



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:35 AM UTC

PDB ID : 6HXI / pdb_00006hxi
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

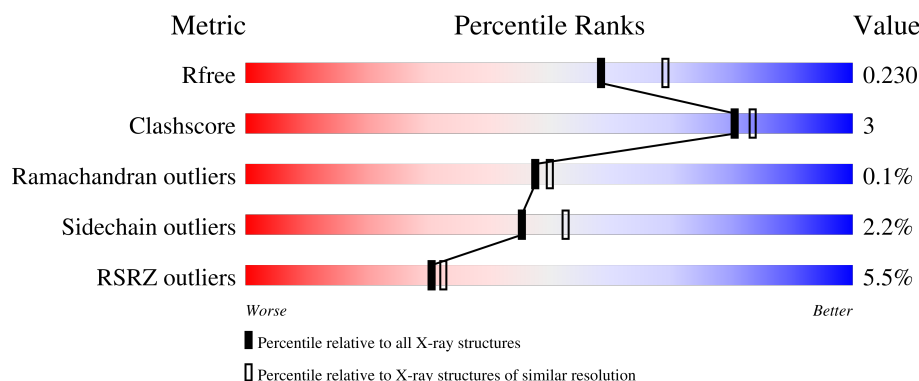
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	14% 80% 10% 10%
1	C	421	7% 84% 13% ..
2	B	631	% 89% 9% .
2	D	631	3% 90% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	SIN	D	702	-	X	-	-

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:

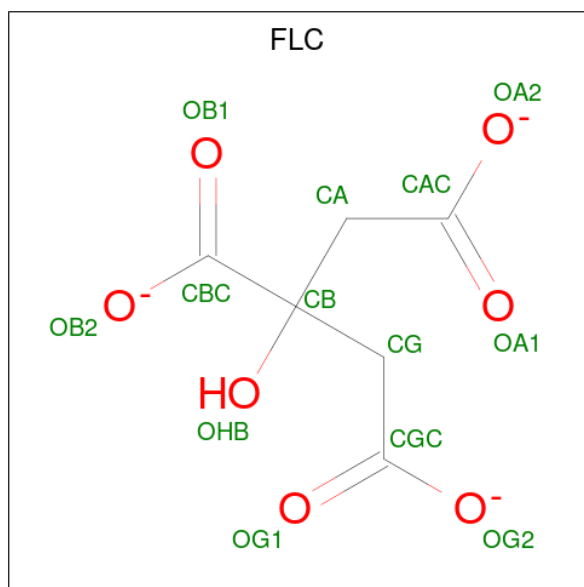
Chain	Residue	Modelled	Actual	Comment	Reference
B	623	GLY	-	expression tag	UNP A0A1V4VDZ9
B	624	GLY	-	expression tag	UNP A0A1V4VDZ9
B	625	SER	-	expression tag	UNP A0A1V4VDZ9
B	626	HIS	-	expression tag	UNP A0A1V4VDZ9
B	627	HIS	-	expression tag	UNP A0A1V4VDZ9
B	628	HIS	-	expression tag	UNP A0A1V4VDZ9
B	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 (CCD ID: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by depositor).

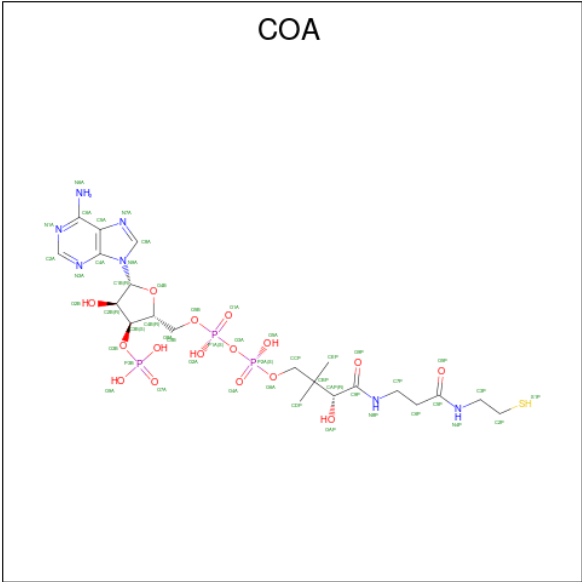


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

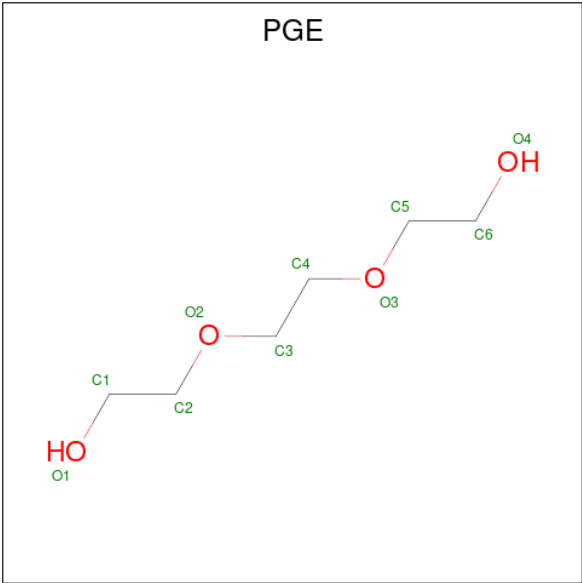
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

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



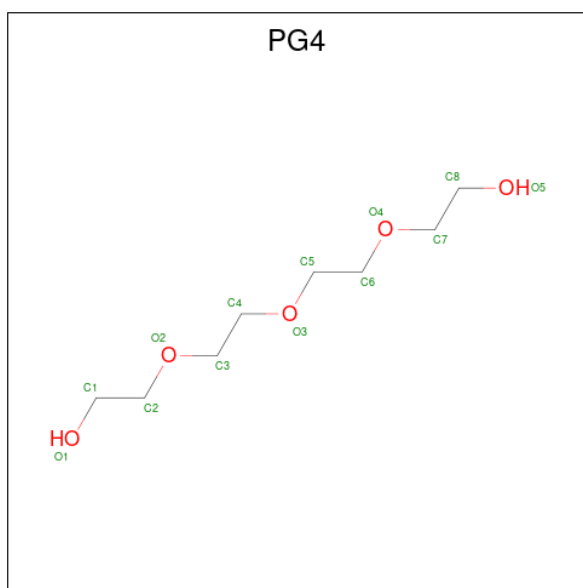
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



