Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 10:17 am BST

PDB ID	:	8P8K
Title	:	Acyl-ACP thioesterase from Lemna paucicostata in complex with a thiazolopyridine
Authors	:	Freigang, J.
Deposited on	:	2023-06-01
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:

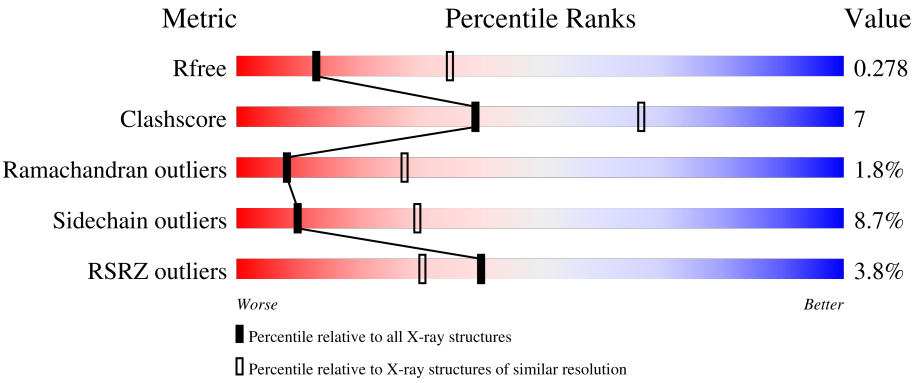
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	AAA	320	3% 67% 16% · 14%
1	BBB	320	4% 66% 17% · 14%

2 Entry composition

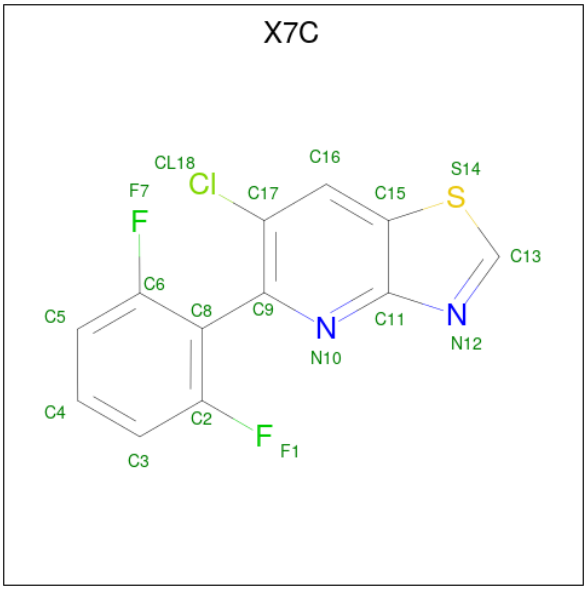
There are 4 unique types of molecules in this entry. The entry contains 4528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-ACP thioesterase.

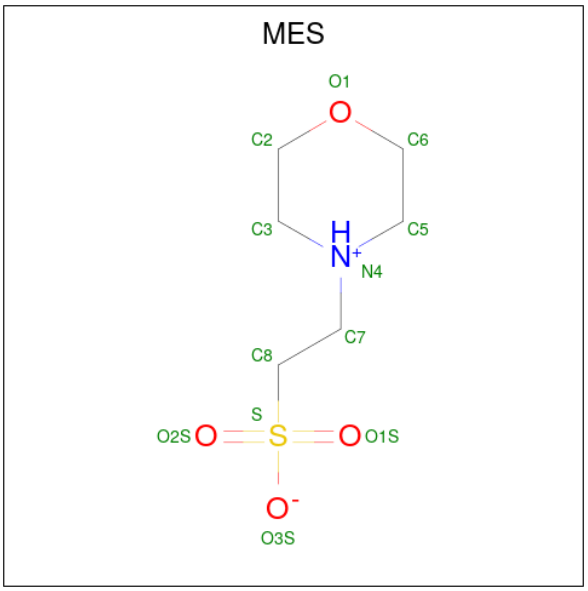
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	276	Total	C	N	O	S	0	0	0
			2238	1403	400	425	10			
1	BBB	276	Total	C	N	O	S	0	0	0
			2238	1403	400	425	10			

