WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 23, 2024 – 04:15 pm BST

PDB ID	:	8QMW
Title	:	Non-obligately L8S8-complex forming RubisCO derived from ancestral sequence reconstruction and rational engineering in L8S8 complex with substitutions R269W, E271R, L273N
Authors	:	Zarzycki, J.; Schulz, L.; Erb, T.J.; Hochberg, G.K.A.
Deposited on	:	2023-09-25
Resolution	:	1.75 Å(reported)

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

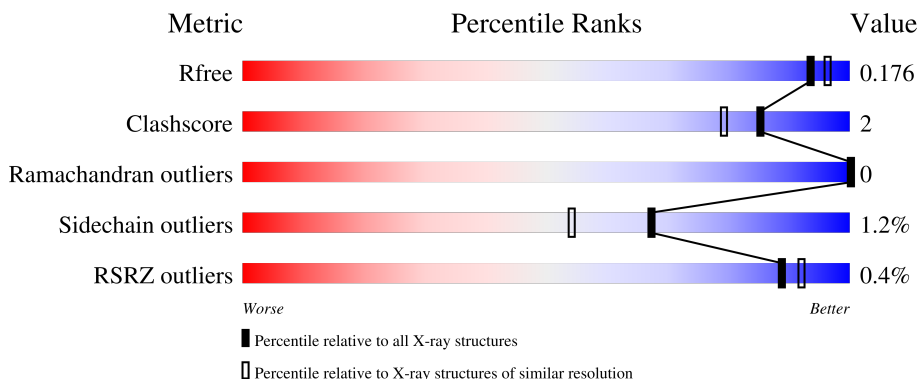|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance ⓘ

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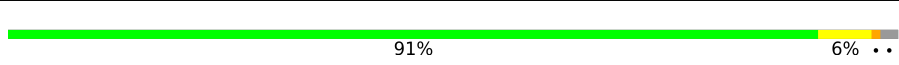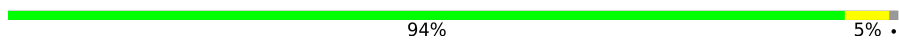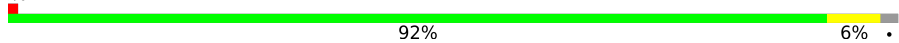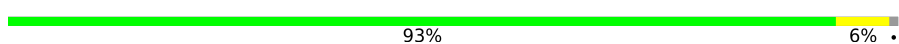*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	Percentile Ranks	Value
Rfree		0.176
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		0.4%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
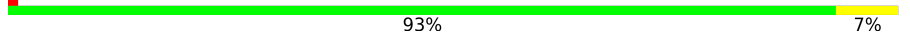
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	457	91% 6% ··
1	B	457	94% 5% ·
1	C	457	% 92% 6% ·
1	D	457	93% 6% ·

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Mol	Chain	Length	Quality of chain
2	E	105	89% 6% 6%
2	F	105	86% 9% 6%
2	G	105	2% 88% 10% •
2	H	105	% 93% 7%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 19717 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 RubisCO large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total 3553	C 2252	N 633	O 653	S 15	0	0	0
1	B	451	Total 3560	C 2257	N 634	O 654	S 15	0	0	0
1	C	449	Total 3544	C 2247	N 632	O 650	S 15	0	0	0
1	D	451	Total 3560	C 2257	N 634	O 654	S 15	0	0	0

- Molecule 2 is a protein called RubisCO small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	99	Total 822	C 532	N 128	O 158	S 4	0	0	0
2	F	99	Total 822	C 532	N 128	O 158	S 4	0	0	0
2	G	102	Total 852	C 550	N 137	O 161	S 4	0	0	0
2	H	105	Total 882	C 568	N 146	O 164	S 4	0	0	0

- Molecule 3 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$) (labeled as "Ligand of Interest" by depositor).
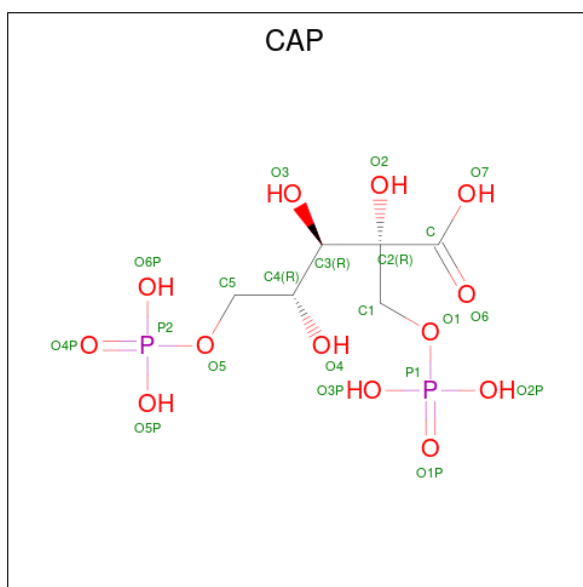
WORLDWIDE wwPDB PROTEIN DATA BANK

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).