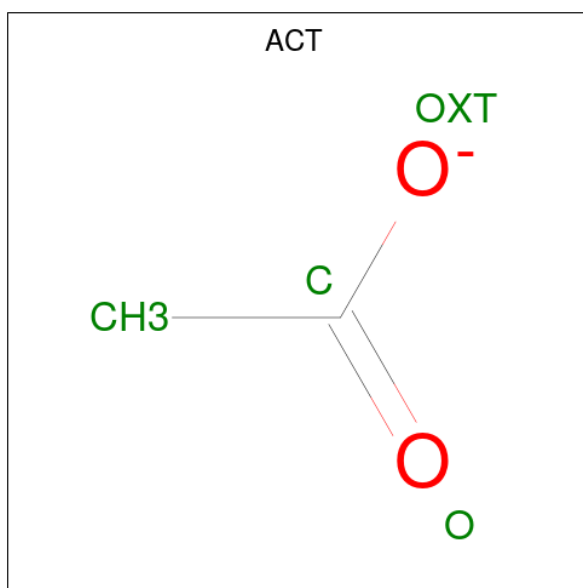
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



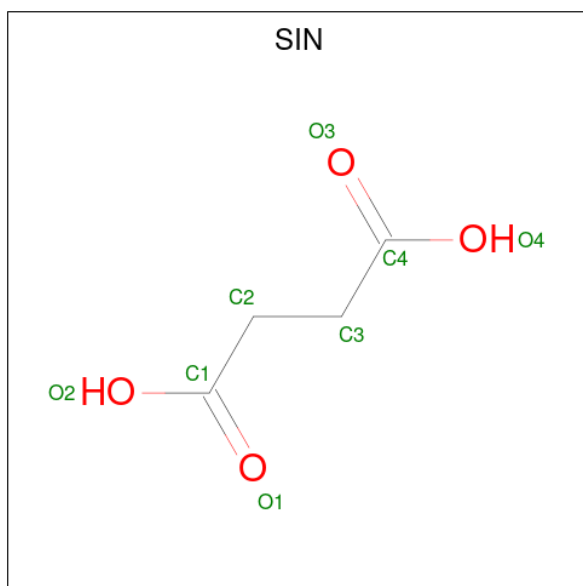
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 9 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



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

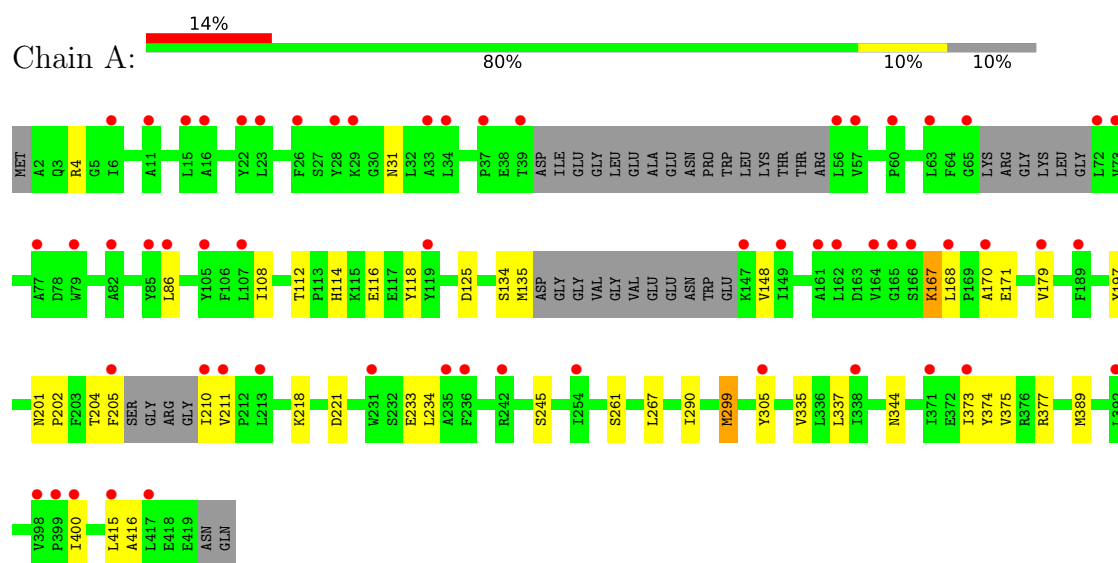
- Molecule 10 is water.

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

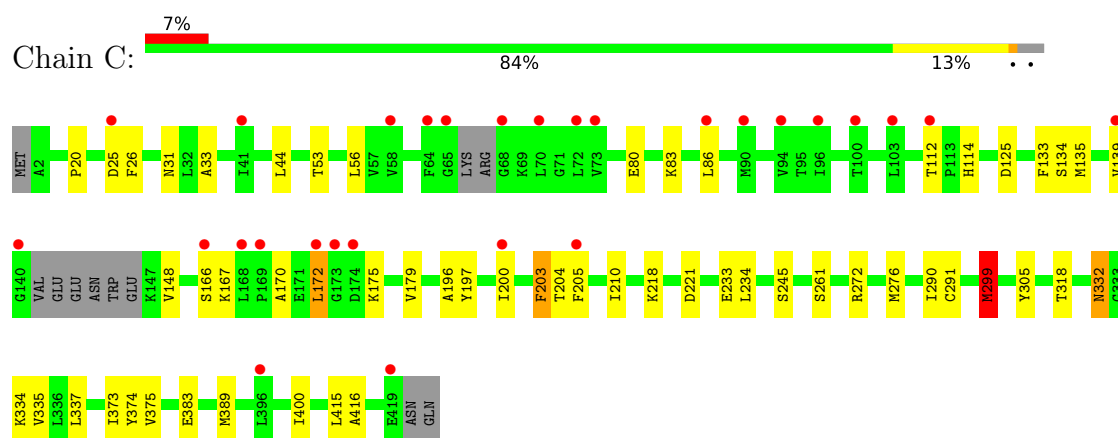
3 Residue-property plots [i](#)

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.