- Molecule 2 is 5-[2,6-bis(fluoranyl)phenyl]-6-chloranyl-[1,3]thiazolo[4,5-b]pyridine (three-letter code: X7C) (formula: $C_{12}H_5ClF_2N_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	Cl	F	N	S	0	0
			18	12	1	2	2	1		
2	BBB	1	Total	C	Cl	F	N	S	0	0
			18	12	1	2	2	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 4 is water.

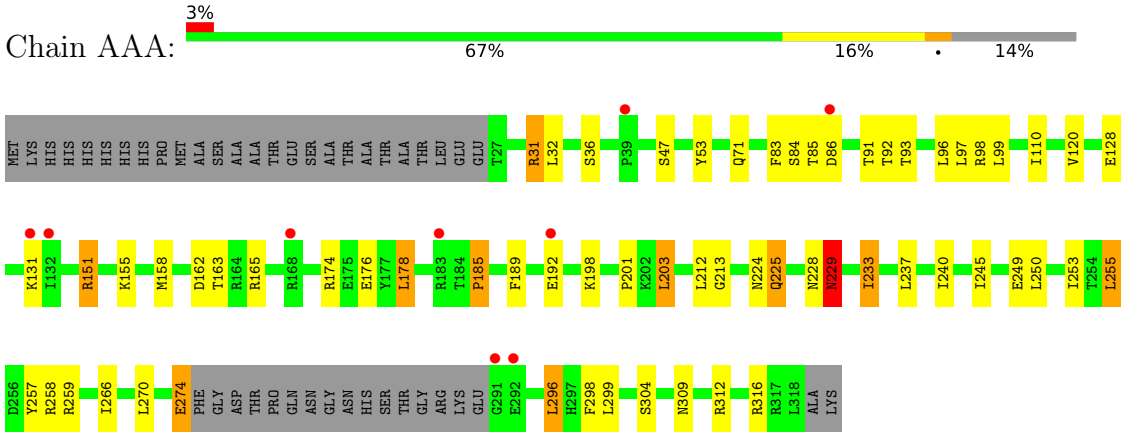
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	2	Total O 2 2	0	0
4	BBB	2	Total O 2 2	0	0

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.

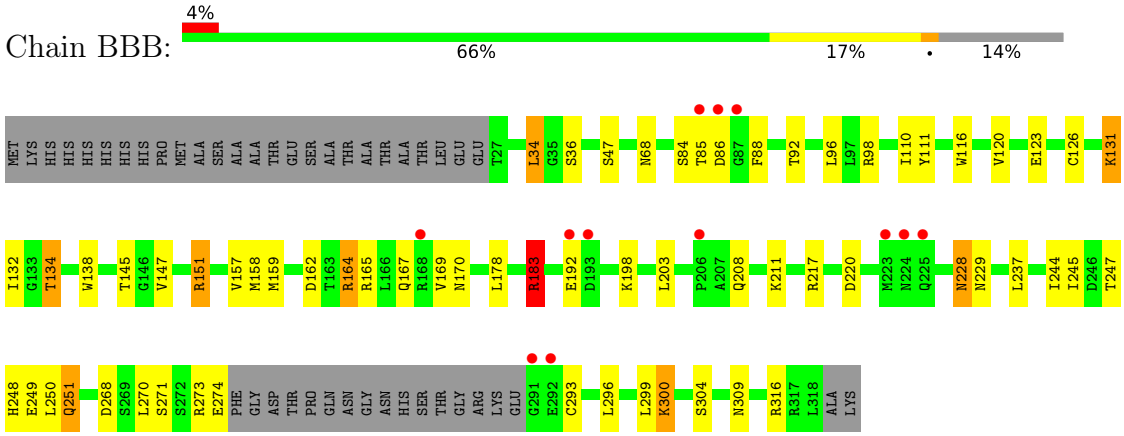
• Molecule 1: Acyl-ACP thioesterase

Chain AAA:



• Molecule 1: Acyl-ACP thioesterase

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.17Å 93.17Å 135.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.13 – 2.80 23.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (23.13-2.80) 98.5 (23.13-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.278 0.223 , 0.278	Depositor DCC
R_{free} test set	864 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 29.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4528	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: X7C, MES

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	AAA	0.64	0/2280	0.82	0/3086
1	BBB	0.64	0/2280	0.86	1/3086 (0.0%)
All	All	0.64	0/4560	0.84	1/6172 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BBB	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	183	ARG	NE-CZ-NH1	-5.57	117.51	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	167	GLN	Peptide

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	AAA	2238	0	2217	36	0
1	BBB	2238	0	2217	32	0
2	AAA	18	0	0	0	0
2	BBB	18	0	0	0	0
3	BBB	12	0	13	1	0
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
All	All	4528	0	4447	66	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 7.

All (66) 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:BBB:228:ASN:HD22	1:BBB:229:ASN:N	1.88	0.70
1:BBB:183:ARG:HA	1:BBB:183:ARG:HE	1.65	0.61
1:BBB:299:LEU:HD22	1:BBB:309:ASN:HD21	1.65	0.61
1:AAA:163:THR:HB	1:AAA:165:ARG:HG3	1.82	0.61
1:AAA:110:ILE:O	1:AAA:316:ARG:NH2	2.35	0.60
1:BBB:249:GLU:OE1	1:BBB:316:ARG:NH1	2.34	0.60
1:AAA:203:LEU:HD12	1:AAA:203:LEU:O	2.02	0.60
1:AAA:249:GLU:OE1	1:AAA:316:ARG:NH1	2.37	0.58
1:AAA:203:LEU:HD12	1:AAA:203:LEU:C	2.25	0.56
1:BBB:268:ASP:HB2	1:BBB:300:LYS:HE2	1.88	0.56
1:AAA:98:ARG:HD3	1:AAA:162:ASP:OD2	2.07	0.54
1:AAA:128:GLU:OE2	1:AAA:174:ARG:HD2	2.08	0.54
1:BBB:126:CYS:SG	1:BBB:134:THR:HG23	2.48	0.53
1:AAA:203:LEU:C	1:AAA:203:LEU:CD1	2.78	0.52
1:AAA:237:LEU:HD21	1:AAA:250:LEU:HD12	1.92	0.51
1:BBB:132:ILE:HG12	1:BBB:157:VAL:HG12	1.91	0.51
1:AAA:151:ARG:HG3	1:AAA:189:PHE:CZ	2.46	0.51
1:AAA:83:PHE:HE1	1:AAA:91:THR:HG22	1.76	0.50
1:BBB:178:LEU:HD22	1:BBB:183:ARG:NH1	2.27	0.50
1:BBB:203:LEU:C	1:BBB:203:LEU:HD12	2.32	0.50
1:AAA:31:ARG:HH11	1:AAA:31:ARG:HG2	1.76	0.50
1:AAA:174:ARG:O	1:AAA:178:LEU:HB2	2.11	0.50
1:BBB:84:SER:O	1:BBB:84:SER:OG	2.28	0.50
1:AAA:163:THR:CB	1:AAA:165:ARG:HG3	2.42	0.50
1:AAA:228:ASN:HD22	1:AAA:229:ASN:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:258:ARG:HG2	1:AAA:259:ARG:HG3	1.94	0.49
