Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:30 pm BST

PDB ID	:	6HXI
Title	:	Structure of ATP citrate lyase from Methanothrix soehngenii in complex with citrate and coenzyme A
Authors	:	Verstraete, K.; Verschueren, K.
Deposited on	:	2018-10-17
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

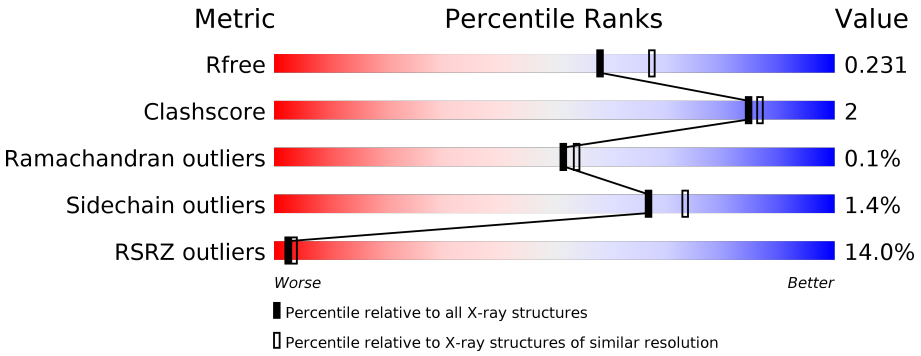
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	421	27% 84% 7% 10%
1	C	421	19% 89% 8% •
2	B	631	6% 91% 6% •
2	D	631	8% 90% 7% •

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16728 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 Citrate lyase, subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	5	0
			3057	1964	492	590	11			
1	C	410	Total	C	N	O	S	0	0	0
			3231	2070	525	625	11			

- Molecule 2 is a protein called Succinyl-CoA ligase (ADP-forming) subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	616	Total	C	N	O	S	0	5	0
			4775	3034	827	886	28			
2	D	616	Total	C	N	O	S	0	4	0
			4764	3028	823	885	28			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	623	GLY	-	expression tag	UNP A0A1V4VDZ9
B	624	GLY	-	expression tag	UNP A0A1V4VDZ9
B	625	SER	-	expression tag	UNP A0A1V4VDZ9
B	626	HIS	-	expression tag	UNP A0A1V4VDZ9
B	627	HIS	-	expression tag	UNP A0A1V4VDZ9
B	628	HIS	-	expression tag	UNP A0A1V4VDZ9
B	629	HIS	-	expression tag	UNP A0A1V4VDZ9
B	630	HIS	-	expression tag	UNP A0A1V4VDZ9
B	631	HIS	-	expression tag	UNP A0A1V4VDZ9
D	623	GLY	-	expression tag	UNP A0A1V4VDZ9
D	624	GLY	-	expression tag	UNP A0A1V4VDZ9
D	625	SER	-	expression tag	UNP A0A1V4VDZ9
D	626	HIS	-	expression tag	UNP A0A1V4VDZ9
D	627	HIS	-	expression tag	UNP A0A1V4VDZ9
D	628	HIS	-	expression tag	UNP A0A1V4VDZ9
D	629	HIS	-	expression tag	UNP A0A1V4VDZ9

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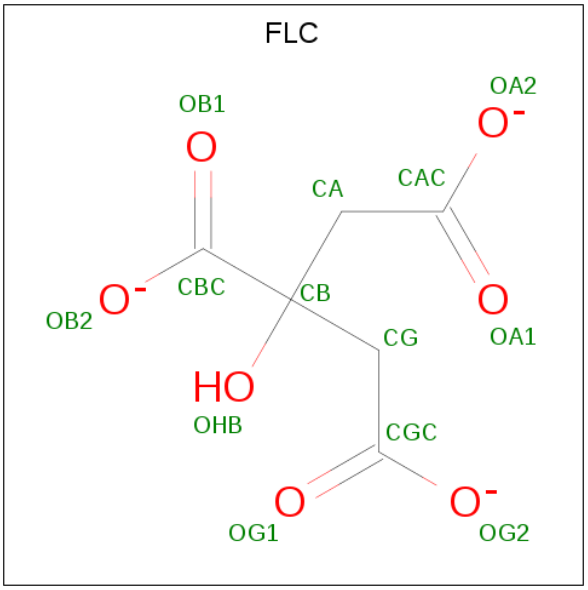
Chain	Residue	Modelled	Actual	Comment	Reference
D	630	HIS	-	expression tag	UNP A0A1V4VDZ9
D	631	HIS	-	expression tag	UNP A0A1V4VDZ9

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by author).

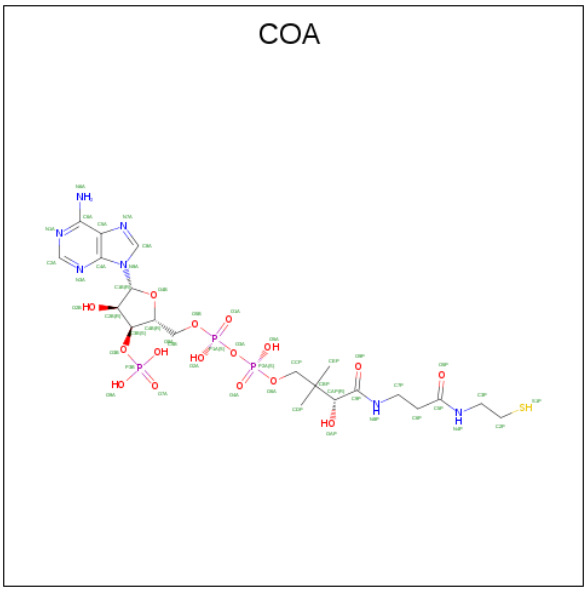


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

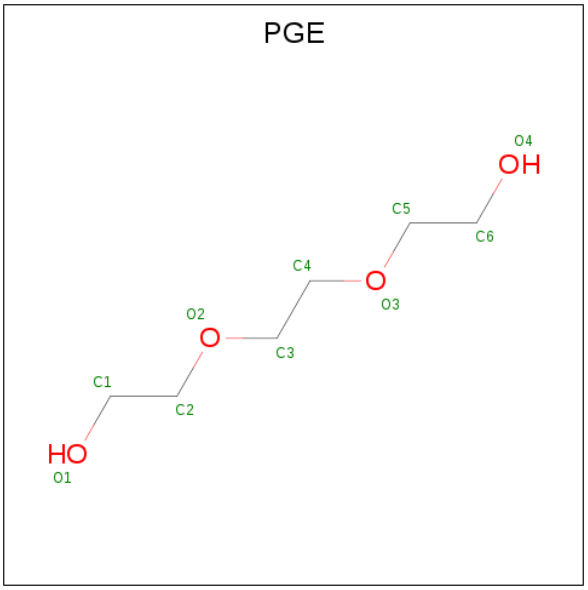
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by author).



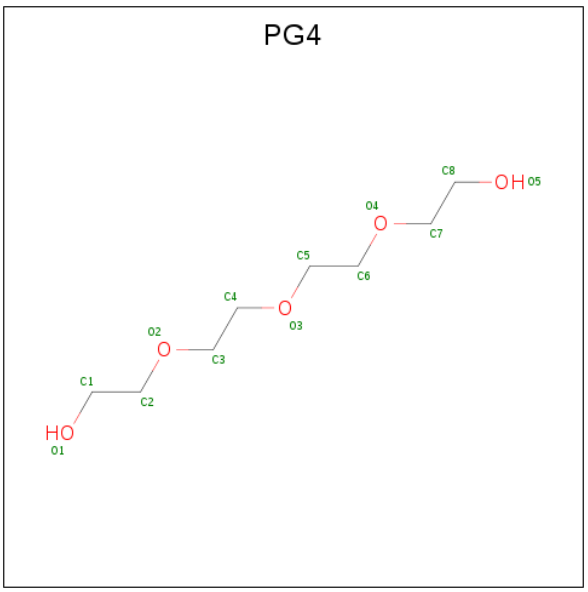
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