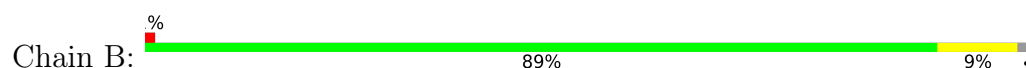
- Molecule 1: Citrate lyase, subunit 1



- Molecule 1: Citrate lyase, subunit 1

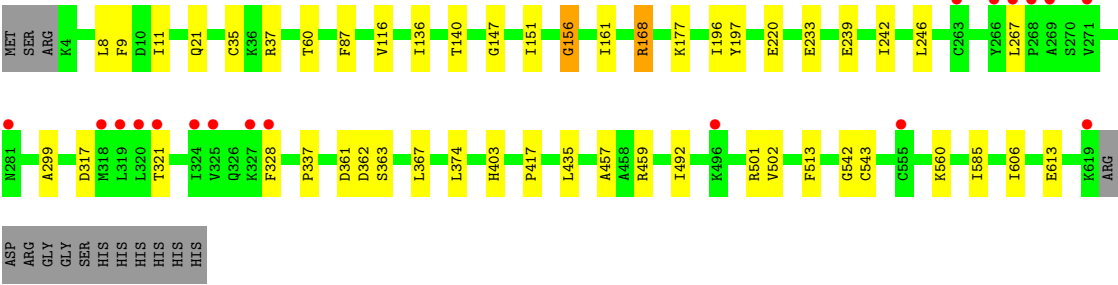
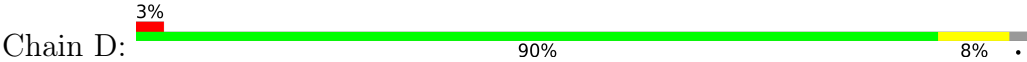


- Molecule 2: Succinyl-CoA ligase (ADP-forming) subunit alpha





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



4 Data and refinement statistics

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 30.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.75-2.10) 99.4 (30.75-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.179 , 0.208 0.200 , 0.230	Depositor DCC
R_{free} test set	6963 reflections (5.00%)	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)	0.33 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PG4, ACT, NA, FLC, COA, 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	0.80	1/3122 (0.0%)	1.30	10/4225 (0.2%)
1	C	0.80	1/3301 (0.0%)	1.32	13/4469 (0.3%)
2	B	0.92	1/4863 (0.0%)	1.27	13/6563 (0.2%)
2	D	0.91	1/4852 (0.0%)	1.27	10/6549 (0.2%)
All	All	0.87	4/16138 (0.0%)	1.29	46/21806 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	212	MET	SD-CE	-6.17	1.64	1.79
1	A	211	VAL	CA-C	6.08	1.56	1.52
2	D	116	VAL	CA-C	5.34	1.57	1.53
1	C	299	MET	SD-CE	-5.08	1.66	1.79

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	328	PHE	CA-CB-CG	7.91	121.71	113.80
1	C	166	SER	CA-C-N	7.47	132.02	122.16
1	C	166	SER	C-N-CA	7.47	132.02	122.16
1	C	332	ASN	CA-CB-CG	7.29	119.89	112.60
2	B	197	TYR	N-CA-C	-7.17	101.72	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	197	TYR	N-CA-C	-6.98	101.99	112.04
1	C	221	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	221	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	210	ILE	CA-C-N	6.58	129.05	123.33
1	A	210	ILE	C-N-CA	6.58	129.05	123.33
1	A	125	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	26	PHE	N-CA-C	-6.40	105.22	113.16
1	C	203	PHE	CA-CB-CG	6.31	120.11	113.80
1	C	125	ASP	CA-CB-CG	6.11	118.71	112.60
2	B	456	ASP	CA-CB-CG	6.06	118.66	112.60
2	B	560	LYS	CA-C-N	5.99	128.23	120.44
2	B	560	LYS	C-N-CA	5.99	128.23	120.44
2	D	560	LYS	CA-C-N	5.76	127.93	120.44
2	D	560	LYS	C-N-CA	5.76	127.93	120.44
1	C	245	SER	CA-C-N	5.75	127.99	120.28
1	C	245	SER	C-N-CA	5.75	127.99	120.28
1	C	112	THR	CB-CA-C	5.72	115.83	110.17
2	D	513	PHE	CA-CB-CG	5.55	119.35	113.80
2	D	156	GLY	N-CA-C	5.48	121.21	111.02
2	B	602	PRO	CA-C-N	5.40	127.78	120.38
2	B	602	PRO	C-N-CA	5.40	127.78	120.38
1	A	245	SER	CA-C-N	5.40	127.51	120.28
1	A	245	SER	C-N-CA	5.40	127.51	120.28
2	B	501	ARG	CA-C-N	5.36	127.42	120.56
2	B	501	ARG	C-N-CA	5.36	127.42	120.56
2	D	362	ASP	CA-C-N	5.31	127.40	120.28
2	D	362	ASP	C-N-CA	5.31	127.40	120.28
1	A	377	ARG	CA-C-N	5.30	127.10	121.48
1	A	377	ARG	C-N-CA	5.30	127.10	121.48
1	A	112	THR	CB-CA-C	5.28	115.40	110.17
2	D	501	ARG	CA-C-N	5.28	127.31	120.56
2	D	501	ARG	C-N-CA	5.28	127.31	120.56
2	B	513	PHE	CA-CB-CG	5.21	119.00	113.80
1	C	56	LEU	CA-C-N	5.11	130.16	122.75
1	C	56	LEU	C-N-CA	5.11	130.16	122.75
2	B	194	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	211	VAL	N-CA-C	5.10	113.68	107.61
2	B	156	GLY	N-CA-C	5.09	120.50	111.02
1	C	196	ALA	N-CA-C	-5.01	107.56	113.97
2	B	441	SER	CA-C-N	5.01	125.40	119.94
2	B	441	SER	C-N-CA	5.01	125.40	119.94

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	19	0
1	C	3231	0	3173	23	0
2	B	4775	0	4848	23	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	84	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 3.