1:AAA:229:ASN:ND2	1:AAA:257:TYR:OH	2.45	0.49
1:BBB:247:THR:OG1	1:BBB:248:HIS:HD2	1.95	0.49
1:AAA:85:THR:HG22	1:AAA:86:ASP:H	1.78	0.49
1:BBB:98:ARG:HD3	1:BBB:162:ASP:OD2	2.13	0.48
1:BBB:34:LEU:N	1:BBB:34:LEU:CD1	2.76	0.48
1:BBB:111:TYR:OH	1:BBB:151:ARG:HD3	2.13	0.48
1:AAA:224:ASN:O	1:AAA:225:GLN:HB2	2.12	0.48
1:BBB:250:LEU:C	1:BBB:250:LEU:HD23	2.34	0.47
1:AAA:250:LEU:HD23	1:AAA:250:LEU:C	2.34	0.47
1:BBB:145:THR:OG1	1:BBB:147:VAL:HG12	2.15	0.47
1:AAA:201:PRO:HG2	1:AAA:296:LEU:HD11	1.98	0.46
1:BBB:271:SER:HA	1:BBB:296:LEU:O	2.17	0.45
1:BBB:47:SER:HA	1:BBB:120:VAL:O	2.17	0.45
1:BBB:268:ASP:HB2	1:BBB:300:LYS:CE	2.46	0.45
1:BBB:110:ILE:O	1:BBB:316:ARG:NH2	2.50	0.45
1:BBB:237:LEU:HD21	1:BBB:250:LEU:HD12	1.97	0.45
1:BBB:250:LEU:HD23	1:BBB:251:GLN:N	2.31	0.45
1:AAA:99:LEU:HD13	1:AAA:158:MET:HE3	1.98	0.45
1:AAA:31:ARG:HG2	1:AAA:31:ARG:NH1	2.32	0.44
1:AAA:47:SER:HA	1:AAA:120:VAL:O	2.17	0.44
1:AAA:213:GLY:HA2	1:AAA:266:ILE:CG2	2.47	0.44
1:AAA:203:LEU:HG	1:AAA:298:PHE:HB2	2.00	0.43
1:AAA:299:LEU:HB2	1:AAA:309:ASN:HB2	1.99	0.43
1:AAA:255:LEU:HD23	1:AAA:255:LEU:HA	1.86	0.43
1:BBB:123:GLU:O	1:BBB:138:TRP:HA	2.18	0.43
1:BBB:208:GLN:HE22	1:BBB:273:ARG:HG3	1.84	0.43
1:AAA:228:ASN:ND2	1:AAA:229:ASN:N	2.65	0.43
1:BBB:183:ARG:HE	1:BBB:183:ARG:CA	2.31	0.42
1:AAA:93:THR:OG1	1:AAA:176:GLU:OE1	2.37	0.42
1:AAA:32:LEU:HD11	3:BBB:402:MES:H62	2.01	0.42
1:BBB:159:MET:SD	1:BBB:164:ARG:HG3	2.60	0.41
1:BBB:247:THR:OG1	1:BBB:248:HIS:CD2	2.73	0.41
1:AAA:233:ILE:HG23	1:AAA:253:ILE:HD13	2.02	0.41
1:AAA:274:GLU:OE2	1:AAA:312:ARG:NH1	2.53	0.41
1:BBB:131:LYS:O	1:BBB:169:VAL:HG23	2.20	0.41
1:BBB:217:ARG:NH2	1:BBB:220:ASP:OD1	2.53	0.41
1:AAA:85:THR:HG23	1:BBB:116:TRP:CE3	2.55	0.41
1:AAA:96:LEU:HD12	1:AAA:96:LEU:HA	1.84	0.41
1:BBB:273:ARG:NH1	1:BBB:293:CYS:HB3	2.36	0.41
1:AAA:53:TYR:CE2	1:BBB:68:ASN:HB3	2.56	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	AAA	272/320 (85%)	261 (96%)	6 (2%)	5 (2%)	8 28
1	BBB	272/320 (85%)	255 (94%)	12 (4%)	5 (2%)	8 28
All	All	544/640 (85%)	516 (95%)	18 (3%)	10 (2%)	8 28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	192	GLU
1	BBB	85	THR
1	BBB	170	ASN
1	BBB	192	GLU
1	AAA	36	SER
1	AAA	225	GLN
1	AAA	229	ASN
1	BBB	36	SER
1	BBB	88	PHE
1	AAA	185	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	AAA	248/282 (88%)	226 (91%)	22 (9%)	9 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	BBB	248/282 (88%)	227 (92%)	21 (8%)	10 31
All	All	496/564 (88%)	453 (91%)	43 (9%)	10 30