B3P
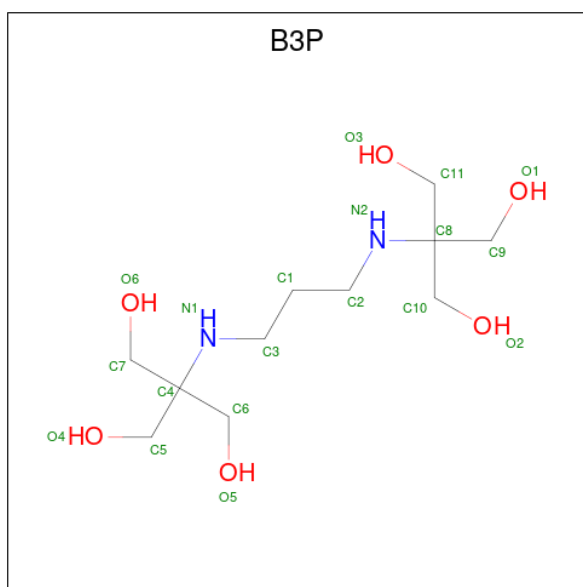
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	19	11	2	6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	402	Total 402	O 402	0	0
6	B	391	Total 391	O 391	0	0
6	C	401	Total 401	O 401	0	0
6	D	419	Total 419	O 419	0	0
6	E	97	Total 97	O 97	0	0
6	F	102	Total 102	O 102	0	0
6	G	105	Total 105	O 105	0	0
6	H	98	Total 98	O 98	0	0

3 Residue-property plots ⓘ

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 =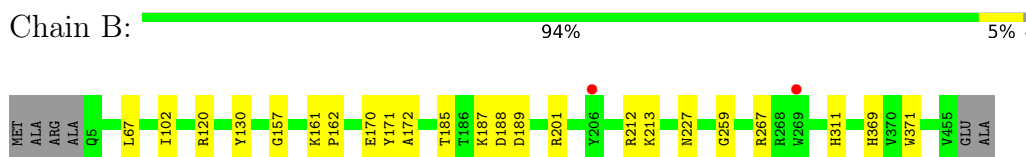 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RubisCO large subunit
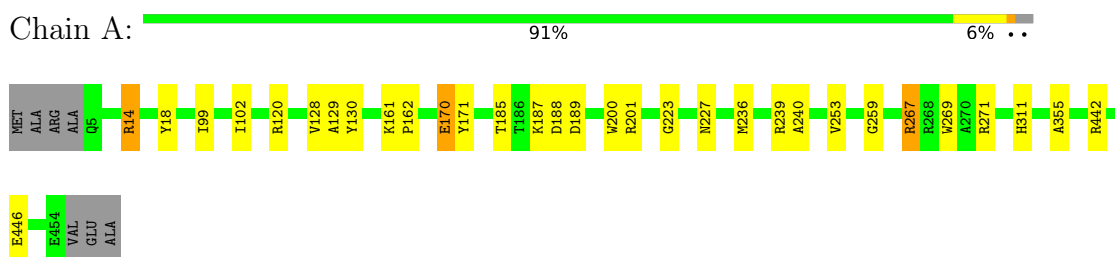
Chain A:

- Molecule 1: RubisCO large subunit

Chain B:

- Molecule 1: RubisCO large subunit

Chain C:

- Molecule 1: RubisCO large subunit

Chain D:

- Molecule 2: RubisCO small subunit

Chain E:

• Molecule 2: RubisCO small subunit

Chain F:

• Molecule 2: RubisCO small subunit

Chain G:

• Molecule 2: RubisCO small subunit

Chain H:
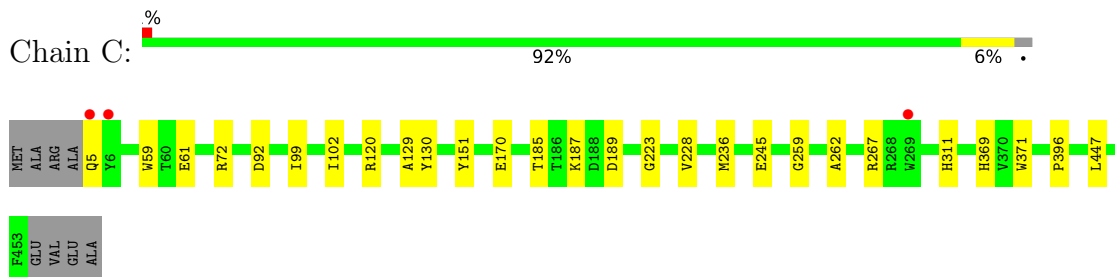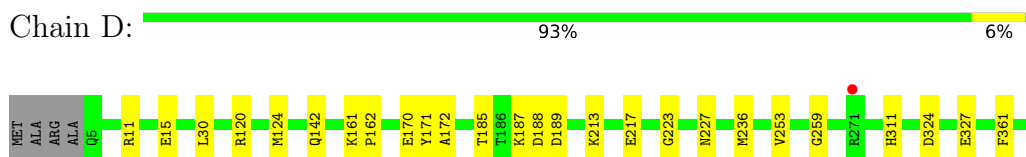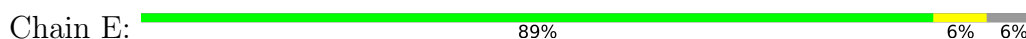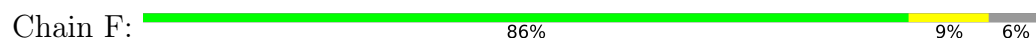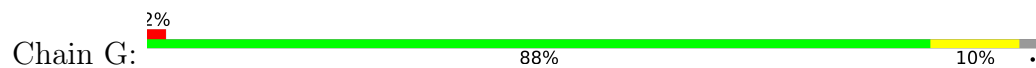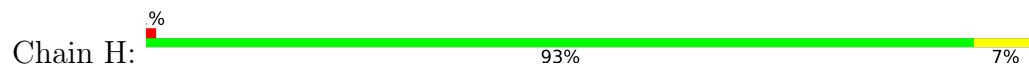
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.01Å 106.44Å 108.49Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	24.88 – 1.75 24.88 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (24.88-1.75) 98.6 (24.88-1.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.145 , 0.174 0.145 , 0.176	Depositor DCC
R_{free} test set	214348 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å²)	16.1	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.41 , 47.9	EDS
L-test for twinning [2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19717	wwPDB-VP
Average B, all atoms (Å²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CAP, B3P, MG, KCX

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	0.65	0/3628	0.76	0/4915
1	B	0.66	0/3635	0.75	0/4925
1	C	0.64	0/3619	0.76	0/4903
1	D	0.65	0/3635	0.76	0/4925
2	E	0.61	0/849	0.65	0/1157
2	F	0.62	0/849	0.65	0/1157
2	G	0.59	0/882	0.65	0/1202
2	H	0.57	0/915	0.62	0/1247
All	All	0.64	0/18012	0.74	0/24431

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	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	267	ARG	Sidechain
1	C	120	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	3553	0	3457	18	0
1	B	3560	0	3466	12	0
1	C	3544	0	3451	16	0
1	D	3560	0	3466	15	0
2	E	822	0	771	5	0
2	F	822	0	771	5	0
2	G	852	0	792	8	0
2	H	882	0	813	5	0
3	A	21	0	7	0	0
3	B	21	0	8	0	0
3	C	21	0	7	0	0
3	D	21	0	8	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
5	C	19	0	26	1	0
6	A	402	0	0	1	0
6	B	391	0	0	2	0
6	C	401	0	0	2	0
6	D	419	0	0	0	0
6	E	97	0	0	0	0
6	F	102	0	0	1	0
6	G	105	0	0	1	0
6	H	98	0	0	0	0
All	All	19717	0	17043	72	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.