All (84) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:375:VAL:HG21	1:C:389:MET:HE2	1.80	0.64
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:375:VAL:HG21	1:A:389:MET:HE2	1.82	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
1:A:290:ILE:HB	1:A:299:MET:HE2	1.88	0.56
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
1:C:135:MET:HE1	1:C:170:ALA:HB3	1.93	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
1:A:167[A]:LYS:HZ1	1:A:179:VAL:HB	1.78	0.49
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
1:A:135:MET:HE1	1:A:170:ALA:HB3	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
2:B:177:LYS:HG3	2:B:212:MET:HE3	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:C:290:ILE:HB	1:C:299:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:267:LEU:HD13	2:D:267:LEU:HD22	2.00	0.43
2:B:361:ASP:OD1	2:B:363:SER:HB2	2.19	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
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
1:C:291:CYS:SG	1:C:299:MET:HE1	2.59	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
2:B:227:MET:HE1	2:B:312:VAL:HG13	2.02	0.41
6:B:703:PGE:H1	10:B:979:HOH:O	2.21	0.41
2:B:212:MET:HE1	2:B:232:GLY:HA2	2.02	0.41
2:B:246:LEU:HD21	2:B:299:ALA:HB2	2.02	0.41
1:C:276:MET:HE1	1:C:318:THR:HG23	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	36	36
1	C	404/421 (96%)	382 (95%)	21 (5%)	1 (0%)	43	44
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%)	48	50

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/353 (92%)	317 (97%)	9 (3%)	38	43
1	C	342/353 (97%)	331 (97%)	11 (3%)	34	38
2	B	503/511 (98%)	493 (98%)	10 (2%)	48	56
2	D	502/511 (98%)	495 (99%)	7 (1%)	59	67
All	All	1673/1728 (97%)	1636 (98%)	37 (2%)	45	53

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	167[A]	LYS
1	A	167[B]	LYS
1	A	168	LEU
1	A	171	GLU
1	A	233	GLU
1	A	234	LEU
1	A	299	MET
1	A	415	LEU
2	B	161	ILE
2	B	168	ARG
2	B	196	ILE
2	B	220	GLU
2	B	455	ASP
2	B	492	ILE
2	B	500	LYS
2	B	555	CYS
2	B	584	LEU
2	B	613	GLU
1	C	53	THR
1	C	139	VAL
1	C	167	LYS
1	C	172	LEU
1	C	210	ILE
1	C	233	GLU
1	C	234	LEU
1	C	299	MET
1	C	332	ASN
1	C	383	GLU
1	C	415	LEU
2	D	161	ILE
2	D	168	ARG
2	D	196	ILE
2	D	220	GLU
2	D	459	ARG
2	D	492	ILE
2	D	613	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	87	ASN
1	A	227	GLN
1	A	330	ASN
1	A	363	GLN
1	A	367	GLN
2	B	314	GLN
1	C	3	GLN
1	C	87	ASN
1	C	227	GLN
1	C	330	ASN
1	C	363	GLN
1	C	367	GLN
1	C	381	ASN
1	C	408	HIS
2	D	314	GLN
2	D	524	GLN
2	D	573	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
5	COA	D	701	-	47,50,50	0.56	1 (2%)	69,75,75	0.53	0
6	PGE	B	703	-	9,9,9	0.13	0	8,8,8	0.22	0
6	PGE	B	702	-	9,9,9	0.18	0	8,8,8	0.51	0
7	PG4	B	704	-	12,12,12	0.16	0	11,11,11	0.15	0
8	ACT	B	706	-	3,3,3	1.56	1 (33%)	3,3,3	0.78	0
9	SIN	D	702	-	7,7,7	2.15	4 (57%)	8,8,8	2.05	4 (50%)
3	FLC	A	501	-	12,12,12	1.12	0	17,17,17	1.17	1 (5%)
3	FLC	C	501	-	12,12,12	1.02	0	17,17,17	1.24	2 (11%)
8	ACT	B	705	-	3,3,3	1.10	0	3,3,3	0.99	0
8	ACT	D	703	-	3,3,3	1.43	0	3,3,3	0.93	0
5	COA	B	701	-	47,50,50	0.43	0	69,75,75	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	COA	D	701	-	-	2/48/64/64	0/3/3/3
6	PGE	B	703	-	-	4/7/7/7	-
6	PGE	B	702	-	-	5/7/7/7	-
7	PG4	B	704	-	-	4/10/10/10	-
9	SIN	D	702	-	-	4/5/5/5	-
3	FLC	A	501	-	-	4/16/16/16	-
3	FLC	C	501	-	-	3/16/16/16	-
5	COA	B	701	-	-	1/48/64/64	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	702	SIN	O1-C1	3.28	1.32	1.22
9	D	702	SIN	O3-C4	3.06	1.32	1.22
9	D	702	SIN	O4-C4	-2.57	1.22	1.30
9	D	702	SIN	O2-C1	-2.35	1.23	1.30
8	B	706	ACT	CH3-C	2.11	1.57	1.49
5	D	701	COA	P3B-O8A	-2.08	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	702	SIN	O3-C4-C3	-2.93	113.81	123.09
9	D	702	SIN	O4-C4-C3	2.88	123.11	114.00
9	D	702	SIN	O1-C1-C2	-2.88	113.95	123.09
9	D	702	SIN	O2-C1-C2	2.88	123.09	114.00
3	C	501	FLC	OB1-CBC-CB	-2.71	116.85	122.09
3	C	501	FLC	OB2-CBC-CB	2.33	117.60	113.14
3	A	501	FLC	OB1-CBC-CB	-2.19	117.85	122.09

There are no chirality outliers.