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	31	ARG
1	AAA	71	GLN
1	AAA	84	SER
1	AAA	92	THR
1	AAA	97	LEU
1	AAA	131	LYS
1	AAA	151	ARG
1	AAA	155	LYS
1	AAA	178	LEU
1	AAA	185	PRO
1	AAA	198	LYS
1	AAA	203	LEU
1	AAA	212	LEU
1	AAA	229	ASN
1	AAA	233	ILE
1	AAA	240	ILE
1	AAA	245	ILE
1	AAA	255	LEU
1	AAA	270	LEU
1	AAA	274	GLU
1	AAA	296	LEU
1	AAA	304	SER
1	BBB	34	LEU
1	BBB	86	ASP
1	BBB	92	THR
1	BBB	96	LEU
1	BBB	131	LYS
1	BBB	134	THR
1	BBB	151	ARG
1	BBB	158	MET
1	BBB	164	ARG
1	BBB	165	ARG
1	BBB	183	ARG
1	BBB	198	LYS
1	BBB	211	LYS
1	BBB	228	ASN

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Mol	Chain	Res	Type
1	BBB	244	ILE
1	BBB	245	ILE
1	BBB	251	GLN
1	BBB	270	LEU
1	BBB	274	GLU
1	BBB	300	LYS
1	BBB	304	SER

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)

3 ligands 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	$\#\|Z\| > 2$
3	MES	BBB	402	-	12,12,12	0.76	0	14,16,16	0.51	0
2	X7C	AAA	401	-	16,20,20	0.87	0	16,29,29	2.40	5 (31%)
2	X7C	BBB	401	-	16,20,20	1.16	2 (12%)	16,29,29	2.41	8 (50%)

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
3	MES	BBB	402	-	-	3/6/14/14	0/1/1/1
2	X7C	AAA	401	-	-	1/4/4/4	0/3/3/3
2	X7C	BBB	401	-	-	0/4/4/4	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	401	X7C	C8-C9	-2.90	1.46	1.50
2	BBB	401	X7C	C8-C6	-2.05	1.36	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	401	X7C	C16-C17-CL18	-5.91	113.33	119.20
2	BBB	401	X7C	C6-C8-C2	5.43	119.89	114.56
2	AAA	401	X7C	C9-N10-C11	4.33	122.06	117.99
2	BBB	401	X7C	C5-C6-C8	-3.79	119.32	123.94
2	AAA	401	X7C	C6-C8-C2	3.46	117.96	114.56
2	BBB	401	X7C	C9-N10-C11	3.21	121.01	117.99
2	BBB	401	X7C	C16-C17-C9	-3.19	119.10	122.00
2	AAA	401	X7C	C3-C2-C8	-3.09	120.17	123.94
2	BBB	401	X7C	C9-C8-C2	-2.46	118.82	121.69
2	AAA	401	X7C	C16-C17-C9	-2.39	119.83	122.00
2	BBB	401	X7C	C16-C17-CL18	-2.23	116.98	119.20
2	BBB	401	X7C	C3-C2-C8	-2.22	121.22	123.94
2	BBB	401	X7C	F7-C6-C5	2.16	123.40	118.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	402	MES	C7-C8-S-O1S
3	BBB	402	MES	C7-C8-S-O2S
3	BBB	402	MES	C7-C8-S-O3S
2	AAA	401	X7C	C6-C8-C9-C17

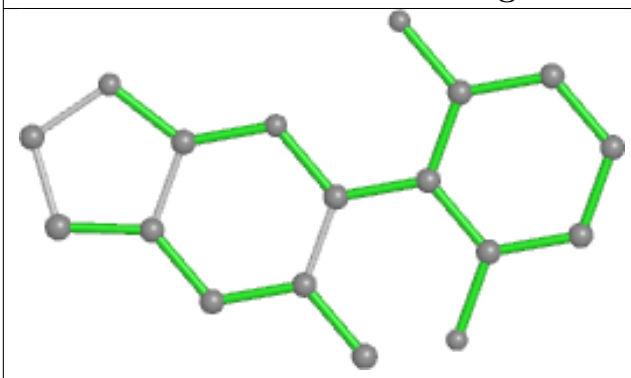
There are no ring outliers.