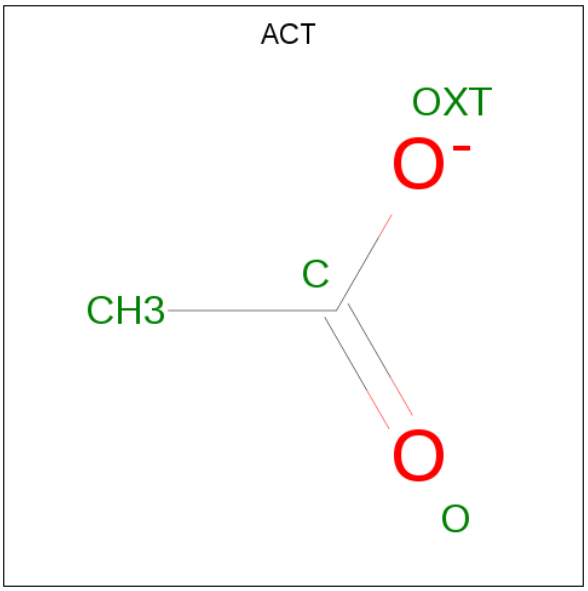
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 13 8 5	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

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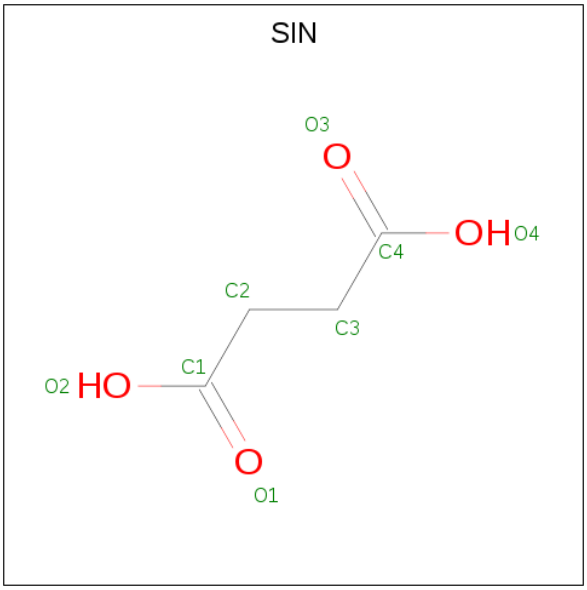
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 4 2 2	0	0

- Molecule 9 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 8 4 4	0	0

- Molecule 10 is water.

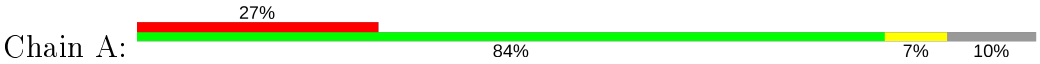
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	76	Total O 76 76	0	0
10	B	298	Total O 298 298	0	0
10	C	93	Total O 93 93	0	0
10	D	257	Total O 257 257	0	0

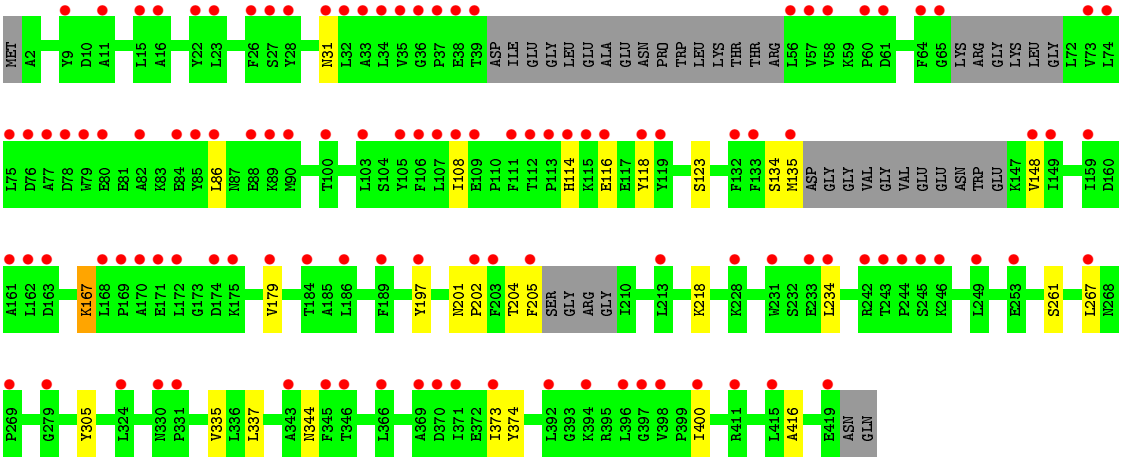
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Citrate lyase, subunit 1

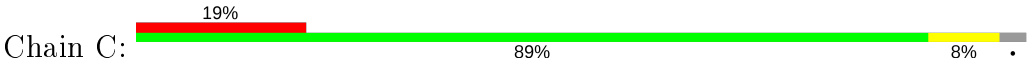
Chain A:

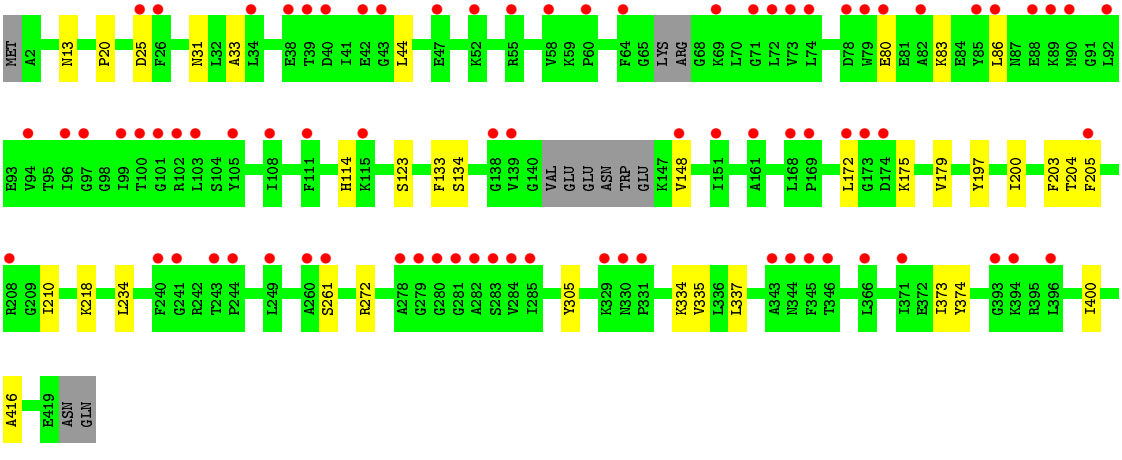




- Molecule 1: Citrate lyase, subunit 1

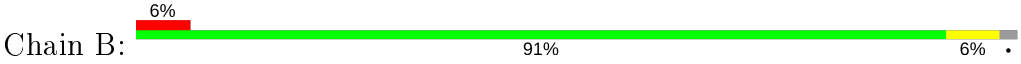
Chain C:

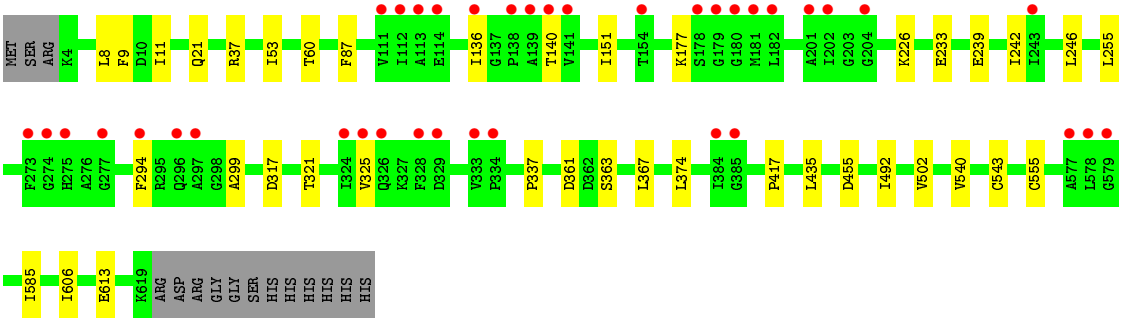




- Molecule 2: Succinyl-CoA ligase (ADP-forming) subunit alpha

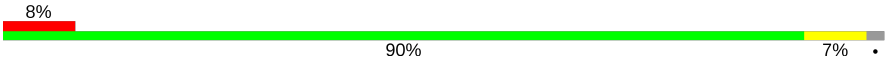
Chain B:

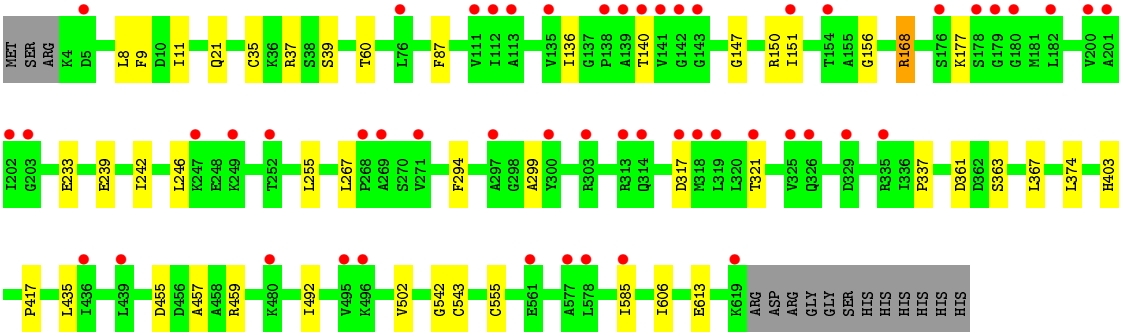




• Molecule 2: Succinyl-CoA ligase (ADP-forming) subunit alpha

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.45Å 275.02Å 72.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.75 – 2.10 39.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.75-2.10) 99.4 (39.08-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.179 , 0.208 0.200 , 0.231	Depositor DCC
R_{free} test set	6963 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16728	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: PGE, NA, COA, PG4, ACT, FLC, SIN

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	0.45	0/3122	0.65	0/4225
1	C	0.45	0/3301	0.66	0/4469
2	B	0.54	0/4863	0.65	0/6563
2	D	0.54	0/4852	0.65	0/6549
All	All	0.51	0/16138	0.65	0/21806

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
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	168	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3057	0	3002	16	0
1	C	3231	0	3173	18	0
2	B	4775	0	4848	20	0
2	D	4764	0	4836	22	0
3	A	13	0	5	0	0
3	C	13	0	5	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	48	0	32	0	0
5	D	48	0	32	0	0
6	B	20	0	28	2	0
7	B	13	0	18	0	0
8	B	8	0	6	0	0
8	D	4	0	3	0	0
9	D	8	0	4	0	0
10	A	76	0	0	0	0
10	B	298	0	0	2	0
10	C	93	0	0	0	0
10	D	257	0	0	1	0
All	All	16728	0	15992	73	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 (73) 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:C:204:THR:HG22	1:C:205:PHE:H	1.44	0.79
1:C:114:HIS:HB2	1:C:204:THR:HG21	1.66	0.78
2:B:540:VAL:HG23	10:B:808:HOH:O	1.84	0.77
2:B:502:VAL:HG13	2:B:543[B]:CYS:SG	2.35	0.67
1:A:167[A]:LYS:HZ1	1:A:179:VAL:HB	1.60	0.67
2:B:367:LEU:HD23	2:B:374:LEU:HD22	1.76	0.66
1:C:172:LEU:HB2	1:C:175:LYS:HB2	1.77	0.66
2:D:8:LEU:HD21	2:D:136:ILE:HD11	1.79	0.65
2:D:367:LEU:HD23	2:D:374:LEU:HD22	1.80	0.64
2:D:502:VAL:HG13	2:D:543[B]:CYS:SG	2.38	0.64
1:C:204:THR:HG22	1:C:205:PHE:N	2.13	0.62
1:A:167[A]:LYS:NZ	1:A:179:VAL:HB	2.15	0.62
2:B:8:LEU:HD21	2:B:136:ILE:HD11	1.83	0.60
1:A:114:HIS:HB2	1:A:204:THR:HG21	1.85	0.59
1:C:204:THR:CG2	1:C:205:PHE:H	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASN:O	2:D:156:GLY:HA2	2.06	0.55
1:C:373:ILE:HB	1:C:400:ILE:HG12	1.89	0.55
1:A:204:THR:HG22	1:A:205:PHE:H	1.71	0.54
1:A:373:ILE:HB	1:A:400:ILE:HG12	1.89	0.54
2:B:606:ILE:HD13	2:D:417:PRO:HG2	1.90	0.53
1:C:335:VAL:HG11	1:C:416:ALA:HB1	1.91	0.53
1:C:33:ALA:HB1	1:C:44:LEU:HD21	1.90	0.51
2:B:9:PHE:CZ	2:B:151:ILE:HD11	2.46	0.50
2:B:239:GLU:HA	2:B:242:ILE:HD12	1.94	0.50
2:D:9:PHE:CZ	2:D:151:ILE:HD11	2.46	0.50
2:B:177:LYS:HD3	2:B:233:GLU:HG2	1.94	0.49
2:D:239:GLU:HA	2:D:242:ILE:HD12	1.94	0.48
2:D:177:LYS:HD3	2:D:233:GLU:HG2	1.96	0.48
2:B:21:GLN:HG3	2:B:87:PHE:CG	2.48	0.47
1:A:86:LEU:HD11	1:A:108:ILE:HD11	1.96	0.47
1:C:80:GLU:HA	1:C:83:LYS:HE3	1.97	0.47
2:D:21:GLN:HG3	2:D:87:PHE:CG	2.50	0.46
1:A:337:LEU:HD23	1:A:374:TYR:HB2	1.96	0.46
2:B:60:THR:HG22	2:B:337:PRO:HG2	1.98	0.46
2:B:317:ASP:O	2:B:321:THR:HG23	2.16	0.45
1:C:337:LEU:HD23	1:C:374:TYR:HB2	1.97	0.45
2:B:417:PRO:HG2	2:D:606:ILE:HD13	1.97	0.45
1:C:261:SER:O	1:C:305:TYR:HA	2.16	0.45
1:A:261:SER:O	1:A:305:TYR:HA	2.17	0.45
2:B:136:ILE:HG22	2:B:140:THR:HG21	1.99	0.44
1:A:134:SER:HB2	1:A:148:VAL:HG22	1.99	0.44
1:C:134:SER:HB2	1:C:148:VAL:HG22	2.00	0.44
2:D:60:THR:HG22	2:D:337:PRO:HG2	2.00	0.44
1:C:272:ARG:HA	1:C:334:LYS:HG2	1.99	0.43
2:D:317:ASP:O	2:D:321:THR:HG23	2.17	0.43
2:D:361:ASP:OD1	2:D:363:SER:HB2	2.18	0.43
2:B:226:LYS:HG3	2:B:325:VAL:HG22	2.00	0.43
1:A:335:VAL:HG11	1:A:416:ALA:HB1	2.00	0.43
2:D:136:ILE:HG22	2:D:140:THR:HG21	2.00	0.43
1:A:118:TYR:HD1	1:A:135:MET:HA	1.84	0.43
2:B:361:ASP:OD1	2:B:363:SER:HB2	2.19	0.43
1:A:267:LEU:HD13	2:D:267:LEU:HD22	2.00	0.43
2:D:403:HIS:HB2	10:D:1025:HOH:O	2.17	0.43
2:D:11:ILE:HG13	2:D:37:ARG:HG2	2.00	0.42
2:B:11:ILE:HG13	2:B:37:ARG:HG2	2.00	0.42
2:B:53:ILE:HG23	6:B:702:PGE:C4	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:HB3	1:A:218:LYS:HB2	2.01	0.42
2:B:435:LEU:HD21	2:B:585:ILE:HG12	2.00	0.42
2:D:9:PHE:HZ	2:D:151:ILE:HD11	1.85	0.42
2:B:9:PHE:HZ	2:B:151:ILE:HD11	1.85	0.41
2:D:246:LEU:HD21	2:D:299:ALA:HB2	2.01	0.41
1:C:200:ILE:CG2	1:C:203:PHE:HB3	2.51	0.41
1:C:133:PHE:CE1	1:C:179:VAL:HG11	2.55	0.41
1:A:201:ASN:HA	1:A:202:PRO:HA	1.90	0.41
1:C:83:LYS:HA	1:C:86:LEU:HD12	2.02	0.41
1:C:20:PRO:HG3	1:C:25:ASP:O	2.21	0.41
1:A:116:GLU:HB2	1:A:204:THR:HG23	2.02	0.41
6:B:703:PGE:H1	10:B:979:HOH:O	2.21	0.41
2:B:246:LEU:HD21	2:B:299:ALA:HB2	2.02	0.41
1:C:197:TYR:HB3	1:C:218:LYS:HB2	2.02	0.40
2:D:35:CYS:SG	2:D:147:GLY:HA2	2.61	0.40
2:D:435:LEU:HD21	2:D:585:ILE:HG12	2.04	0.40
2:D:457:ALA:CB	2:D:542:GLY:HA2	2.51	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	376/421 (89%)	349 (93%)	26 (7%)	1 (0%)	41	41
1	C	404/421 (96%)	382 (95%)	21 (5%)	1 (0%)	47	49
2	B	619/631 (98%)	610 (98%)	9 (2%)	0	100	100
2	D	618/631 (98%)	609 (98%)	9 (2%)	0	100	100
All	All	2017/2104 (96%)	1950 (97%)	65 (3%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	C	31	ASN