All (27) torsion outliers are listed below:

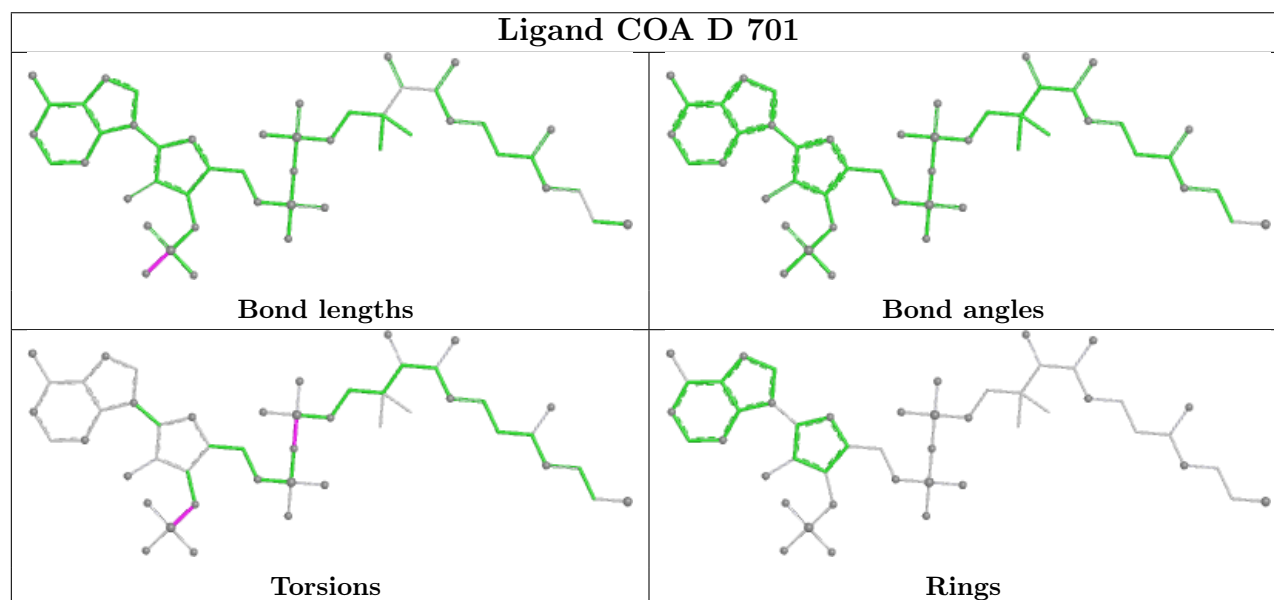
Mol	Chain	Res	Type	Atoms
3	C	501	FLC	CA-CB-CG-CGC
3	C	501	FLC	CBC-CB-CG-CGC
3	A	501	FLC	CA-CB-CG-CGC
3	C	501	FLC	OHB-CB-CG-CGC
3	A	501	FLC	CBC-CB-CG-CGC
6	B	702	PGE	O2-C3-C4-O3
6	B	702	PGE	O3-C5-C6-O4
5	B	701	COA	P1A-O3A-P2A-O6A
7	B	704	PG4	C8-C7-O4-C6
7	B	704	PG4	C5-C6-O4-C7
7	B	704	PG4	O3-C5-C6-O4
3	A	501	FLC	OHB-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
9	D	702	SIN	C2-C3-C4-O4
9	D	702	SIN	O1-C1-C2-C3
9	D	702	SIN	C2-C3-C4-O3
9	D	702	SIN	O2-C1-C2-C3
5	D	701	COA	P1A-O3A-P2A-O6A
6	B	703	PGE	C3-C4-O3-C5
6	B	703	PGE	O1-C1-C2-O2
5	D	701	COA	C3B-O3B-P3B-O9A
6	B	702	PGE	C6-C5-O3-C4
6	B	702	PGE	C3-C4-O3-C5
3	A	501	FLC	CB-CA-CAC-OA1
6	B	703	PGE	O2-C3-C4-O3

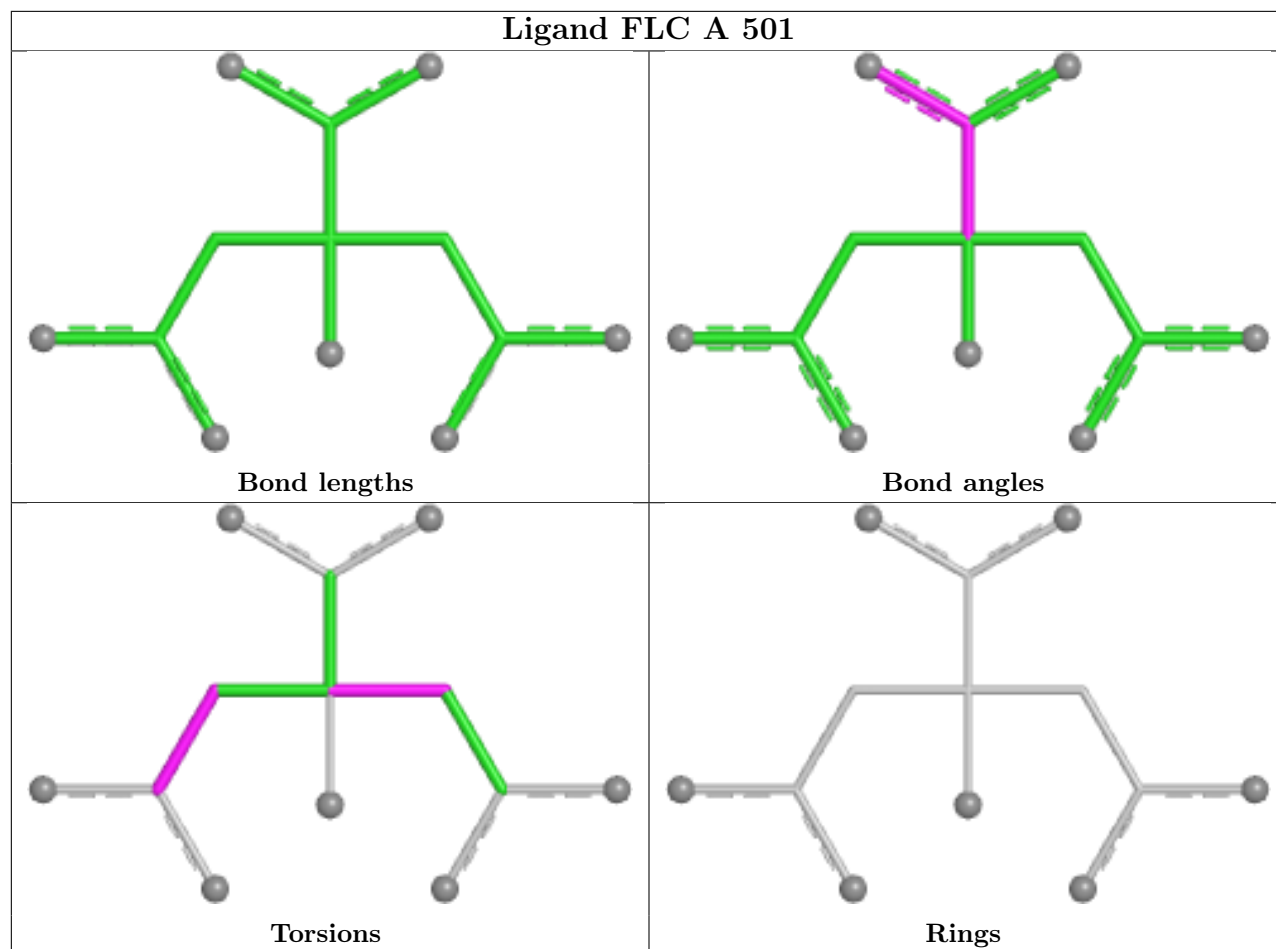
There are no ring outliers.

