



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:24 PM UTC

PDB ID : 5MAC / pdb_00005mac
Title : Crystal structure of decameric Methanococcoides burtonii Rubisco complexed with 2-carboxyarabinitol biphosphate
Authors : Gunn, L.H.; Valegard, K.; Andersson, I.
Deposited on : 2016-11-03
Resolution : 2.60 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)
Xtrriage (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

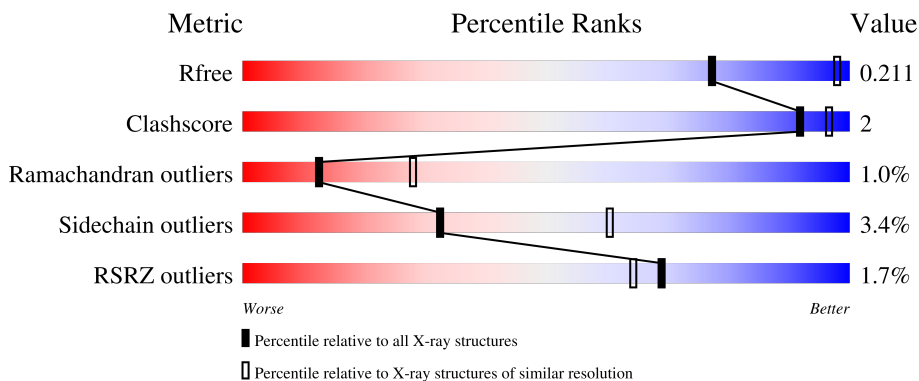
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	474	 90% 9% .
1	B	474	 88% 11% .
1	C	474	 90% 9% .
1	D	474	 89% 10% .
1	E	474	 90% 9% .

2 Entry composition [i](#)

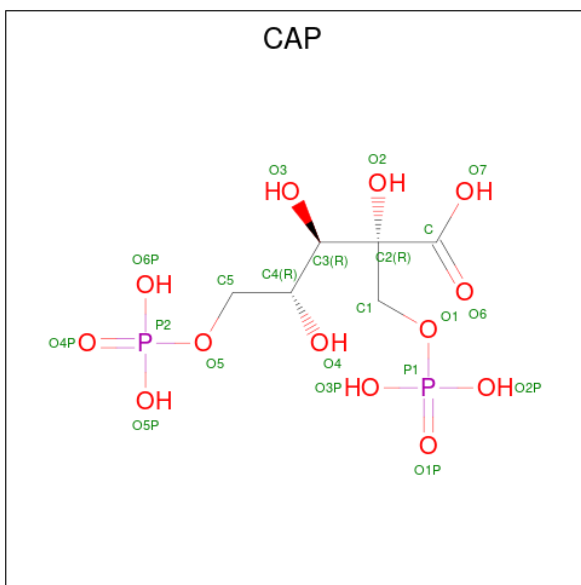
There are 5 unique types of molecules in this entry. The entry contains 19036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribulose-1,5-bisphosphate carboxylase-oxygenase type III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	473	Total 3732	C 2382	N 621	O 703	S 26	0	3	0
1	B	473	Total 3721	C 2376	N 617	O 702	S 26	0	2	0
1	C	472	Total 3724	C 2378	N 619	O 701	S 26	0	3	0
1	D	473	Total 3721	C 2376	N 617	O 702	S 26	0	2	0
1	E	472	Total 3724	C 2377	N 620	O 702	S 25	0	3	0

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	Total 21	C 6	O 13	P 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	B	1	21	6	13	2	0	0
2	C	1	21	6	13	2	0	0
2	D	1	21	6	13	2	0	0
2	E	1	21	6	13	2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0
3	E	2	2	2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0
4	E	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	86	86	86	0	0

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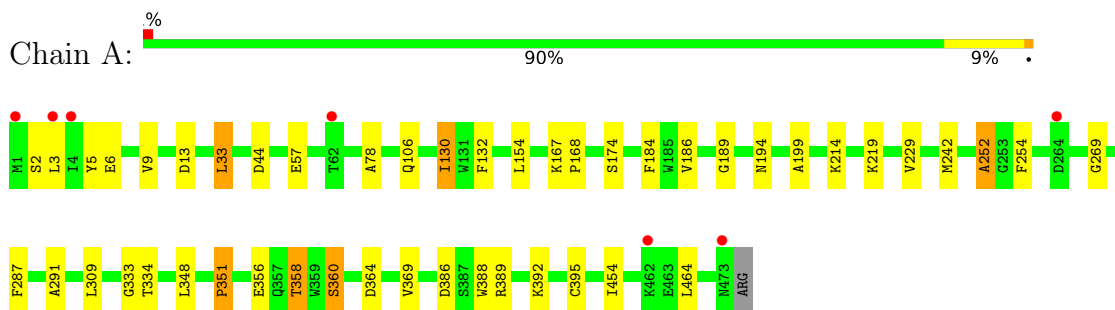
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	85	Total 85	O 85	0	0
5	C	50	Total 50	O 50	0	0
5	D	45	Total 45	O 45	0	0
5	E	28	Total 28	O 28	0	0

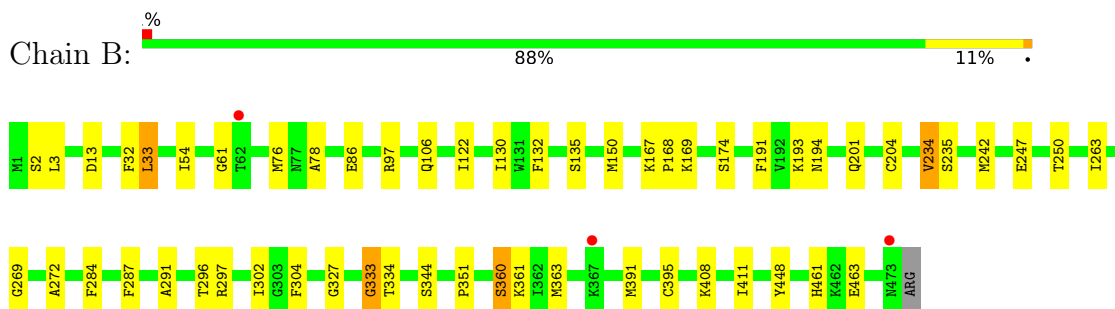
3 Residue-property plots [i](#)

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.

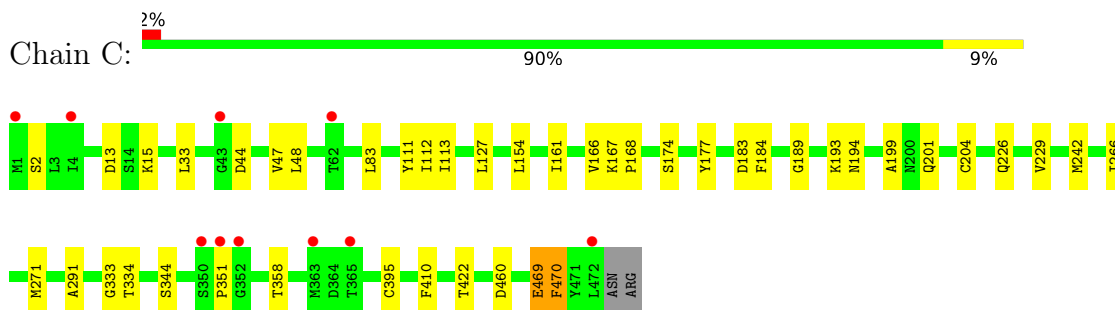
- Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III



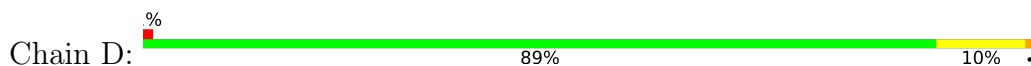
- Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III