1 monomer is involved in 1 short contact:

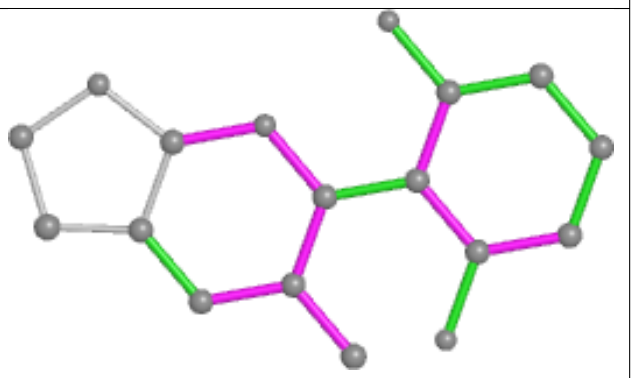
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	402	MES	1	0

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 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.

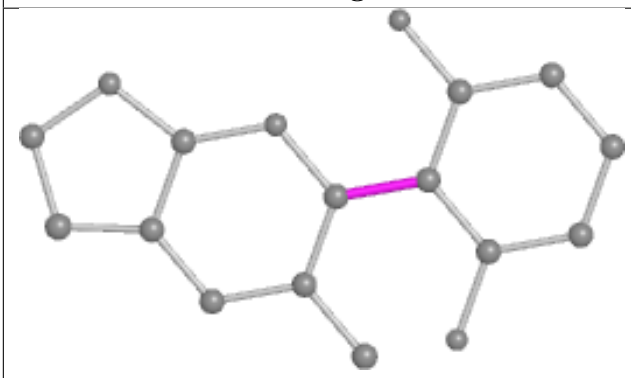
Ligand X7C AAA 401



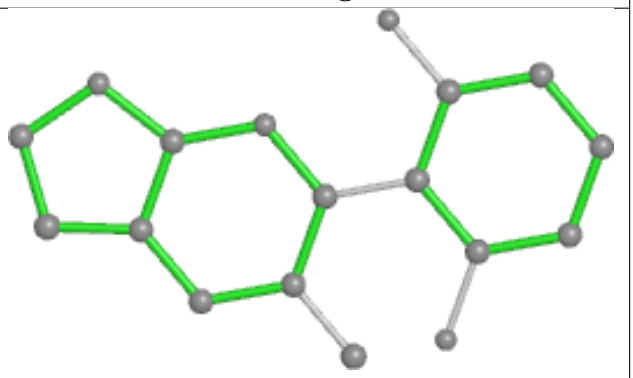
Bond lengths



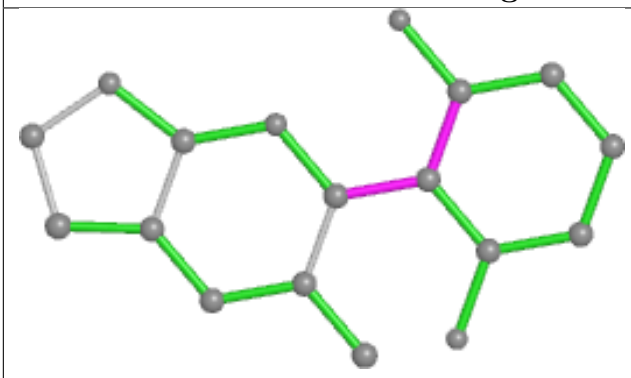
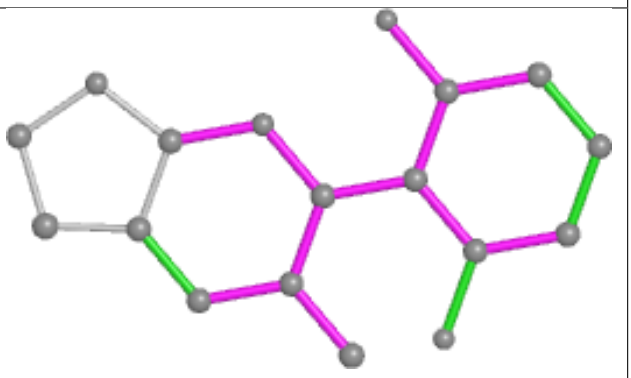
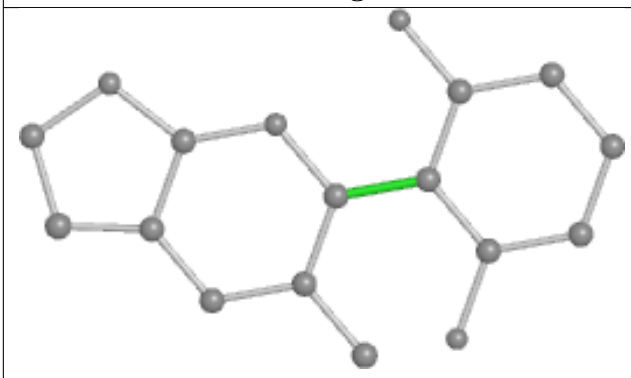
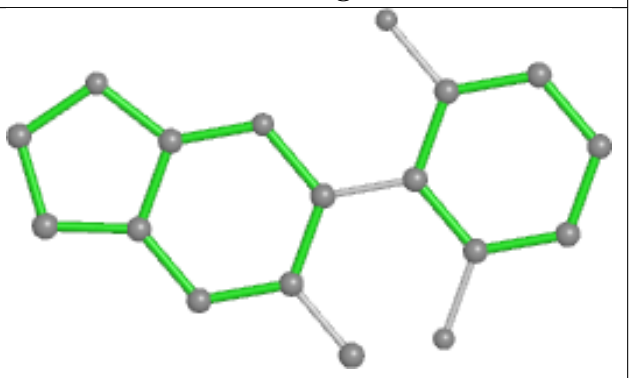
Bond angles



Torsions



Rings

Ligand X7C BBB 401	
 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	AAA	276/320 (86%)	-0.20	9 (3%)	46	36	20, 36, 71, 109	0
1	BBB	276/320 (86%)	-0.08	12 (4%)	35	25	18, 40, 72, 96	0
All	All	552/640 (86%)	-0.14	21 (3%)	40	30	18, 38, 72, 109	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	291	GLY	9.5
1	AAA	131	LYS	5.1
1	BBB	224	ASN	3.5
1	AAA	39	PRO	3.4
1	BBB	85	THR	2.9
1	BBB	87	GLY	2.9
1	AAA	292	GLU	2.9
1	AAA	192	GLU	2.6
1	AAA	183	ARG	2.6
1	BBB	192	GLU	2.6
1	BBB	168	ARG	2.6
1	AAA	168	ARG	2.6
1	AAA	291	GLY	2.5
1	BBB	225	GLN	2.5
1	AAA	132	ILE	2.5
1	BBB	193	ASP	2.4
1	BBB	206	PRO	2.4
1	BBB	292	GLU	2.2
1	BBB	86	ASP	2.2
1	AAA	86	ASP	2.1
1	BBB	223	MET	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)

