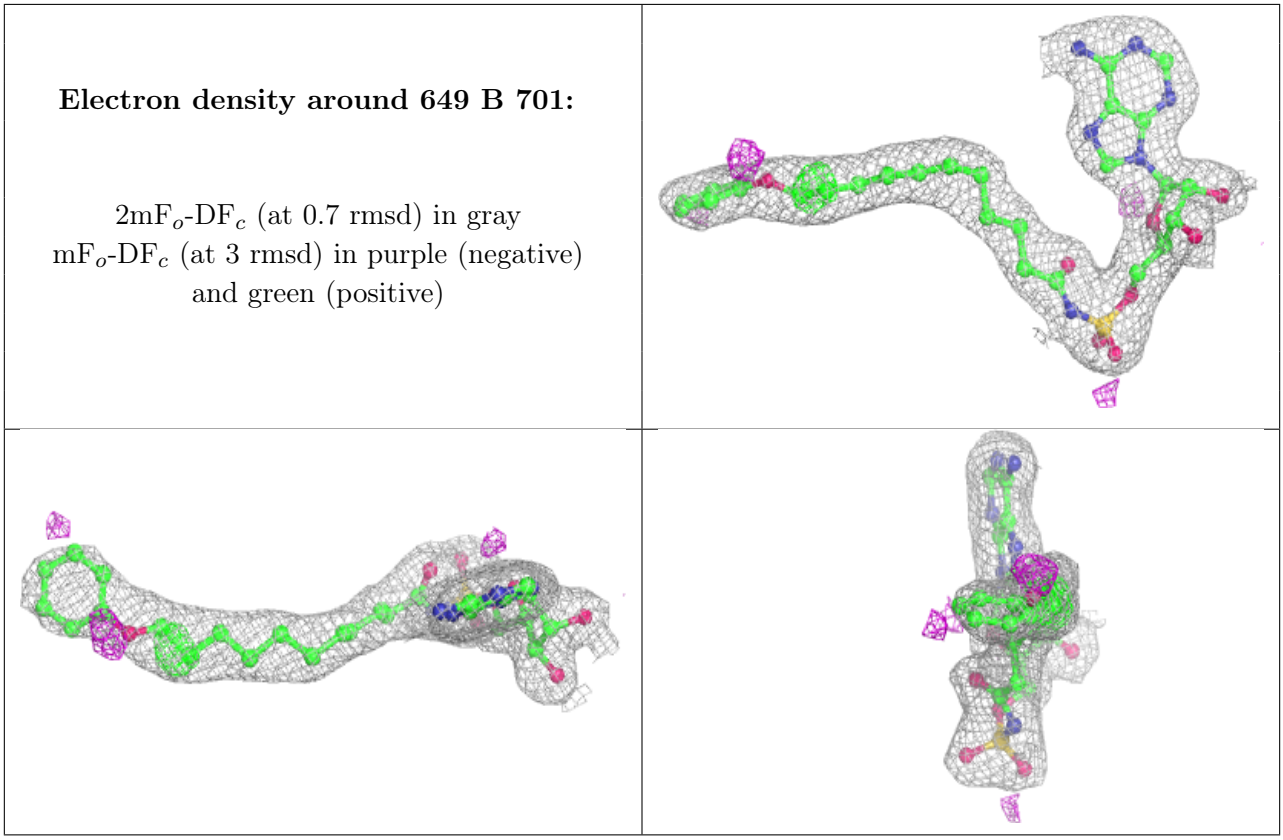
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	703	5/5	0.69	0.24	73,82,83,109	0
3	SO4	D	702	5/5	0.79	0.18	99,100,115,117	0
3	SO4	B	703	5/5	0.84	0.15	89,97,107,109	0
3	SO4	C	702	5/5	0.87	0.15	85,92,99,105	0
4	CL	B	702	1/1	0.87	0.15	79,79,79,79	0
3	SO4	A	702	5/5	0.88	0.13	97,99,107,111	0
5	GOL	C	703	6/6	0.88	0.12	67,74,75,80	0
2	649	B	701	42/42	0.96	0.16	27,31,52,55	0
2	649	A	701	42/42	0.96	0.18	22,25,46,49	0
2	649	D	701	42/42	0.97	0.15	29,40,58,64	0
2	649	C	701	42/42	0.97	0.16	27,31,61,64	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.