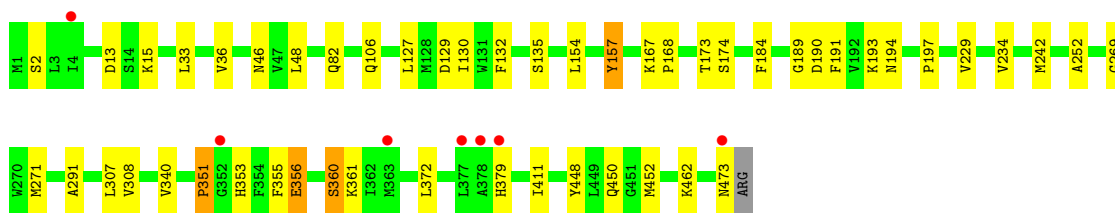


- Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III

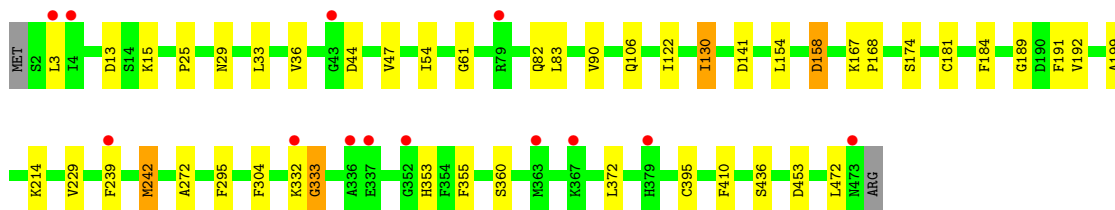
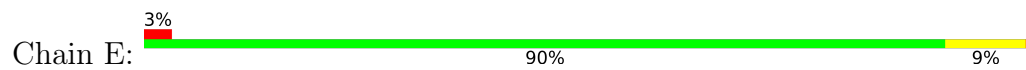


- Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III





● Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	273.76Å 273.76Å 96.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.37 – 2.60 48.37 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.37-2.60) 99.7 (48.37-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.61Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.189 , 0.225 (Not available) , 0.211	Depositor DCC
R_{free} test set	6337 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtrriage
Anisotropy	0.154	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19036	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: CL, KCX, MG, CAP

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	0.90	1/3810 (0.0%)	1.28	19/5161 (0.4%)
1	B	0.90	1/3799 (0.0%)	1.29	22/5147 (0.4%)
1	C	0.87	1/3802 (0.0%)	1.22	11/5150 (0.2%)
1	D	0.85	0/3799	1.28	18/5147 (0.3%)
1	E	0.85	2/3802 (0.1%)	1.24	12/5151 (0.2%)
All	All	0.87	5/19012 (0.0%)	1.26	82/25756 (0.3%)

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	A	0	2
1	B	0	2
1	D	0	2
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	MET	SD-CE	-6.37	1.63	1.79
1	E	242	MET	SD-CE	-5.75	1.65	1.79
1	C	266	ILE	CG1-CD1	-5.14	1.31	1.51
1	E	130	ILE	CG1-CD1	-5.10	1.31	1.51
1	B	391	MET	SD-CE	-5.08	1.66	1.79