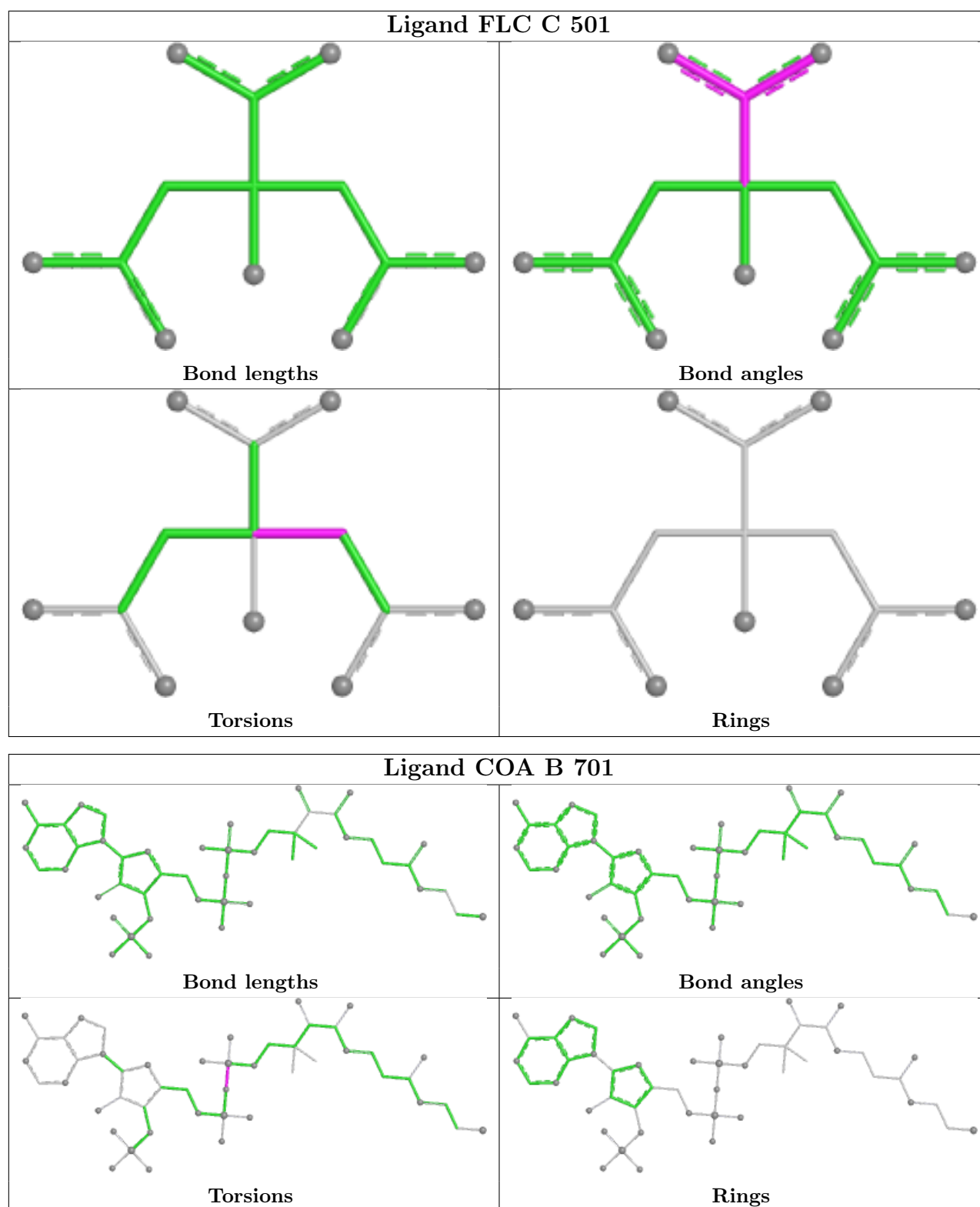
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	703	PGE	1	0
6	B	702	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	381/421 (90%)	1.06	58 (15%) 5 5	43, 82, 124, 164	5 (1%)
1	C	410/421 (97%)	0.59	28 (6%) 23 25	39, 72, 114, 145	0
2	B	616/631 (97%)	-0.14	7 (1%) 78 80	19, 46, 84, 112	5 (0%)
2	D	616/631 (97%)	0.05	18 (2%) 53 56	17, 51, 98, 163	4 (0%)
All	All	2023/2104 (96%)	0.29	111 (5%) 30 32	17, 59, 110, 164	14 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166[A]	SER	7.5
1	A	65	GLY	5.2
1	C	65	GLY	5.1
1	C	140	GLY	4.9
1	A	165[A]	GLY	4.2
1	C	41	ILE	4.2
1	C	68	GLY	4.1
1	A	170	ALA	4.0
1	A	205	PHE	3.9
1	A	371	ILE	3.8
1	A	168	LEU	3.7
1	A	16	ALA	3.5
1	A	86	LEU	3.4
1	C	139	VAL	3.4
2	D	269	ALA	3.4
1	A	72	LEU	3.3
1	C	172	LEU	3.3
1	A	39	THR	3.2
2	D	268	PRO	3.2
1	C	96	ILE	3.1
1	C	169	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	73	VAL	3.1
1	C	70	LEU	3.1
1	A	392	LEU	3.1
1	A	26	PHE	3.0
1	C	86	LEU	3.0
1	A	28	TYR	3.0
2	D	271	VAL	3.0
1	A	210	ILE	2.9
1	A	119	TYR	2.9
1	A	235	ALA	2.9
1	A	105	TYR	2.9
1	C	25	ASP	2.8
1	A	11	ALA	2.8
1	A	164[A]	VAL	2.8
1	C	173	GLY	2.8
2	D	266	TYR	2.8
2	D	619	LYS	2.7
1	A	56	LEU	2.7
1	A	107	LEU	2.7
1	C	100	THR	2.7
1	A	400	ILE	2.7
1	A	63	LEU	2.7
1	A	417	LEU	2.7
1	A	373	ILE	2.7
2	D	555	CYS	2.7
1	A	79	TRP	2.7
1	A	189	PHE	2.6
2	D	281	ASN	2.6
1	A	179	VAL	2.6
1	A	161	ALA	2.6
1	A	15	LEU	2.6
1	A	398	VAL	2.6
2	B	618	CYS	2.6
2	D	320	LEU	2.5
1	A	23	LEU	2.5
2	B	619	LYS	2.5
1	A	415	LEU	2.5
1	C	58	VAL	2.4
2	B	555	CYS	2.4
1	A	60	PRO	2.4
1	A	34	LEU	2.4
2	D	318	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	213	LEU	2.4
2	D	321	THR	2.4
1	A	399	PRO	2.4
1	A	82	ALA	2.4
1	A	162	LEU	2.4
1	A	236	PHE	2.4
1	A	6	ILE	2.4
1	A	77	ALA	2.3
1	A	338	ILE	2.3
2	B	324	ILE	2.3
2	D	324	ILE	2.3
2	B	297	ALA	2.3
2	D	328	PHE	2.3
1	A	211	VAL	2.3
1	A	231	TRP	2.3
2	D	496	LYS	2.3
1	C	168	LEU	2.3
1	A	57	VAL	2.2
2	D	319	LEU	2.2
1	A	242	ARG	2.2
1	C	200	ILE	2.2
1	A	33	ALA	2.2
1	C	396	LEU	2.2
1	C	64	PHE	2.1
2	B	325	VAL	2.1
2	B	4	LYS	2.1
1	C	94	VAL	2.1
1	C	72	LEU	2.1
2	D	327	LYS	2.1
2	D	263	CYS	2.1
1	C	174	ASP	2.1
1	A	85	TYR	2.1
1	A	22	TYR	2.1
1	A	37	PRO	2.1
1	A	305	TYR	2.1
1	A	147	LYS	2.1
1	A	73	VAL	2.1
2	D	325	VAL	2.1
1	C	419	GLU	2.0
1	C	103	LEU	2.0
1	A	149	ILE	2.0
1	A	254	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	205	PHE	2.0
1	C	90	MET	2.0
1	C	166	SER	2.0
2	D	267	LEU	2.0
1	A	29	LYS	2.0
1	C	112	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