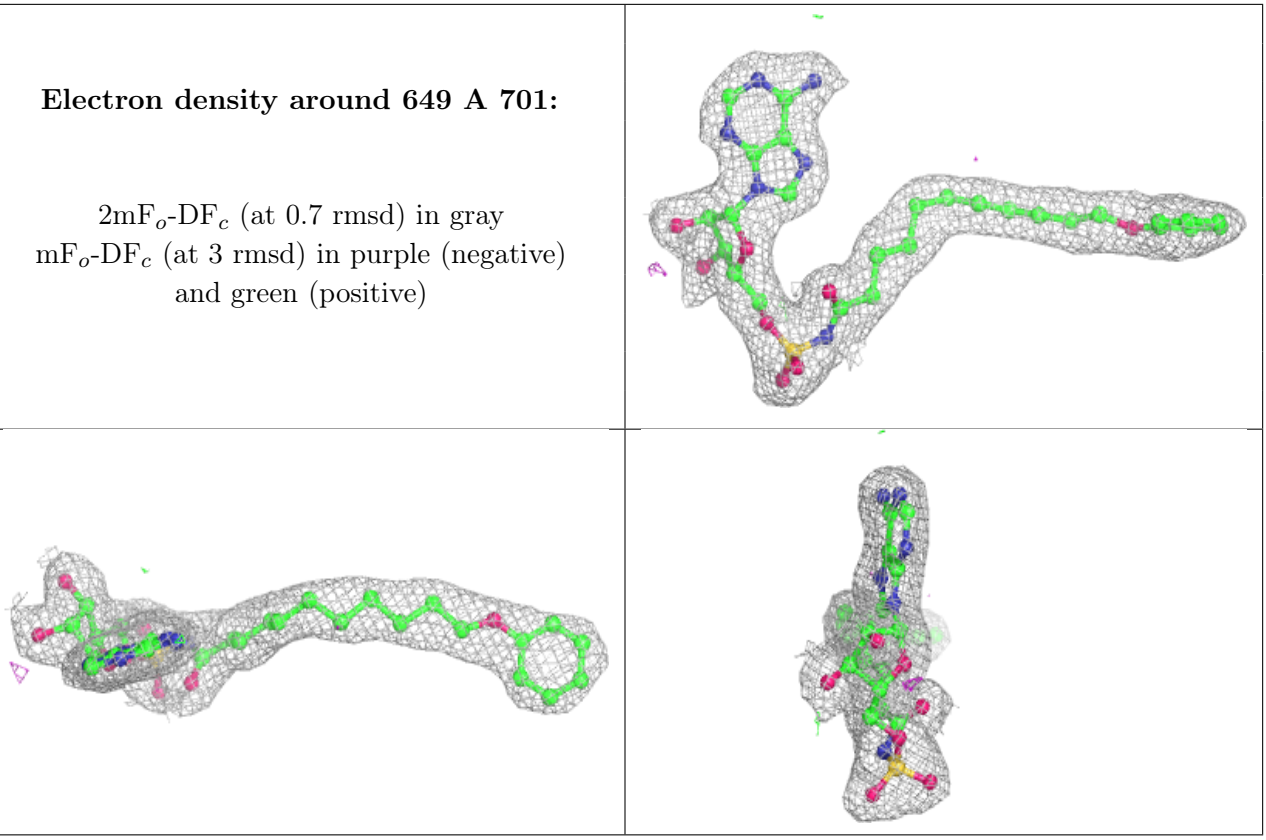
Electron density around 649 B 701:

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



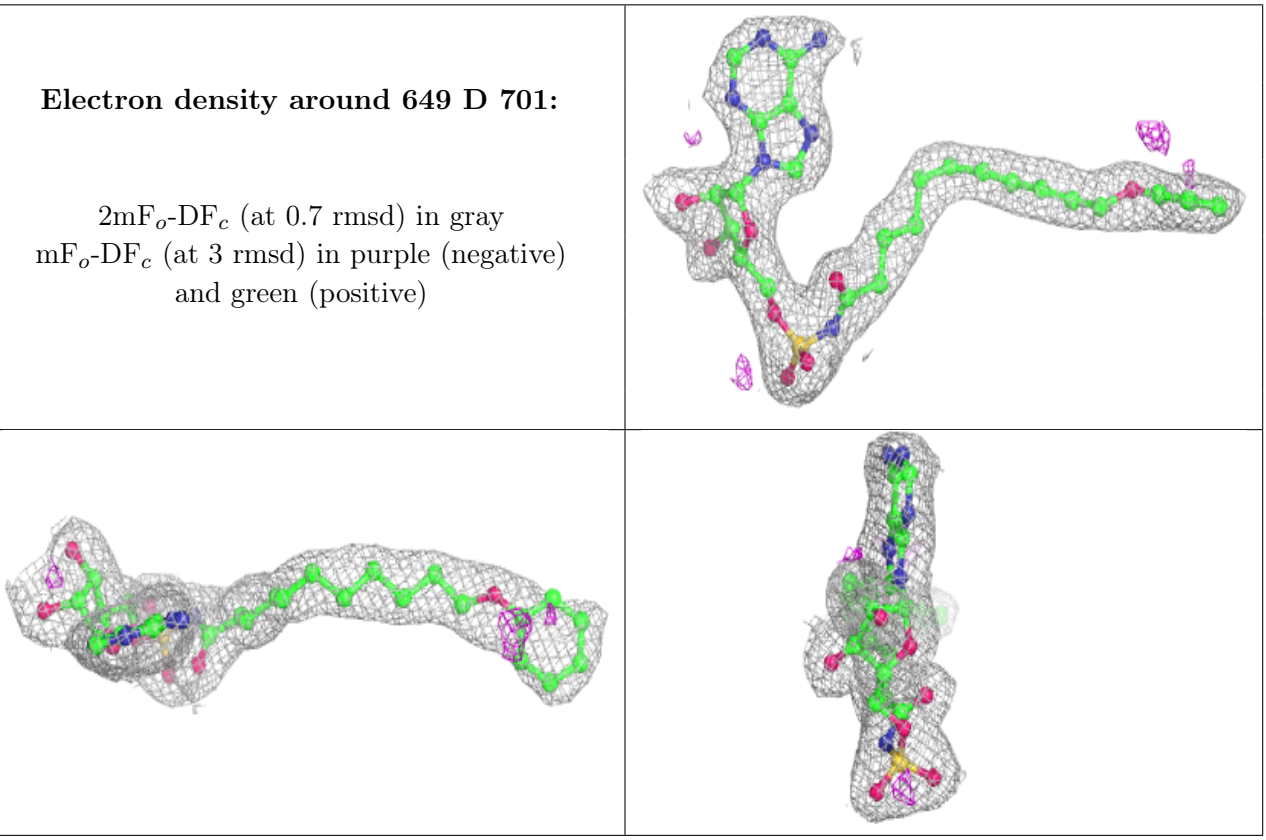
Electron density around 649 A 701:

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



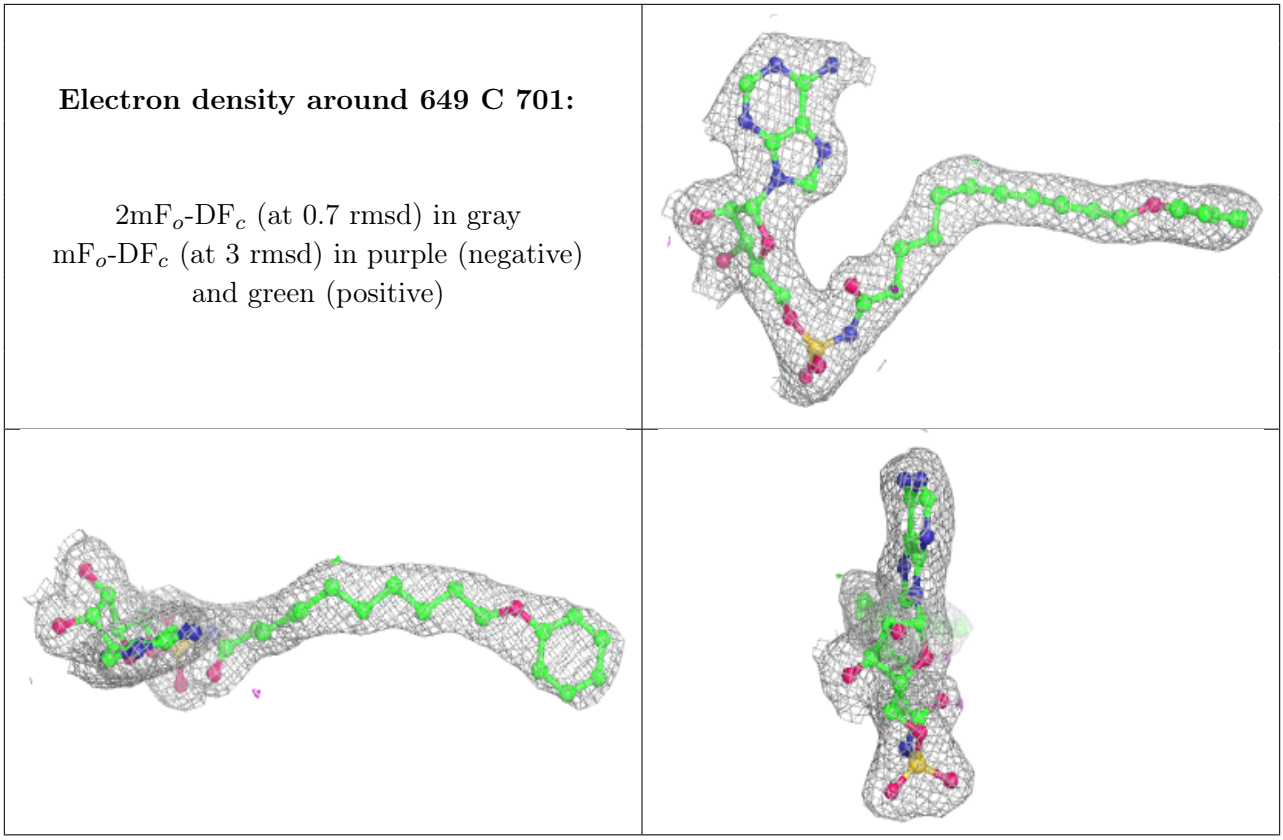
Electron density around 649 D 701:

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



Electron density around 649 C 701:

$2mF_o$-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.