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	SER	CA-C-N	13.15	145.37	121.70
1	A	360	SER	C-N-CA	13.15	145.37	121.70
1	D	360	SER	CA-C-N	12.27	144.97	121.54
1	D	360	SER	C-N-CA	12.27	144.97	121.54
1	B	360	SER	CA-C-N	12.20	144.85	121.54
1	B	360	SER	C-N-CA	12.20	144.85	121.54
1	E	360	SER	CA-C-N	11.16	141.78	121.70
1	E	360	SER	C-N-CA	11.16	141.78	121.70
1	D	252	ALA	N-CA-C	7.63	122.69	113.23
1	B	13	ASP	CA-CB-CG	7.08	119.68	112.60
1	B	191	PHE	CA-CB-CG	6.74	120.54	113.80
1	B	351	PRO	N-CA-C	6.62	122.73	113.53
1	A	252	ALA	N-CA-C	6.59	121.06	112.89
1	A	13	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	334	THR	N-CA-C	6.55	118.76	108.55
1	B	334	THR	N-CA-C	6.50	118.68	108.55
1	A	392	LYS	CA-C-N	6.47	130.02	120.90
1	A	392	LYS	C-N-CA	6.47	130.02	120.90
1	C	334	THR	N-CA-C	6.42	118.57	108.55
1	C	183	ASP	CA-CB-CG	6.41	119.01	112.60
1	E	158	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	13	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	287	PHE	CA-CB-CG	6.26	120.06	113.80
1	B	33	LEU	N-CA-C	-6.25	99.05	109.24
1	E	360	SER	CA-C-O	-6.16	113.71	120.43
1	B	296	THR	N-CA-C	6.02	120.69	113.23
1	A	351	PRO	N-CA-C	6.01	122.06	113.47
1	B	32	PHE	N-CA-C	5.96	119.26	109.72
1	B	78	ALA	N-CA-C	-5.93	101.70	110.48
1	A	252	ALA	CA-C-N	5.88	132.29	121.70
1	A	252	ALA	C-N-CA	5.88	132.29	121.70
1	A	360	SER	CA-C-O	-5.86	113.91	120.54
1	A	351	PRO	CA-C-N	5.84	132.21	121.70
1	A	351	PRO	C-N-CA	5.84	132.21	121.70
1	E	13	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	351	PRO	N-CA-C	5.82	121.20	113.40
1	A	287	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	33	LEU	N-CA-C	-5.72	98.42	108.20
1	D	360	SER	CA-C-O	-5.65	114.11	120.32
1	D	462	LYS	N-CA-C	5.62	117.41	111.28
1	B	395	CYS	N-CA-C	5.61	116.72	109.65
1	B	351	PRO	CA-C-N	5.60	131.77	121.70
1	B	351	PRO	C-N-CA	5.60	131.77	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	ALA	CA-C-N	5.59	131.76	121.70
1	D	252	ALA	C-N-CA	5.59	131.76	121.70
1	D	351	PRO	CA-C-N	5.57	131.73	121.70
1	D	351	PRO	C-N-CA	5.57	131.73	121.70
1	C	395	CYS	N-CA-C	5.57	116.66	109.65
1	E	29	ASN	CA-CB-CG	5.53	118.13	112.60
1	C	351	PRO	CA-C-N	5.50	131.60	121.70
1	C	351	PRO	C-N-CA	5.50	131.60	121.70
1	D	157	TYR	N-CA-C	-5.50	100.38	108.79
1	C	161	ILE	N-CA-C	-5.48	102.45	109.30
1	E	158	ASP	N-CA-C	-5.47	95.68	111.00
1	D	157	TYR	CA-C-N	5.44	131.50	121.70
1	D	157	TYR	C-N-CA	5.44	131.50	121.70
1	E	61	GLY	N-CA-C	5.43	120.01	112.57
1	C	358	THR	N-CA-C	-5.39	99.95	108.73
1	B	234	VAL	N-CA-CB	-5.36	105.35	112.26
1	C	13	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	78	ALA	N-CA-C	-5.31	102.42	110.28
1	A	360	SER	O-C-N	-5.30	117.18	123.22
1	E	395	CYS	N-CA-C	5.28	116.31	109.65
1	A	358	THR	N-CA-C	-5.26	99.94	108.52
1	C	410	PHE	CA-CB-CG	-5.26	108.53	113.80
1	D	190	ASP	CA-CB-CG	5.22	117.82	112.60
1	E	191	PHE	CA-CB-CG	5.21	119.02	113.80
1	E	410	PHE	CA-CB-CG	-5.20	108.60	113.80
1	B	463	GLU	CB-CG-CD	5.17	121.39	112.60
1	D	269	GLY	N-CA-C	5.14	117.27	112.08
1	E	141	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	191	PHE	CA-CB-CG	5.08	118.88	113.80
1	D	46	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	297	ARG	CA-C-N	5.06	127.31	120.38
1	B	297	ARG	C-N-CA	5.06	127.31	120.38
1	B	304	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	395	CYS	N-CA-C	5.04	116.87	109.42
1	D	129	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	461	HIS	CA-C-N	5.01	127.25	120.38
1	B	461	HIS	C-N-CA	5.01	127.25	120.38
1	B	61	GLY	N-CA-C	5.00	119.71	112.81
1	C	194	ASN	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	SER	Peptide,Mainchain
1	B	360	SER	Peptide,Mainchain
1	D	360	SER	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3732	0	3651	12	0
1	B	3721	0	3639	17	0
1	C	3724	0	3645	12	0
1	D	3721	0	3639	14	0
1	E	3724	0	3639	10	0
2	A	21	0	7	0	0
2	B	21	0	8	0	0
2	C	21	0	7	0	0
2	D	21	0	8	0	0
2	E	21	0	9	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	86	0	0	0	0
5	B	85	0	0	0	0
5	C	50	0	0	0	0
5	D	45	0	0	0	0
5	E	28	0	0	0	0
All	All	19036	0	18252	59	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 (59) 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:E:242:MET:HE1	1:E:272:ALA:HB1	1.76	0.67
1:E:154:LEU:HD21	1:E:229:VAL:HG23	1.80	0.63
1:D:36:VAL:HG23	1:D:355:PHE:CE2	2.36	0.60
1:A:154:LEU:HD21	1:A:229:VAL:HG23	1.85	0.57
1:C:48:LEU:HD13	1:C:83:LEU:HD11	1.87	0.56
1:C:271:MET:HE1	1:D:242:MET:SD	2.48	0.54
1:A:386:ASP:HA	1:A:388:TRP:CZ3	2.43	0.53
1:E:36:VAL:HG23	1:E:355:PHE:CE2	2.45	0.52
1:D:154:LEU:HD21	1:D:229:VAL:HG23	1.91	0.51
1:B:54:ILE:HD11	1:B:122:ILE:HG21	1.92	0.51
1:A:5:TYR:O	1:A:9:VAL:HG23	2.12	0.49
1:D:127:LEU:HD23	1:D:308:VAL:HG11	1.94	0.49
1:B:135:SER:HA	1:D:173:THR:HG21	1.93	0.49
1:E:167:LYS:HA	1:E:168:PRO:C	2.38	0.48
1:D:351:PRO:O	1:D:356:GLU:HA	2.14	0.47
1:B:242:MET:HE1	1:B:272:ALA:HB1	1.95	0.47
1:D:184:PHE:CE2	1:D:189:GLY:HA3	2.50	0.46
1:E:295:PHE:CD1	1:E:304:PHE:CE2	3.03	0.46
1:C:242:MET:HB2	1:D:271:MET:HE1	1.98	0.45
1:B:201:GLN:HB2	1:B:204[A]:CYS:SG	2.56	0.45
1:B:327:GLY:HA3	1:B:333:GLY:O	2.17	0.45
1:C:469:GLU:O	1:C:470:PHE:CB	2.64	0.45
1:C:154:LEU:HD21	1:C:229:VAL:HG23	1.99	0.45
1:B:130:ILE:HD13	1:B:132:PHE:CZ	2.52	0.45
1:B:150:MET:HE3	1:B:284:PHE:CD1	2.52	0.44
1:D:167:LYS:HA	1:D:168:PRO:C	2.43	0.44
1:E:181:CYS:SG	1:E:192:VAL:HG11	2.58	0.44
1:B:76:MET:HE1	1:B:97:ARG:CB	2.48	0.44
1:A:130:ILE:HD13	1:A:132:PHE:CZ	2.53	0.44
1:A:167:LYS:HA	1:A:168:PRO:C	2.43	0.44
1:E:54:ILE:HD11	1:E:122:ILE:HG21	2.00	0.44
1:A:184:PHE:CE2	1:A:189:GLY:HA3	2.53	0.43
1:E:184:PHE:CE2	1:E:189:GLY:HA3	2.53	0.43
1:B:54:ILE:HD11	1:B:122:ILE:CG2	2.48	0.43
1:B:167:LYS:HA	1:B:168:PRO:C	2.43	0.43
1:C:166:VAL:HG11	1:C:177:TYR:CD1	2.53	0.43
1:B:76:MET:HE1	1:B:97:ARG:HB3	1.99	0.43
1:D:450:GLN:HG3	1:D:452:MET:HE3	2.01	0.43
1:B:411:ILE:HG21	1:B:448:TYR:CZ	2.54	0.43
1:B:242:MET:CE	1:B:263:ILE:HD13	2.49	0.42
1:C:113:ILE:HD12	1:C:113:ILE:O	2.20	0.42
1:E:239[A]:PHE:CD2	1:E:239[A]:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:HA	1:A:369:VAL:HG11	2.01	0.42
1:D:130:ILE:HD13	1:D:132:PHE:CZ	2.53	0.42
1:D:340:VAL:HG11	1:D:353:HIS:ND1	2.34	0.42
1:A:252:ALA:HB3	1:A:254:PHE:CD2	2.55	0.42
1:B:247:GLU:HA	1:B:250:THR:HB	2.02	0.42
1:C:111:TYR:CZ	1:D:197:PRO:HB2	2.54	0.42
1:C:112:ILE:HD12	1:C:127:LEU:HD21	2.02	0.42
1:C:167:LYS:HA	1:C:168:PRO:C	2.45	0.41
1:C:201:GLN:HB2	1:C:204[A]:CYS:SG	2.60	0.41
1:E:332:LYS:HA	1:E:333:GLY:HA3	1.91	0.41
1:A:351:PRO:O	1:A:356:GLU:HA	2.21	0.41
1:C:184:PHE:CE2	1:C:189:GLY:HA3	2.56	0.41
1:A:269:GLY:HA3	1:B:269:GLY:HA3	2.01	0.41
1:D:411:ILE:HG21	1:D:448:TYR:CZ	2.56	0.41
1:A:348:LEU:O	1:A:358:THR:HA	2.21	0.41
1:B:242:MET:HE1	1:B:263:ILE:HD13	2.03	0.41
1:A:57:GLU:O	1:B:169:LYS:HE3	2.20	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	473/474 (100%)	446 (94%)	22 (5%)	5 (1%)	11 25
1	B	472/474 (100%)	443 (94%)	25 (5%)	4 (1%)	16 34
1	C	472/474 (100%)	452 (96%)	14 (3%)	6 (1%)	9 21
1	D	472/474 (100%)	441 (93%)	28 (6%)	3 (1%)	21 42
1	E	472/474 (100%)	443 (94%)	24 (5%)	5 (1%)	11 25
All	All	2361/2370 (100%)	2225 (94%)	113 (5%)	23 (1%)	12 28

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	B	2	SER
1	B	361	LYS
1	C	2	SER
1	C	470	PHE
1	D	2	SER
1	D	361	LYS
1	C	44	ASP
1	E	3	LEU
1	A	44	ASP
1	A	291	ALA
1	A	333	GLY
1	B	333	GLY
1	C	333	GLY
1	B	291	ALA
1	C	291	ALA
1	D	291	ALA
1	E	44	ASP
1	E	199	ALA
1	A	199	ALA
1	C	199	ALA
1	E	333	GLY
1	E	25	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/395 (100%)	383 (96%)	14 (4%)	32	59
1	B	396/395 (100%)	384 (97%)	12 (3%)	36	64
1	C	396/395 (100%)	387 (98%)	9 (2%)	44	71
1	D	396/395 (100%)	381 (96%)	15 (4%)	29	56
1	E	396/395 (100%)	380 (96%)	16 (4%)	28	55
All	All	1981/1975 (100%)	1915 (97%)	66 (3%)	32	61

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	GLU
1	A	33	LEU
1	A	106	GLN
1	A	130	ILE
1	A	174	SER
1	A	186	VAL
1	A	194	ASN
1	A	214	LYS
1	A	219	LYS
1	A	309	LEU
1	A	389	ARG
1	A	454	ILE
1	A	464	LEU
1	B	3	LEU
1	B	33	LEU
1	B	86	GLU
1	B	106	GLN
1	B	174	SER
1	B	194	ASN
1	B	234	VAL
1	B	235	SER
1	B	302	ILE
1	B	344	SER
1	B	363	MET
1	B	408	LYS
1	C	15	LYS
1	C	33	LEU
1	C	47	VAL
1	C	174	SER
1	C	226	GLN
1	C	344	SER
1	C	422	THR
1	C	460	ASP
1	C	469	GLU
1	D	15	LYS
1	D	33	LEU
1	D	48	LEU
1	D	82	GLN
1	D	106	GLN
1	D	135	SER
1	D	157	TYR