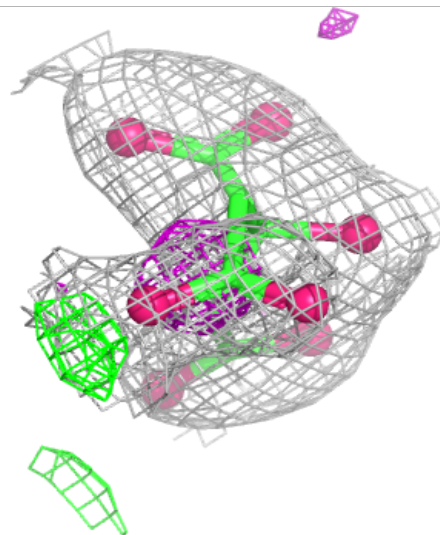
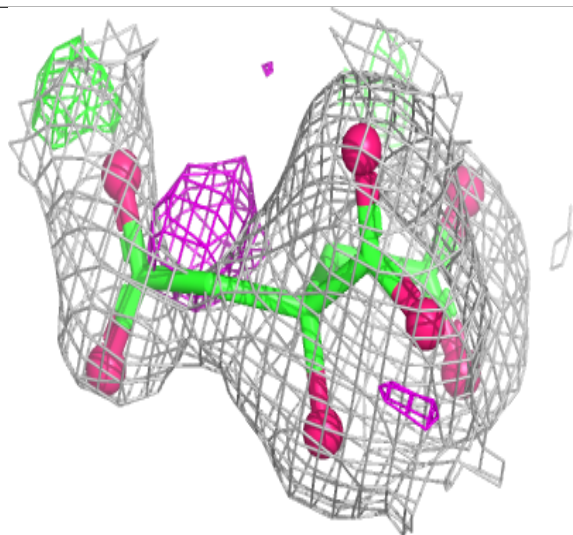
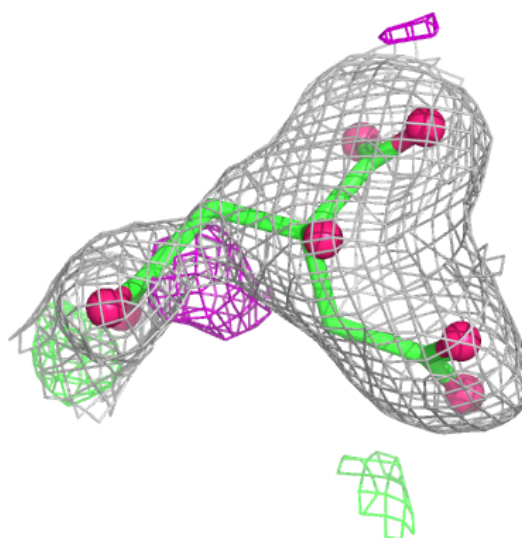
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	ACT	B	706	4/4	0.68	0.21	61,66,67,72	0
8	ACT	D	703	4/4	0.73	0.19	60,64,66,66	0
8	ACT	B	705	4/4	0.80	0.12	67,69,69,70	0
9	SIN	D	702	8/8	0.82	0.15	67,71,80,82	0
3	FLC	A	501	13/13	0.86	0.11	61,64,76,78	0
7	PG4	B	704	13/13	0.88	0.11	54,60,67,70	0
6	PGE	B	703	10/10	0.91	0.11	43,52,60,60	0
3	FLC	C	501	13/13	0.92	0.09	45,53,63,64	0
4	NA	C	502	1/1	0.94	0.07	41,41,41,41	0
4	NA	A	502	1/1	0.96	0.06	46,46,46,46	0
5	COA	D	701	48/48	0.96	0.07	41,51,58,68	0
6	PGE	B	702	10/10	0.96	0.06	43,46,48,49	0
5	COA	B	701	48/48	0.97	0.05	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.