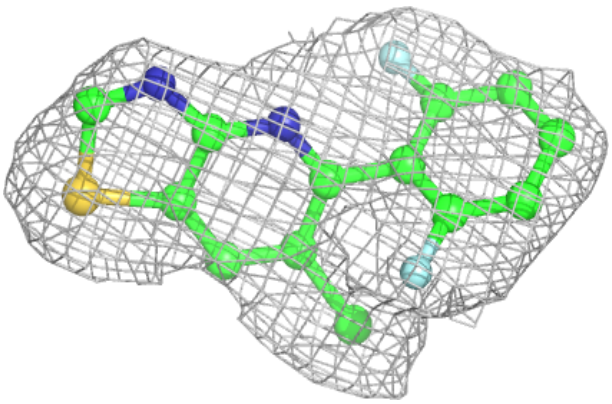
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

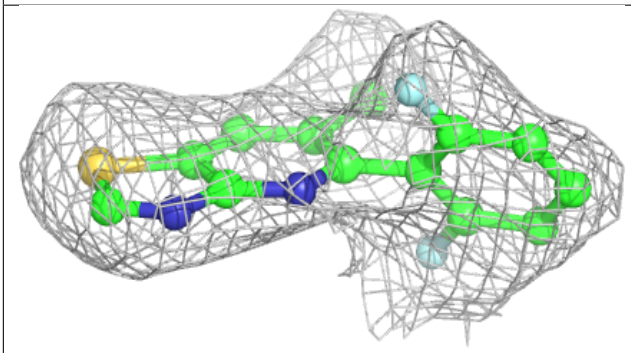
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	BBB	402	12/12	0.96	0.17	14,15,15,15	12
2	X7C	BBB	401	18/18	0.97	0.13	28,29,34,37	0
2	X7C	AAA	401	18/18	0.97	0.14	31,35,39,42	0

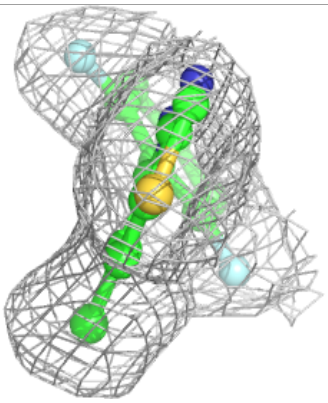
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around X7C BBB 401:

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

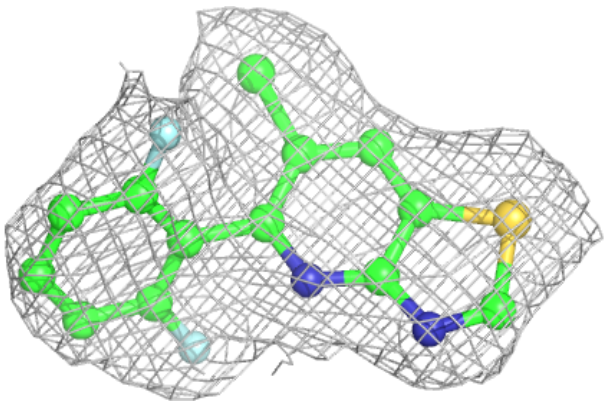


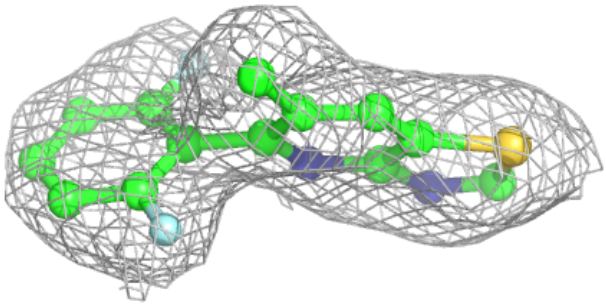


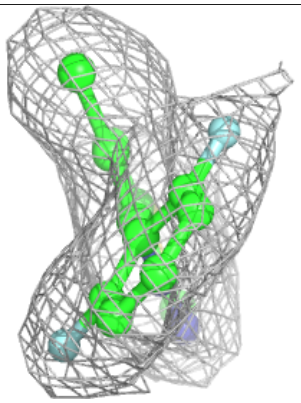


Electron density around X7C AAA 401:

$2mF_o$-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.