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Mol	Chain	Res	Type
1	D	174	SER
1	D	194	ASN
1	D	234	VAL
1	D	307	LEU
1	D	356	GLU
1	D	372	LEU
1	D	379	HIS
1	D	473	ASN
1	E	15	LYS
1	E	33	LEU
1	E	47	VAL
1	E	82	GLN
1	E	83	LEU
1	E	90	VAL
1	E	106	GLN
1	E	130	ILE
1	E	158	ASP
1	E	174	SER
1	E	214	LYS
1	E	353	HIS
1	E	372	LEU
1	E	436	SER
1	E	453	ASP
1	E	472	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	226	GLN
1	B	251	ASN
1	C	82	GLN
1	C	226	GLN
1	C	403	ASN
1	E	29	ASN
1	E	139	GLN
1	E	298	GLN
1	E	473	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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$
1	KCX	B	193	3,1	10,11,12	2.97	1 (10%)	6,12,14	1.88	1 (16%)
1	KCX	A	193	3,1	10,11,12	1.08	0	6,12,14	0.92	0
1	KCX	D	193	3,1	10,11,12	2.36	2 (20%)	6,12,14	1.33	0
1	KCX	E	193	3,1	10,11,12	0.65	0	6,12,14	0.79	0
1	KCX	C	193	3,1	10,11,12	1.01	0	6,12,14	1.03	1 (16%)

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
1	KCX	B	193	3,1	-	0/9/10/12	-
1	KCX	A	193	3,1	-	0/9/10/12	-
1	KCX	D	193	3,1	-	0/9/10/12	-
1	KCX	E	193	3,1	-	1/9/10/12	-
1	KCX	C	193	3,1	-	1/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	KCX	OQ1-CX	8.91	1.38	1.21
1	D	193	KCX	OQ1-CX	6.51	1.33	1.21
1	D	193	KCX	CB-CA	2.60	1.57	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	KCX	OQ1-CX-NZ	-4.36	118.30	124.92
1	C	193	KCX	CD-CE-NZ	2.03	117.88	112.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	193	KCX	CE-CD-CG-CB
1	E	193	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 15 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CAP	D	501	3	18,20,20	0.70	0	23,31,31	1.29	2 (8%)
2	CAP	A	501	3	18,20,20	0.71	0	23,31,31	1.16	1 (4%)
2	CAP	E	501	3	18,20,20	0.73	0	23,31,31	1.16	2 (8%)
2	CAP	C	501	3	18,20,20	0.87	1 (5%)	23,31,31	1.27	3 (13%)
2	CAP	B	501	3	18,20,20	0.88	1 (5%)	23,31,31	1.48	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	D	501	3	-	3/29/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	A	501	3	-	8/29/29/29	-
2	CAP	E	501	3	-	9/29/29/29	-
2	CAP	C	501	3	-	10/29/29/29	-
2	CAP	B	501	3	-	8/29/29/29	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	CAP	C2-C	-2.31	1.51	1.53
2	B	501	CAP	C2-C	-2.23	1.51	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	CAP	O7-C-C2	4.33	121.31	114.06
2	D	501	CAP	O7-C-C2	3.74	120.32	114.06
2	B	501	CAP	O6-C-C2	-2.87	116.97	122.32
2	E	501	CAP	O7-C-C2	2.46	118.18	114.06
2	C	501	CAP	O7-C-C2	2.39	118.06	114.06
2	A	501	CAP	O7-C-C2	2.30	117.92	114.06
2	E	501	CAP	O6P-P2-O5	-2.18	100.98	106.67
2	D	501	CAP	O2-C2-C1	-2.13	103.67	108.72
2	C	501	CAP	C2-C3-C4	2.12	118.26	114.03
2	C	501	CAP	O3-C3-C4	2.10	113.63	109.13
2	B	501	CAP	O6P-P2-O5P	2.00	115.31	107.80

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CAP	O3-C3-C4-O4
2	B	501	CAP	O6-C-C2-O2
2	B	501	CAP	O3-C3-C4-O4
2	C	501	CAP	O6-C-C2-C3
2	C	501	CAP	O6-C-C2-O2
2	C	501	CAP	O7-C-C2-O2
2	C	501	CAP	C2-C3-C4-O4
2	C	501	CAP	O3-C3-C4-O4
2	E	501	CAP	O6-C-C2-C3
2	E	501	CAP	O6-C-C2-O2

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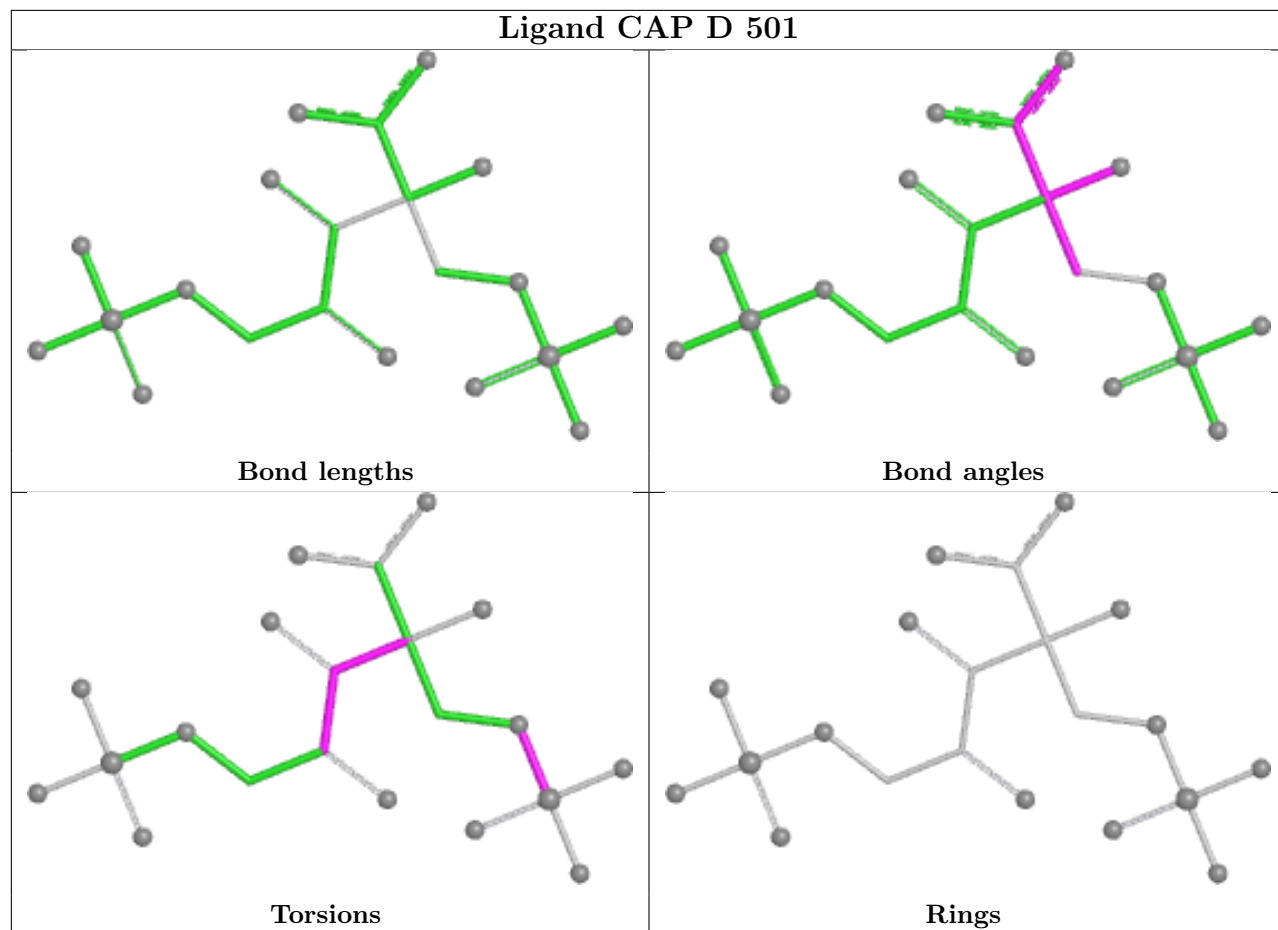
Mol	Chain	Res	Type	Atoms
2	E	501	CAP	O3-C3-C4-O4
2	E	501	CAP	O7-C-C2-O2
2	C	501	CAP	O6-C-C2-C1
2	A	501	CAP	O6-C-C2-O2
2	A	501	CAP	O6-C-C2-C3
2	D	501	CAP	C1-O1-P1-O3P
2	A	501	CAP	O6-C-C2-C1
2	C	501	CAP	O7-C-C2-C1
2	E	501	CAP	O6-C-C2-C1
2	E	501	CAP	O7-C-C2-C1
2	A	501	CAP	O7-C-C2-O2
2	A	501	CAP	O2-C2-C3-C4
2	B	501	CAP	O2-C2-C3-C4
2	C	501	CAP	O2-C2-C3-C4
2	D	501	CAP	O2-C2-C3-C4
2	E	501	CAP	O2-C2-C3-C4
2	A	501	CAP	O7-C-C2-C3
2	B	501	CAP	O7-C-C2-C3
2	C	501	CAP	O7-C-C2-C3
2	E	501	CAP	O7-C-C2-C3
2	D	501	CAP	O3-C3-C4-O4
2	C	501	CAP	C4-C5-O5-P2
2	A	501	CAP	O7-C-C2-C1
2	B	501	CAP	O7-C-C2-O2
2	B	501	CAP	C2-C3-C4-O4
2	B	501	CAP	O6-C-C2-C3
2	B	501	CAP	O7-C-C2-C1
2	E	501	CAP	O4-C4-C5-O5