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	326/353 (92%)	322 (99%)	4 (1%)	71	77
1	C	342/353 (97%)	338 (99%)	4 (1%)	71	77
2	B	503/511 (98%)	497 (99%)	6 (1%)	71	77
2	D	502/511 (98%)	492 (98%)	10 (2%)	55	60
All	All	1673/1728 (97%)	1649 (99%)	24 (1%)	67	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	SER
1	A	167[A]	LYS
1	A	167[B]	LYS
1	A	234	LEU
2	B	255	LEU
2	B	294	PHE
2	B	455	ASP
2	B	492	ILE
2	B	555	CYS
2	B	613	GLU
1	C	13	ASN
1	C	123	SER
1	C	210	ILE
1	C	234	LEU
2	D	39	SER
2	D	150	ARG
2	D	168	ARG
2	D	255	LEU
2	D	294	PHE
2	D	455	ASP

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Mol	Chain	Res	Type
2	D	459	ARG
2	D	492	ILE
2	D	555	CYS
2	D	613	GLU

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
8	ACT	B	706	-	1,3,3	6.80	1 (100%)	0,3,3	0.00	-
6	PGE	B	702	-	9,9,9	0.18	0	8,8,8	0.51	0
8	ACT	D	703	-	1,3,3	6.24	1 (100%)	0,3,3	0.00	-
9	SIN	D	702	-	1,7,7	0.13	0	2,8,8	0.81	0
3	FLC	C	501	-	3,12,12	0.41	0	3,17,17	0.91	0
5	COA	D	701	-	41,50,50	0.70	1 (2%)	52,75,75	0.76	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	COA	B	701	-	41,50,50	0.61	0	52,75,75	0.74	2 (3%)
7	PG4	B	704	-	12,12,12	0.16	0	11,11,11	0.15	0
6	PGE	B	703	-	9,9,9	0.14	0	8,8,8	0.22	0
8	ACT	B	705	-	1,3,3	4.67	1 (100%)	0,3,3	0.00	-
3	FLC	A	501	-	3,12,12	0.44	0	3,17,17	1.45	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	B	702	-	-	5/7/7/7	-
9	SIN	D	702	-	-	0/1/5/5	-
3	FLC	C	501	-	-	3/6/16/16	-
5	COA	D	701	-	-	3/44/64/64	0/3/3/3
5	COA	B	701	-	-	2/44/64/64	0/3/3/3
7	PG4	B	704	-	-	5/10/10/10	-
6	PGE	B	703	-	-	4/7/7/7	-
3	FLC	A	501	-	-	3/6/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	706	ACT	CH3-C	6.80	1.57	1.48
8	D	703	ACT	CH3-C	6.24	1.56	1.48
8	B	705	ACT	CH3-C	4.67	1.54	1.48
5	D	701	COA	P3B-O8A	-2.02	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	701	COA	P2A-O3A-P1A	2.59	141.71	132.83
3	A	501	FLC	CB-CG-CGC	2.34	118.72	114.98
5	B	701	COA	P2A-O3A-P1A	2.31	140.74	132.83
5	D	701	COA	C5A-C6A-N6A	2.17	123.65	120.35
5	B	701	COA	C5A-C6A-N6A	2.10	123.55	120.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	FLC	CA-CB-CG-CGC
3	C	501	FLC	CBC-CB-CG-CGC
3	C	501	FLC	OHB-CB-CG-CGC
3	A	501	FLC	CA-CB-CG-CGC
6	B	702	PGE	O2-C3-C4-O3
6	B	702	PGE	O3-C5-C6-O4
5	B	701	COA	P1A-O3A-P2A-O6A
3	A	501	FLC	OHB-CB-CG-CGC
7	B	704	PG4	O3-C5-C6-O4
7	B	704	PG4	C8-C7-O4-C6
7	B	704	PG4	C5-C6-O4-C7
5	D	701	COA	C3B-O3B-P3B-O9A
3	A	501	FLC	CBC-CB-CG-CGC
7	B	704	PG4	C3-C4-O3-C5
6	B	703	PGE	C1-C2-O2-C3
6	B	702	PGE	C4-C3-O2-C2
6	B	703	PGE	C3-C4-O3-C5
5	D	701	COA	P1A-O3A-P2A-O6A
6	B	702	PGE	C6-C5-O3-C4
6	B	702	PGE	C3-C4-O3-C5
6	B	703	PGE	O1-C1-C2-O2
5	D	701	COA	CCP-O6A-P2A-O4A
5	B	701	COA	CCP-O6A-P2A-O4A
6	B	703	PGE	O2-C3-C4-O3
7	B	704	PG4	O2-C3-C4-O3

There are no ring outliers.

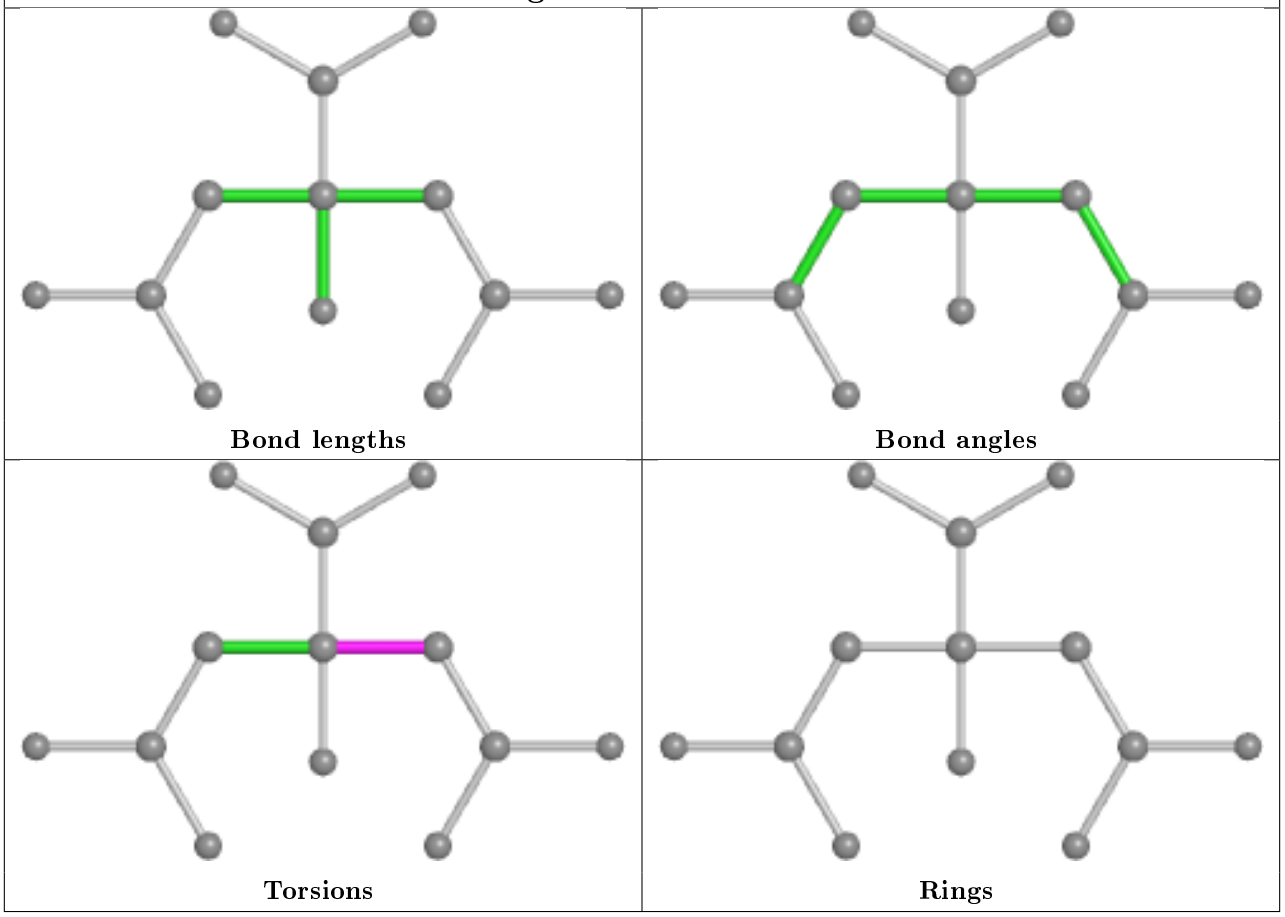
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	702	PGE	1	0
6	B	703	PGE	1	0