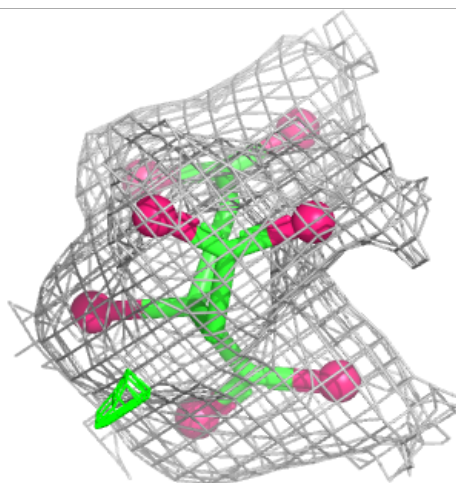
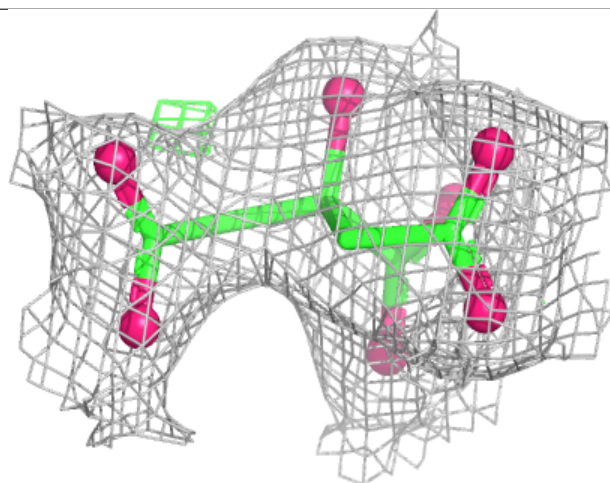
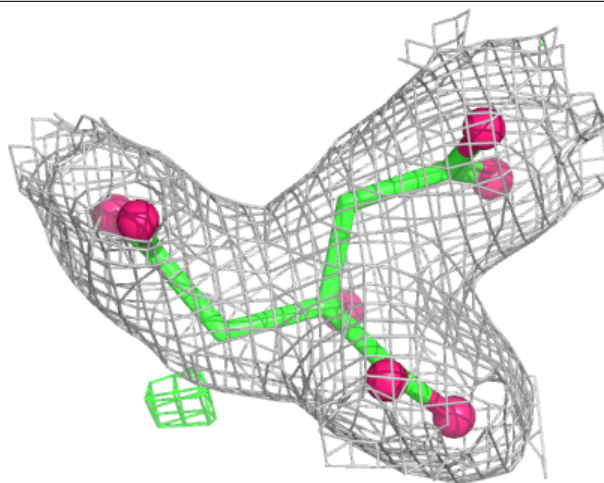
Electron density around FLC A 501:

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



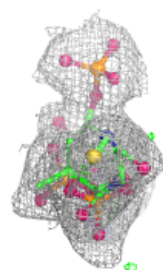
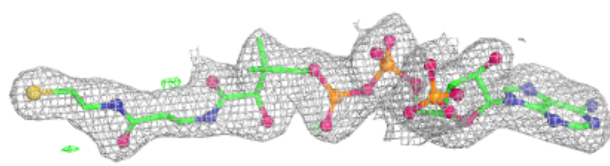
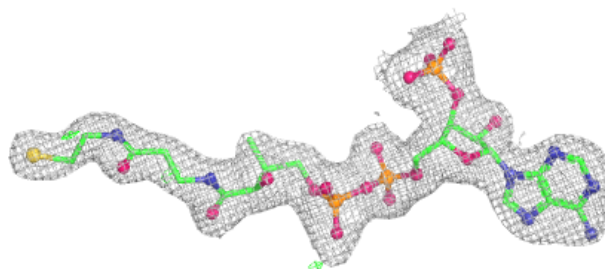
Electron density around FLC C 501:

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

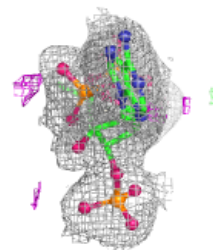
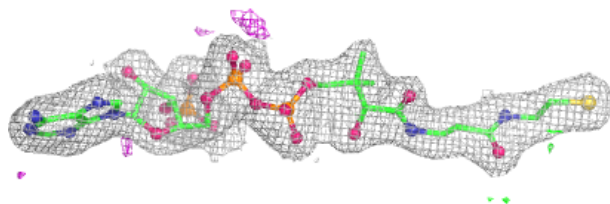
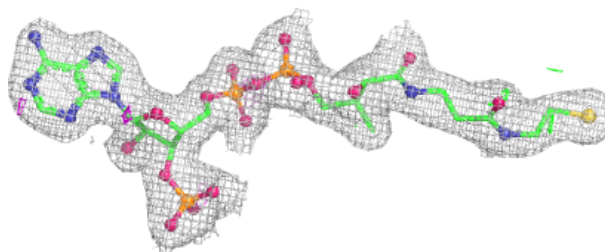


Electron density around COA D 701:

$2mF_o-DF_c$ (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.