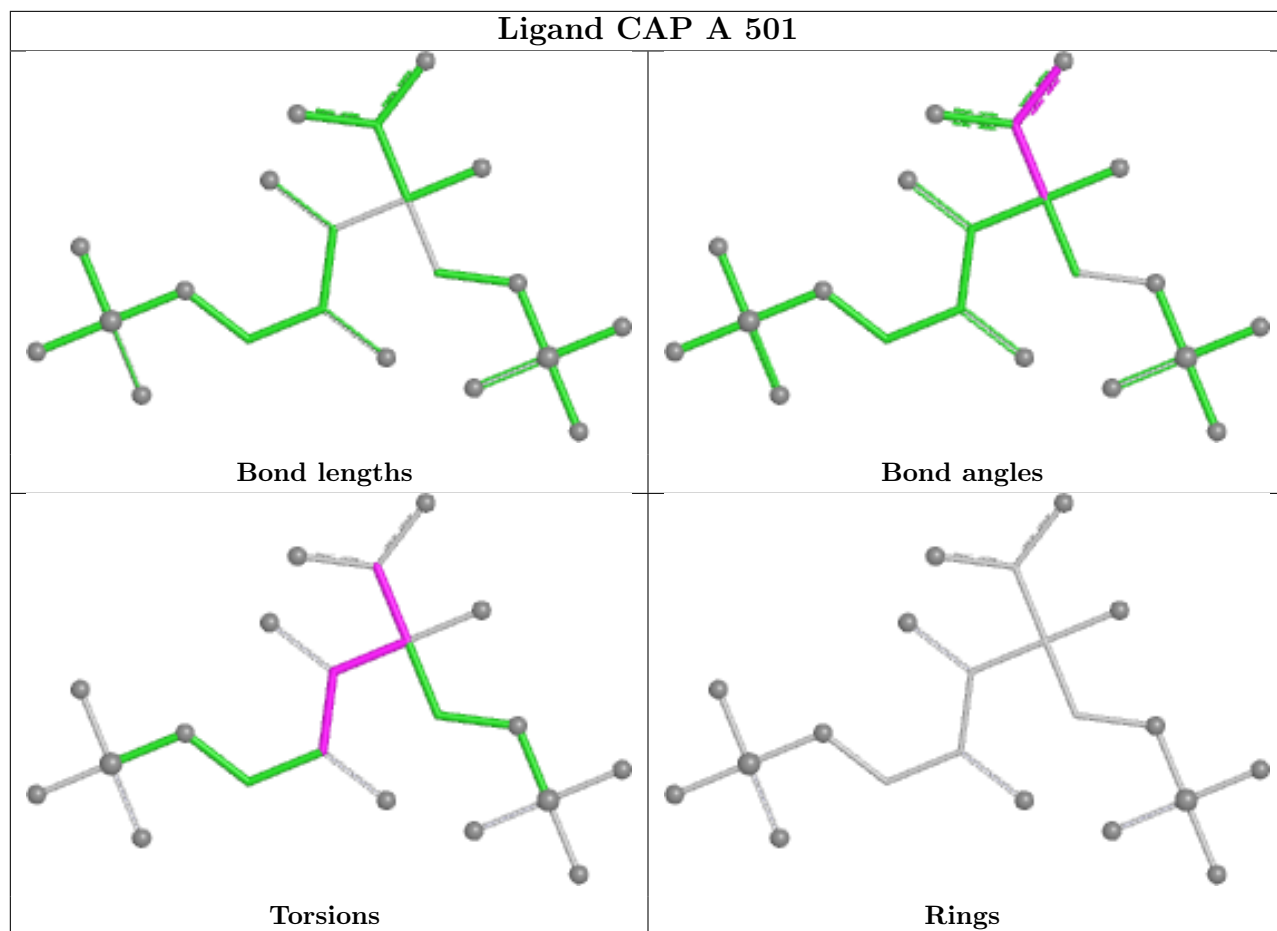
There are no ring outliers.

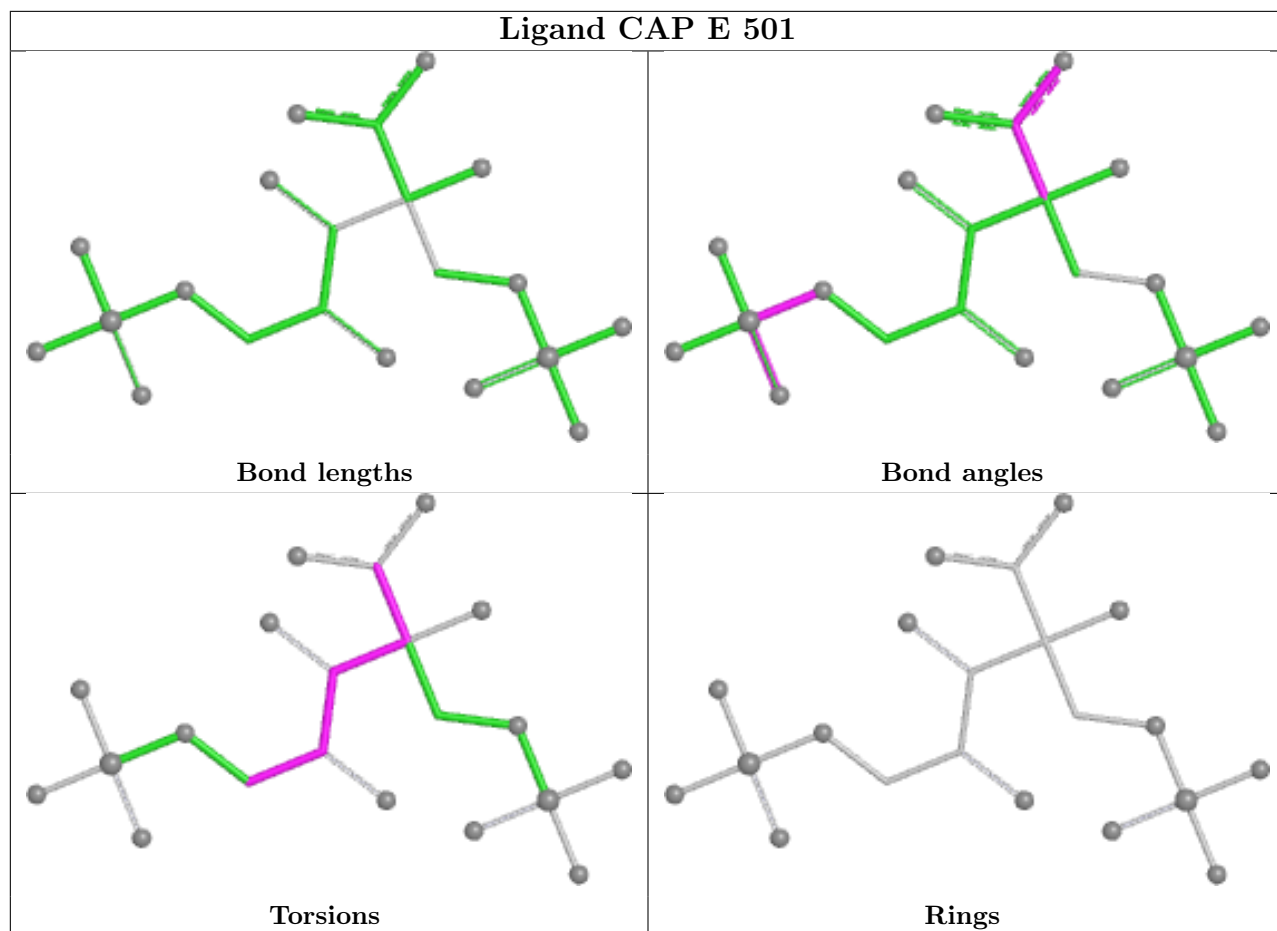
No monomer is involved in short contacts.