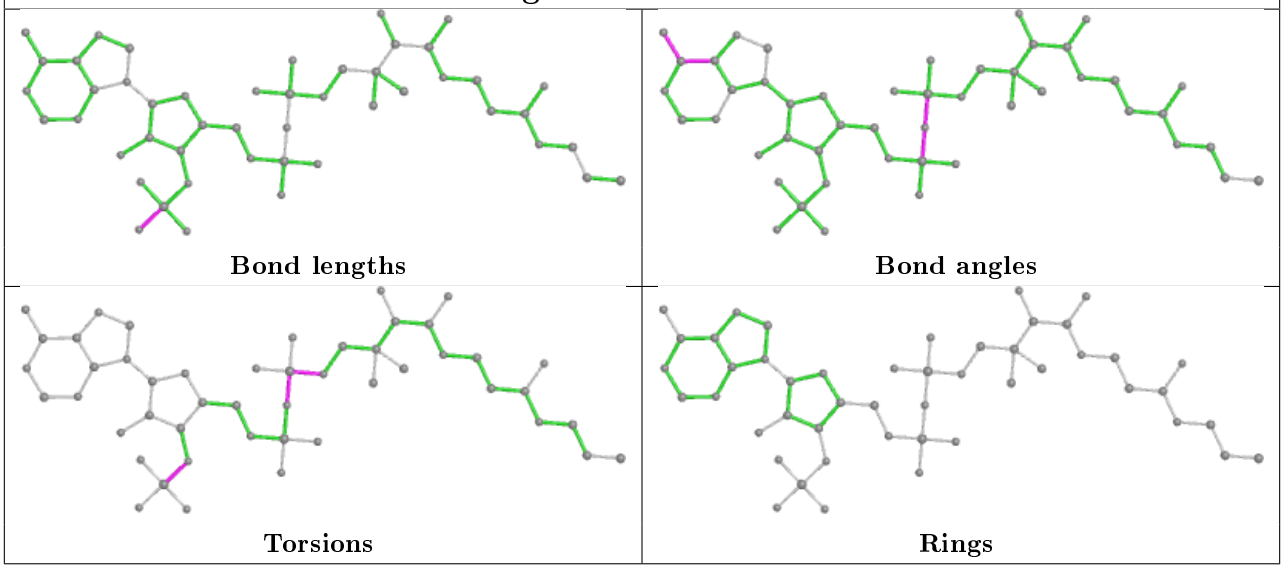
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FLC C 501



Ligand COA D 701



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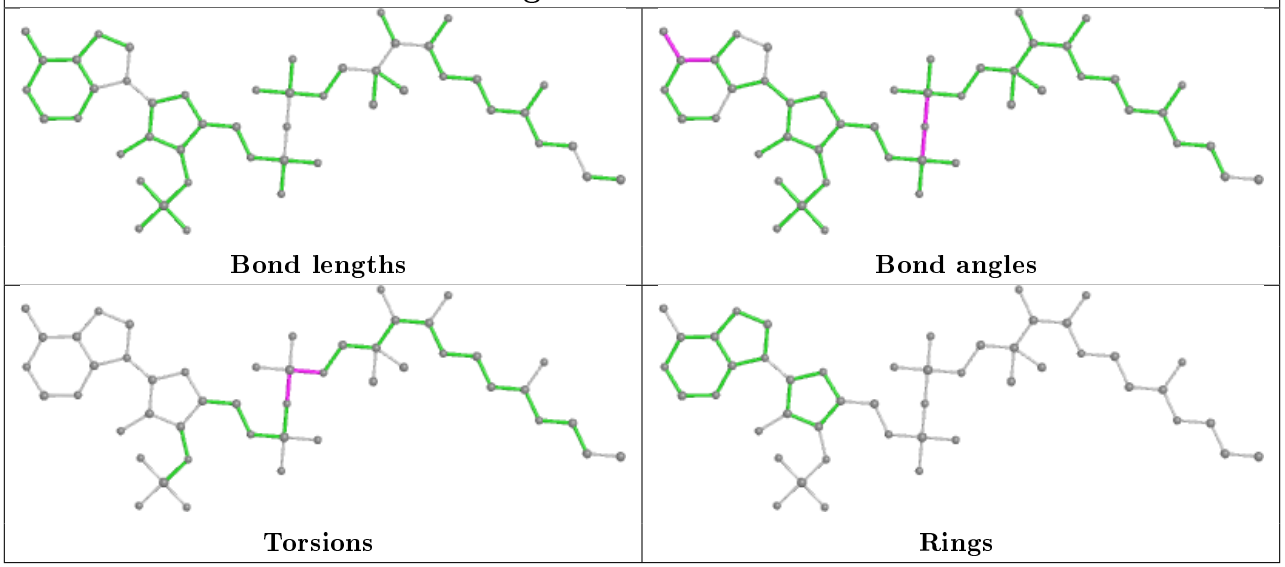

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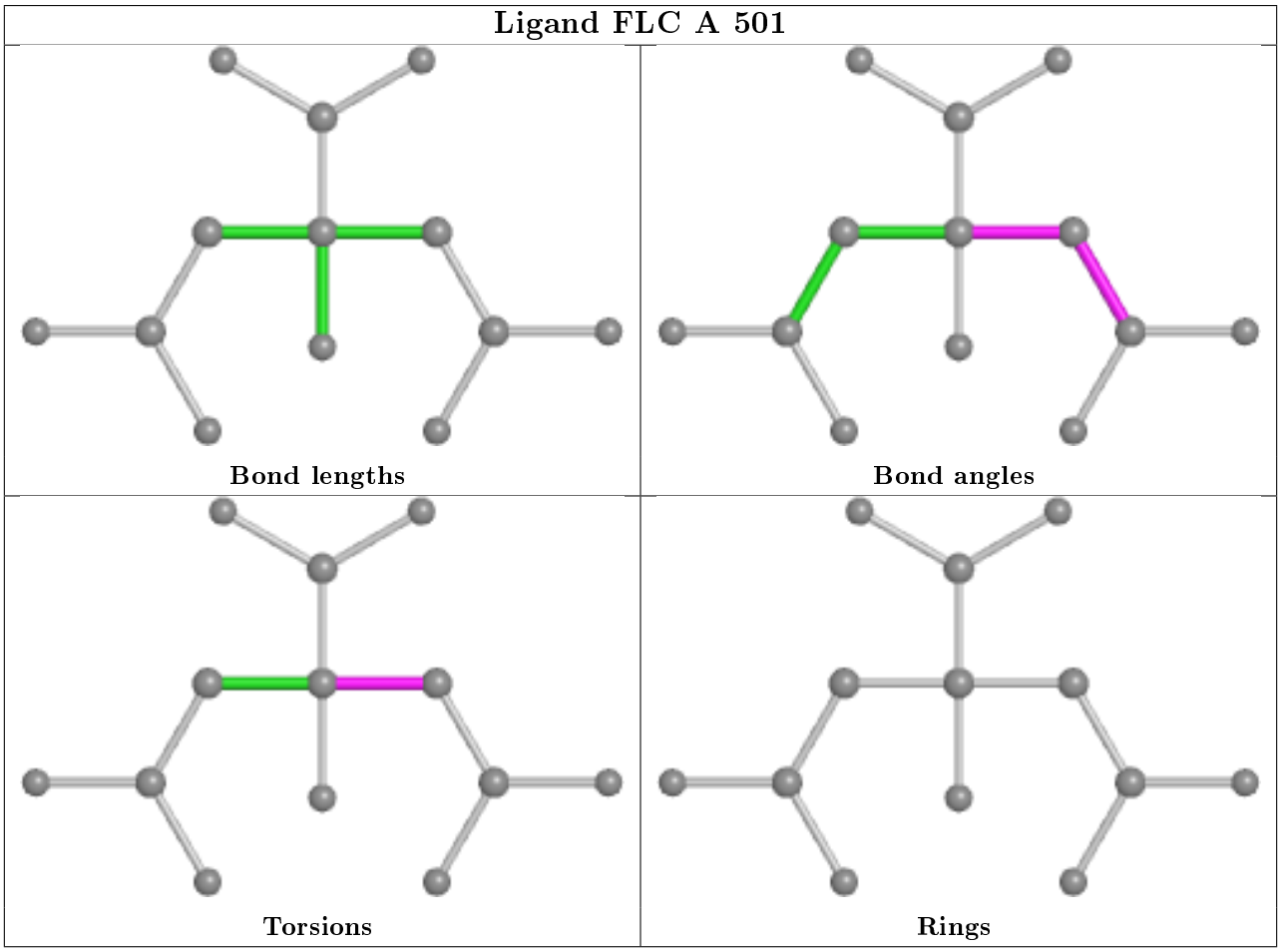

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	381/421 (90%)	1.51	114 (29%) 0 0	49, 84, 124, 164	0
1	C	410/421 (97%)	0.83	80 (19%) 1 1	39, 72, 114, 145	0
2	B	616/631 (97%)	0.43	38 (6%) 20 25	20, 46, 84, 112	0
2	D	616/631 (97%)	0.51	52 (8%) 11 14	17, 51, 98, 163	0
All	All	2023/2104 (96%)	0.74	284 (14%) 2 3	17, 59, 110, 164	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	10.8
1	A	56	LEU	8.9
1	A	105	TYR	8.5
1	A	85	TYR	7.8
1	A	170	ALA	7.6
1	A	75	LEU	7.5
1	A	161	ALA	7.2
1	A	26	PHE	7.1
1	A	82	ALA	7.0
1	A	111	PHE	6.8
1	A	80	GLU	6.8
1	C	100	THR	6.3
1	A	171	GLU	6.0
1	A	60	PRO	6.0
1	C	174	ASP	5.8
1	C	73	VAL	5.8
1	A	23	LEU	5.7
1	A	168	LEU	5.7
1	A	205	PHE	5.6
1	A	76	ASP	5.5
1	A	162	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	90	MET	5.3
1	A	392	LEU	5.3
2	D	325	VAL	5.3
1	A	37	PRO	5.2
1	A	118	TYR	5.0
2	B	325	VAL	4.9
1	A	398	VAL	4.9
1	A	115	LYS	4.8
1	C	86	LEU	4.8
1	A	64	PHE	4.7
1	A	35	VAL	4.6
1	A	119	TYR	4.6
1	C	96	ILE	4.6
1	A	108	ILE	4.5
1	C	396	LEU	4.5
1	A	112	THR	4.5
1	A	77	ALA	4.5
2	B	140	THR	4.4
1	A	28	TYR	4.4
2	D	318	MET	4.4
1	A	32	LEU	4.4
1	A	57	VAL	4.4
1	A	249	LEU	4.3
1	C	74	LEU	4.3
1	A	38	GLU	4.2
1	A	79	TRP	4.2
1	A	233	GLU	4.2
2	B	178	SER	4.1
2	D	141	VAL	4.1
1	A	100	THR	4.1
1	A	331	PRO	4.0
1	A	396	LEU	4.0
1	A	243	THR	4.0
1	C	85	TYR	4.0
1	C	101	GLY	3.9
2	B	294	PHE	3.9
2	D	202	ILE	3.9
1	C	40	ASP	3.9
1	A	74	LEU	3.9
1	A	106	PHE	3.9
1	A	148	VAL	3.9
1	C	64	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	179	VAL	3.8
1	A	169	PRO	3.8
1	A	103	LEU	3.8
2	D	249	LYS	3.8
1	C	240	PHE	3.6
1	A	135	MET	3.6
2	B	297	ALA	3.6
2	D	139	ALA	3.6
2	B	329	ASP	3.6
2	D	112	ILE	3.6
1	A	36	GLY	3.6
2	B	179	GLY	3.5
1	A	371	ILE	3.5
1	C	25	ASP	3.5
2	B	180	GLY	3.5
1	C	281	GLY	3.5
1	A	159	ILE	3.5
2	B	112	ILE	3.5
1	C	282	ALA	3.5
1	C	244	PRO	3.4
1	A	246	LYS	3.4
2	D	319	LEU	3.4
1	A	163[A]	ASP	3.4
1	A	84	GLU	3.4
1	C	58	VAL	3.4
1	C	43	GLY	3.4
1	A	244	PRO	3.3
2	B	243	ILE	3.3
2	D	314	GLN	3.3
2	B	139	ALA	3.3
1	C	331	PRO	3.3
1	A	11	ALA	3.3
1	C	72	LEU	3.3
2	D	140	THR	3.2
1	A	415	LEU	3.2
2	D	247	LYS	3.2
1	A	9	TYR	3.2
2	D	303	ARG	3.2
1	C	366	LEU	3.2
2	B	141	VAL	3.2
1	A	27	SER	3.2
1	A	34	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	34	LEU	3.2
2	B	334	PRO	3.1
1	A	15	LEU	3.1
1	A	114	HIS	3.1
1	A	346	THR	3.1
1	C	169	PRO	3.1
1	A	172	LEU	3.1
1	C	111	PHE	3.1
2	B	384	ILE	3.1
1	A	242	ARG	3.1
2	D	203	GLY	3.1
1	A	373	ILE	3.1
2	D	154	THR	3.1
1	A	174	ASP	3.1
1	C	69	LYS	3.0
1	A	78	ASP	3.0
2	D	179	GLY	3.0
1	A	73	VAL	3.0
2	B	333	VAL	3.0
2	B	182	LEU	3.0
2	D	300	TYR	3.0
1	A	113	PRO	3.0
1	A	22	TYR	3.0
1	A	61	ASP	3.0
1	A	89	LYS	3.0
2	D	326	GLN	3.0
1	C	55	ARG	2.9
1	C	94	VAL	2.9
2	D	151	ILE	2.9
1	A	397	GLY	2.9
1	A	107	LEU	2.9
1	A	58	VAL	2.8
2	D	269	ALA	2.8
1	C	103	LEU	2.8
2	B	202	ILE	2.8
2	D	201	ALA	2.8
1	C	241	GLY	2.8
1	A	133	PHE	2.8
1	C	393	GLY	2.8
2	B	274	GLY	2.8
1	C	38	GLU	2.8
1	C	89	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	201	ALA	2.7
1	A	39	THR	2.7
1	A	109	GLU	2.7
1	C	208	ARG	2.7
1	C	71	GLY	2.7
1	C	280	GLY	2.7
1	C	346	THR	2.7
1	C	249	LEU	2.7
1	A	411	ARG	2.7
2	B	579	GLY	2.7
1	C	139	VAL	2.7
1	C	394	LYS	2.7
1	A	370	ASP	2.7
2	D	76	LEU	2.7
1	A	33	ALA	2.6
1	A	231	TRP	2.6
1	A	253	GLU	2.6
1	C	279	GLY	2.6
1	C	105	TYR	2.6
1	C	161	ALA	2.6
1	A	132	PHE	2.6
1	C	26	PHE	2.6
1	A	324	LEU	2.6
2	D	578	LEU	2.6
1	A	394	LYS	2.6
2	D	496	LYS	2.6
1	A	31	ASN	2.6
2	D	268	PRO	2.6
1	C	90	MET	2.5
2	D	585	ILE	2.5
1	A	345	PHE	2.5
1	C	345	PHE	2.5
2	D	138	PRO	2.5
2	B	324	ILE	2.5
2	D	329	ASP	2.5
1	C	79	TRP	2.5
1	C	285	ILE	2.5
2	D	480	LYS	2.5
2	D	335	ARG	2.5
1	C	173	GLY	2.5
2	D	142	GLY	2.5
1	C	47	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	330	ASN	2.5
1	A	88	GLU	2.5
2	B	577	ALA	2.5
2	D	317	ASP	2.4
1	A	400	ILE	2.4
1	C	371	ILE	2.4
2	D	113	ALA	2.4
2	B	273	PHE	2.4
2	B	154	THR	2.4
1	A	279	GLY	2.4
1	C	138	GLY	2.4
1	C	278	ALA	2.4
1	C	343	ALA	2.4
2	B	578	LEU	2.4
2	B	111	VAL	2.4
1	C	42	GLU	2.4
2	B	204	GLY	2.4
1	C	39	THR	2.4
1	C	205	PHE	2.4
2	B	296	GLN	2.4
2	B	326	GLN	2.4
1	C	344	ASN	2.3
2	D	5	ASP	2.3
2	B	114	GLU	2.3
2	D	200	VAL	2.3
1	C	243	THR	2.3
1	A	330	ASN	2.3
1	C	102	ARG	2.3
1	A	189	PHE	2.3
1	A	202	PRO	2.3
2	B	328	PHE	2.3
1	C	168	LEU	2.3
2	D	313	ARG	2.3
2	D	619	LYS	2.3
2	D	436	ILE	2.3
2	B	277	GLY	2.3
1	A	269	PRO	2.3
2	D	143	GLY	2.3
1	A	149	ILE	2.3
1	A	186	LEU	2.2
1	C	88	GLU	2.2
1	A	16	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	181	MET	2.2
1	A	366	LEU	2.2
2	D	182	LEU	2.2
2	D	297	ALA	2.2
2	D	577	ALA	2.2
2	D	252	THR	2.2
1	A	116	GLU	2.2
2	B	275	HIS	2.2
2	D	111	VAL	2.2
1	C	283	SER	2.2
1	A	343	ALA	2.2
1	C	82	ALA	2.2
2	B	113	ALA	2.2
1	A	234	LEU	2.2
1	C	329	LYS	2.2
2	D	271	VAL	2.2
1	A	65	GLY	2.2
1	C	92	LEU	2.2
1	A	419	GLU	2.2
2	D	135	VAL	2.2
1	C	52	LYS	2.2
1	C	284	VAL	2.2
1	A	175	LYS	2.2
1	C	99	ILE	2.1
2	D	561	GLU	2.1
1	A	369	ALA	2.1
1	C	97	GLY	2.1
1	A	228	LYS	2.1
1	A	267	LEU	2.1
1	C	172	LEU	2.1
1	C	80	GLU	2.1
2	D	495	VAL	2.1
2	D	321	THR	2.1
1	C	151	ILE	2.1
1	A	213	LEU	2.1
1	A	245	SER	2.1
1	C	60	PRO	2.1
1	C	261	SER	2.1
2	B	136	ILE	2.1
1	A	197	TYR	2.1
2	B	385	GLY	2.1
1	A	184	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	148	VAL	2.0
2	D	180	GLY	2.0
1	C	78	ASP	2.0
2	D	178	SER	2.0
1	C	115	LYS	2.0
2	B	138	PRO	2.0
2	D	439	LEU	2.0
1	C	260	ALA	2.0
1	A	203	PHE	2.0
2	D	176	SER	2.0
1	C	108	ILE	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 carbohydrates 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
8	ACT	D	703	4/4	0.72	0.23	60,64,66,66	0
9	SIN	D	702	8/8	0.80	0.28	67,71,80,82	0
8	ACT	B	706	4/4	0.84	0.32	61,66,67,72	0
4	NA	C	502	1/1	0.90	0.19	41,41,41,41	0
7	PG4	B	704	13/13	0.91	0.16	54,60,67,70	0
3	FLC	A	501	13/13	0.91	0.28	61,64,76,78	0
8	ACT	B	705	4/4	0.91	0.16	67,69,69,70	0
6	PGE	B	703	10/10	0.92	0.18	43,52,60,60	0
4	NA	A	502	1/1	0.93	0.10	46,46,46,46	0
6	PGE	B	702	10/10	0.95	0.10	43,46,48,49	0
3	FLC	C	501	13/13	0.95	0.34	45,53,63,64	0
5	COA	D	701	48/48	0.95	0.14	41,51,58,68	0