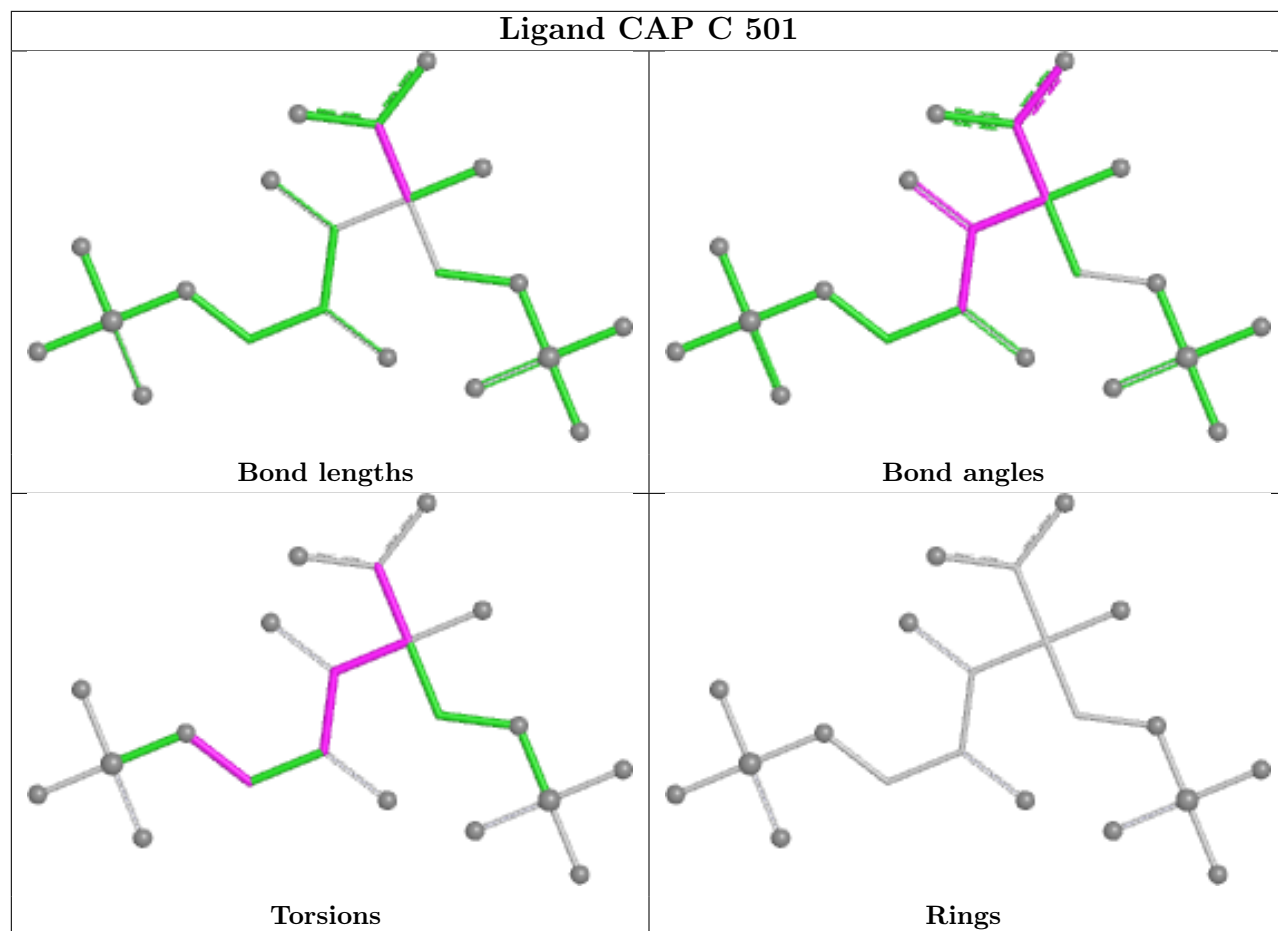
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

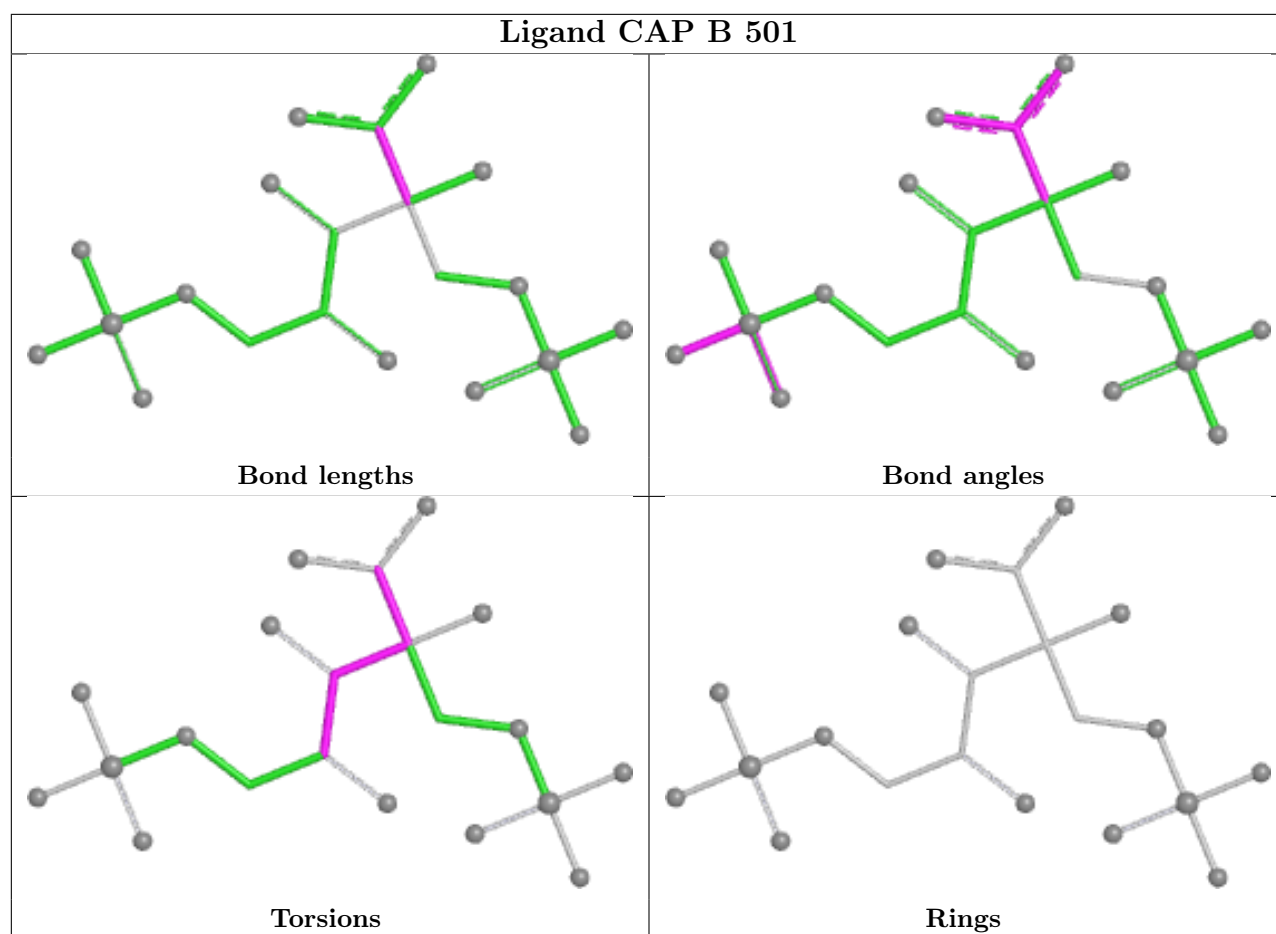
equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	472/474 (99%)	-0.09	7 (1%) 72 68	23, 55, 75, 107	3 (0%)
1	B	472/474 (99%)	-0.08	3 (0%) 85 83	24, 55, 73, 98	2 (0%)
1	C	471/474 (99%)	0.22	10 (2%) 63 58	28, 64, 84, 110	3 (0%)
1	D	472/474 (99%)	0.19	7 (1%) 72 68	28, 62, 81, 121	2 (0%)
1	E	471/474 (99%)	0.40	13 (2%) 55 49	36, 72, 92, 113	3 (0%)
All	All	2358/2370 (99%)	0.13	40 (1%) 69 64	23, 61, 84, 121	13 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	239[A]	PHE	5.5
1	E	3	LEU	4.7
1	E	79[A]	ARG	4.3
1	D	473	ASN	4.0
1	A	3	LEU	3.9
1	C	352	GLY	3.8
1	A	473	ASN	3.5
1	C	1	MET	3.5
1	D	377	LEU	3.4
1	D	4	ILE	3.3
1	E	4	ILE	3.3
1	E	352	GLY	3.1
1	C	4	ILE	3.0
1	C	62	THR	3.0
1	E	367	LYS	2.9
1	C	363	MET	2.8
1	D	363	MET	2.8
1	B	473	ASN	2.7
1	A	462	LYS	2.7
1	D	378	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	363	MET	2.6
1	E	43	GLY	2.6
1	D	379	HIS	2.6
1	D	352	GLY	2.6
1	C	365	THR	2.5
1	B	367	LYS	2.5
1	C	472	LEU	2.5
1	E	336	ALA	2.5
1	C	350	SER	2.4
1	A	4	ILE	2.3
1	A	1	MET	2.3
1	C	351	PRO	2.3
1	E	473	ASN	2.3
1	A	264	ASP	2.2
1	A	62	THR	2.1
1	E	332	LYS	2.1
1	E	379	HIS	2.1
1	C	43	GLY	2.1
1	E	337	GLU	2.0
1	B	62	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	A	193	12/13	0.96	0.09	47,52,55,56	0
1	KCX	C	193	12/13	0.96	0.10	60,63,63,65	0
1	KCX	E	193	12/13	0.96	0.08	57,61,66,66	0
1	KCX	D	193	12/13	0.97	0.08	48,48,52,55	0
1	KCX	B	193	12/13	0.97	0.07	45,47,51,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

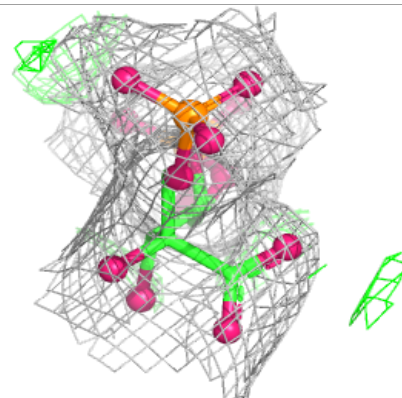
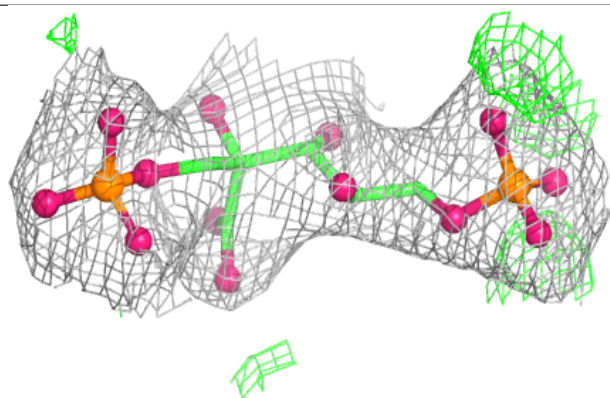
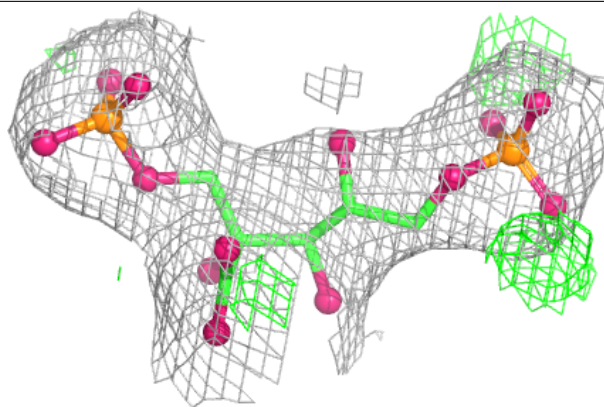
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CAP	E	501	21/21	0.94	0.09	75,78,80,80	0
4	CL	E	504	1/1	0.94	0.15	63,63,63,63	0
2	CAP	C	501	21/21	0.96	0.08	62,66,73,74	0
4	CL	D	504	1/1	0.97	0.13	61,61,61,61	0
2	CAP	D	501	21/21	0.97	0.06	54,61,63,64	0
3	MG	B	503	1/1	0.98	0.08	46,46,46,46	0
3	MG	C	503	1/1	0.98	0.15	50,50,50,50	0
2	CAP	B	501	21/21	0.98	0.06	52,60,65,67	0
2	CAP	A	501	21/21	0.98	0.05	50,55,60,63	0
3	MG	C	502	1/1	0.99	0.03	58,58,58,58	0
3	MG	A	503	1/1	0.99	0.11	41,41,41,41	0
3	MG	D	503	1/1	0.99	0.06	53,53,53,53	0
3	MG	E	502	1/1	0.99	0.04	62,62,62,62	0
3	MG	E	503	1/1	0.99	0.13	57,57,57,57	0
4	CL	A	504	1/1	0.99	0.12	49,49,49,49	0
4	CL	B	504	1/1	0.99	0.14	48,48,48,48	0
4	CL	C	504	1/1	0.99	0.10	49,49,49,49	0
3	MG	B	502	1/1	0.99	0.05	59,59,59,59	0
3	MG	A	502	1/1	0.99	0.03	46,46,46,46	0
3	MG	D	502	1/1	1.00	0.02	55,55,55,55	0

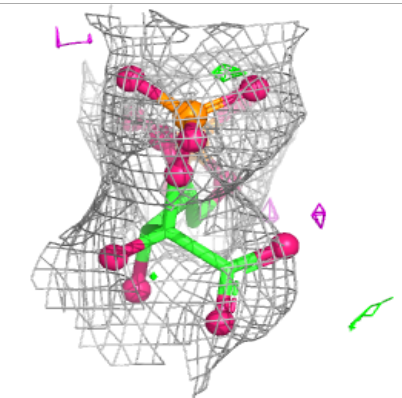
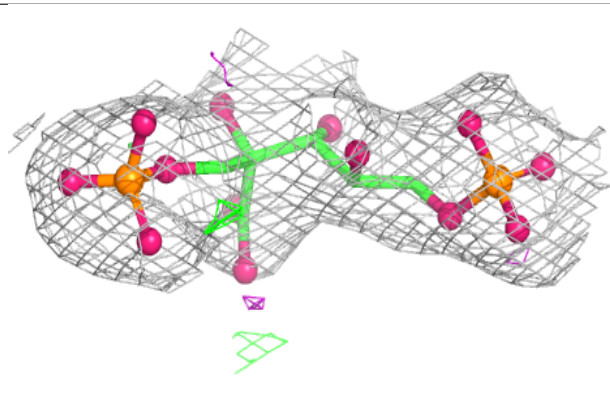
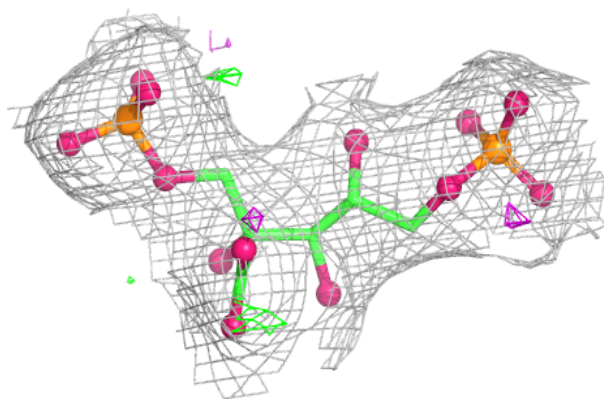
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