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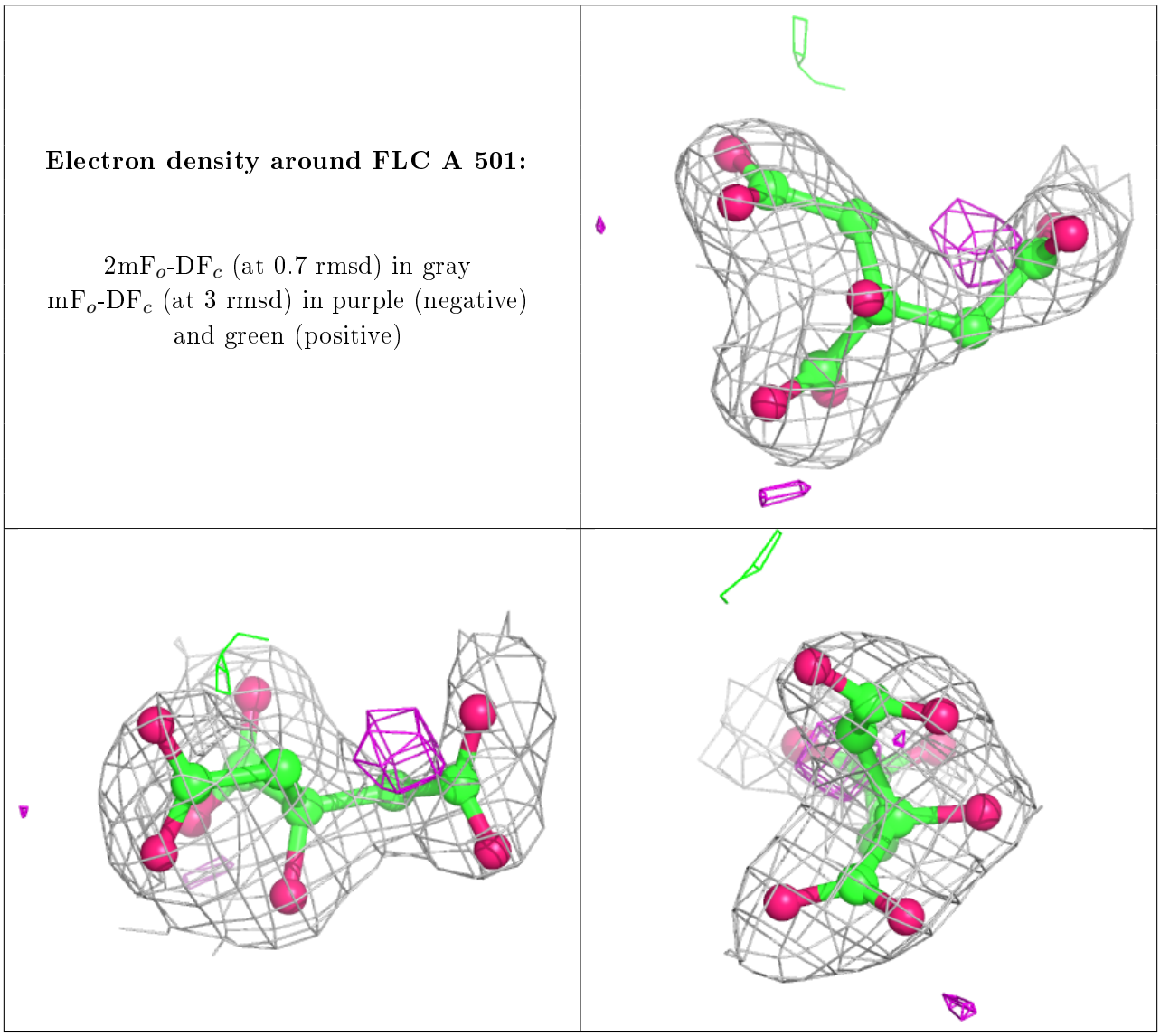
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	COA	B	701	48/48	0.95	0.14	29,40,51,58	0

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.

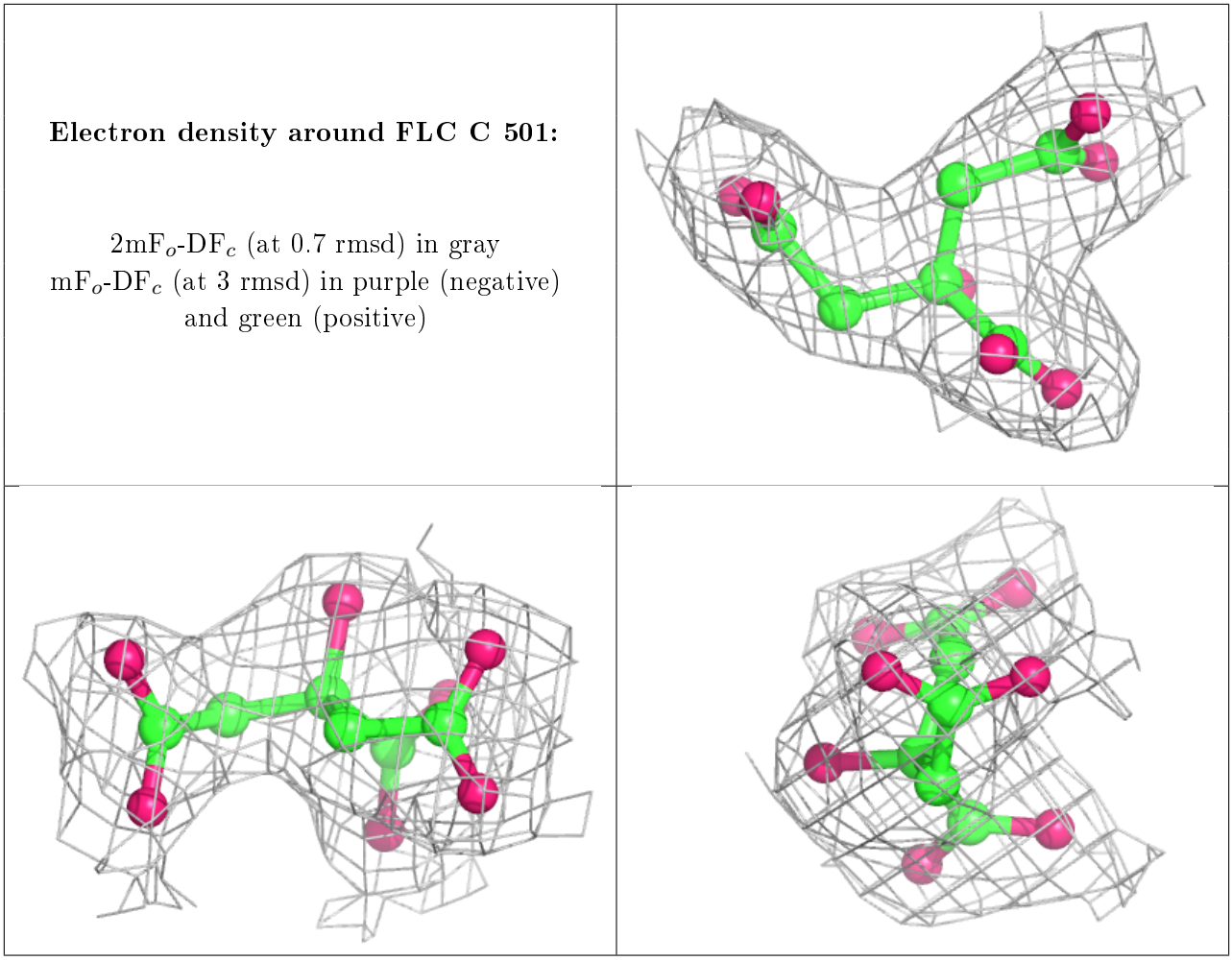
Electron density around FLC A 501:

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



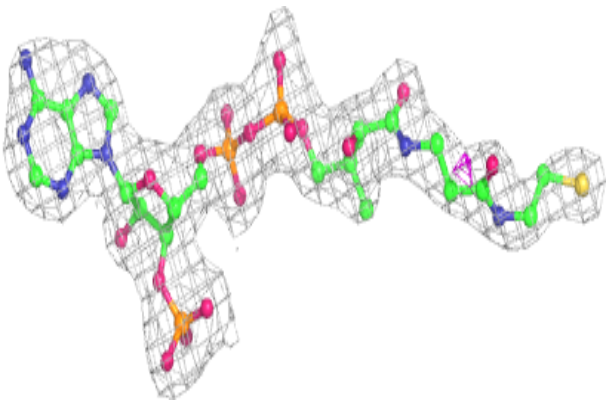
Electron density around FLC C 501:

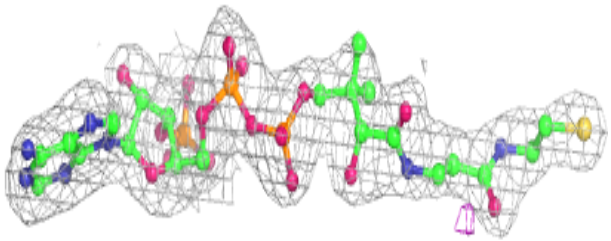
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

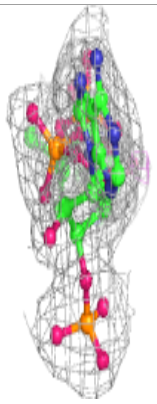


Electron density around COA D 701:

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

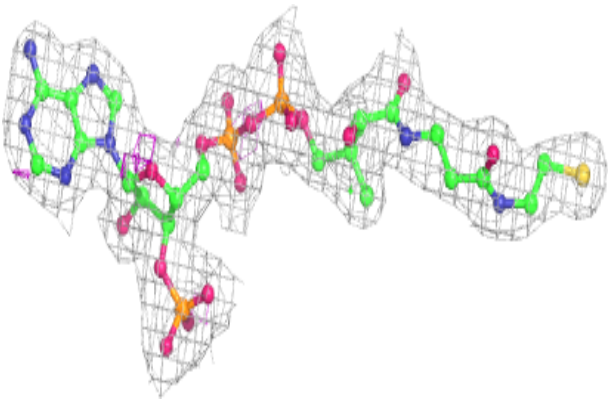


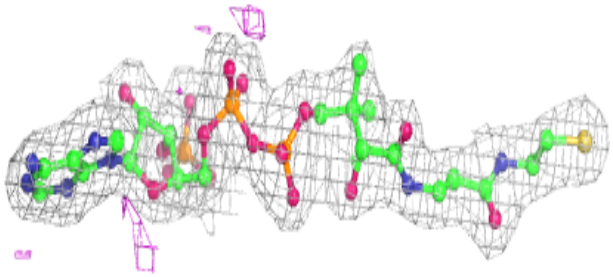


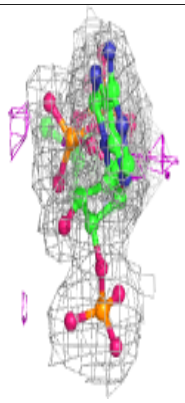


Electron density around COA B 701:

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







6.5 Other polymers (i)

There are no such residues in this entry.