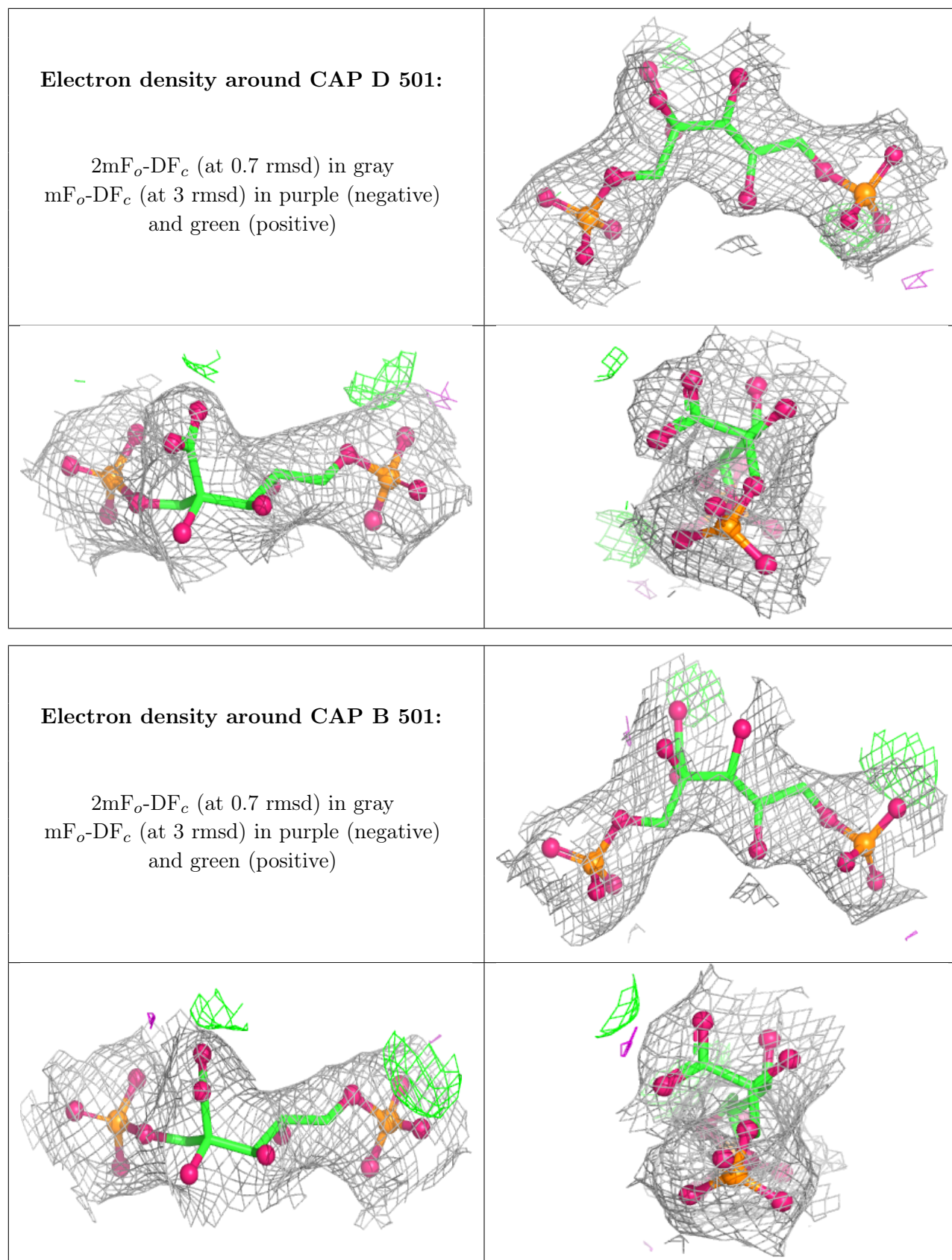
Electron density around CAP E 501:

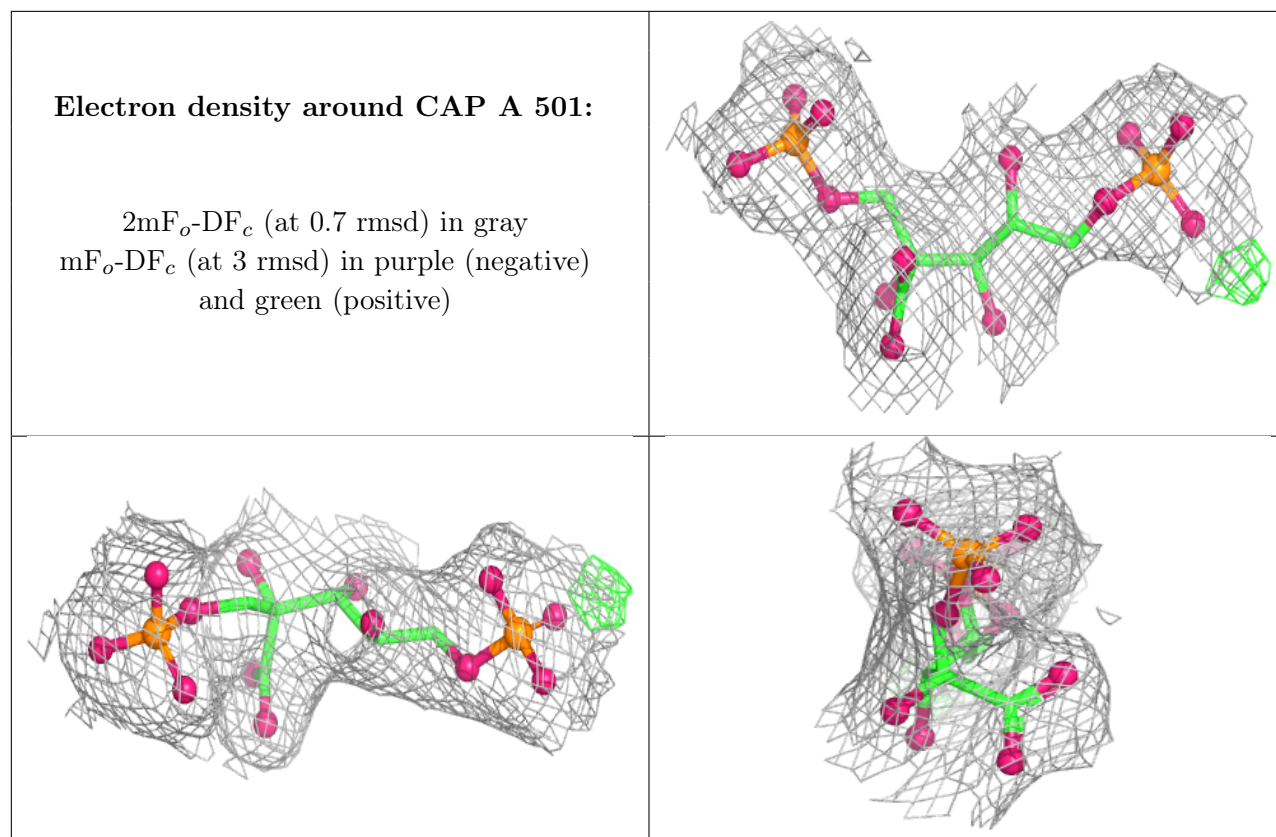
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CAP 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)







6.5 Other polymers [i](#)

There are no such residues in this entry.