The worst 5 of 72 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:102:ILE:HD11	1:C:130:TYR:HE2	1.60	0.67
1:B:201:ARG:NH2	6:B:602:HOH:O	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HD11	1:A:130:TYR:HE2	1.65	0.60
1:A:201:ARG:NH2	6:A:604:HOH:O	2.31	0.59
2:G:70:ARG:NH1	6:G:202:HOH:O	2.36	0.58

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	447/457 (98%)	432 (97%)	15 (3%)	0	100	100
1	B	448/457 (98%)	433 (97%)	15 (3%)	0	100	100
1	C	446/457 (98%)	431 (97%)	15 (3%)	0	100	100
1	D	448/457 (98%)	434 (97%)	14 (3%)	0	100	100
2	E	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
2	F	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
2	G	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
2	H	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
All	All	2186/2248 (97%)	2111 (97%)	75 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	359/363 (99%)	354 (99%)	5 (1%)	62	49
1	B	360/363 (99%)	355 (99%)	5 (1%)	62	49
1	C	358/363 (99%)	354 (99%)	4 (1%)	70	58
1	D	360/363 (99%)	355 (99%)	5 (1%)	62	49
2	E	89/95 (94%)	89 (100%)	0	100	100
2	F	89/95 (94%)	88 (99%)	1 (1%)	70	58
2	G	92/95 (97%)	91 (99%)	1 (1%)	70	58
2	H	95/95 (100%)	95 (100%)	0	100	100
All	All	1802/1832 (98%)	1781 (99%)	21 (1%)	67	54

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	120	ARG
1	D	311	HIS
2	G	87	ARG
1	D	361	PHE
1	D	189	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	100	HIS

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	C	187	1,4	9,11,12	1.59	2 (22%)	5,12,14	1.64	1 (20%)
1	KCX	B	187	1,4	9,11,12	2.12	2 (22%)	5,12,14	1.28	1 (20%)
1	KCX	A	187	1,4	9,11,12	2.30	4 (44%)	5,12,14	3.56	1 (20%)
1	KCX	D	187	1,4	9,11,12	2.61	4 (44%)	5,12,14	4.11	1 (20%)

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	C	187	1,4	-	0/9/10/12	-
1	KCX	B	187	1,4	-	0/9/10/12	-
1	KCX	A	187	1,4	-	0/9/10/12	-
1	KCX	D	187	1,4	-	0/9/10/12	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	KCX	CB-CA	5.34	1.60	1.53
1	D	187	KCX	CB-CA	4.86	1.60	1.53
1	D	187	KCX	OQ1-CX	4.28	1.29	1.21
1	A	187	KCX	OQ1-CX	4.19	1.29	1.21
1	A	187	KCX	CB-CA	3.65	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	187	KCX	OQ1-CX-NZ	-9.10	110.85	124.96
1	A	187	KCX	OQ1-CX-NZ	-7.71	113.00	124.96
1	C	187	KCX	OQ1-CX-NZ	-3.47	119.58	124.96
1	B	187	KCX	OQ1-CX-NZ	-2.48	121.11	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 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	#$\|Z\| > 2$
3	CAP	A	501	4	17,20,20	1.41	3 (17%)	22,31,31	0.98	2 (9%)
5	B3P	C	503	-	18,18,18	0.25	0	21,23,23	1.54	2 (9%)
3	CAP	C	501	4	17,20,20	1.54	3 (17%)	22,31,31	1.01	2 (9%)
3	CAP	D	501	4	17,20,20	1.37	2 (11%)	22,31,31	0.97	2 (9%)
3	CAP	B	501	4	17,20,20	1.36	2 (11%)	22,31,31	0.97	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAP	A	501	4	-	7/29/29/29	-
5	B3P	C	503	-	-	3/28/28/28	-
3	CAP	C	501	4	-	7/29/29/29	-
3	CAP	D	501	4	-	7/29/29/29	-
3	CAP	B	501	4	-	7/29/29/29	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	CAP	O6-C	3.56	1.33	1.22
3	C	501	CAP	O6-C	3.47	1.33	1.22
3	A	501	CAP	P1-O1P	3.06	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	CAP	P1-O1P	3.01	1.60	1.50
3	D	501	CAP	P1-O1P	2.90	1.59	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	503	B3P	C2-N2-C8	-5.51	108.27	116.08
5	C	503	B3P	C3-N1-C4	-3.08	111.71	116.08
3	C	501	CAP	P2-O5-C5	-2.66	110.96	118.30
3	B	501	CAP	P2-O5-C5	-2.59	111.16	118.30
3	A	501	CAP	P2-O5-C5	-2.47	111.48	118.30

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

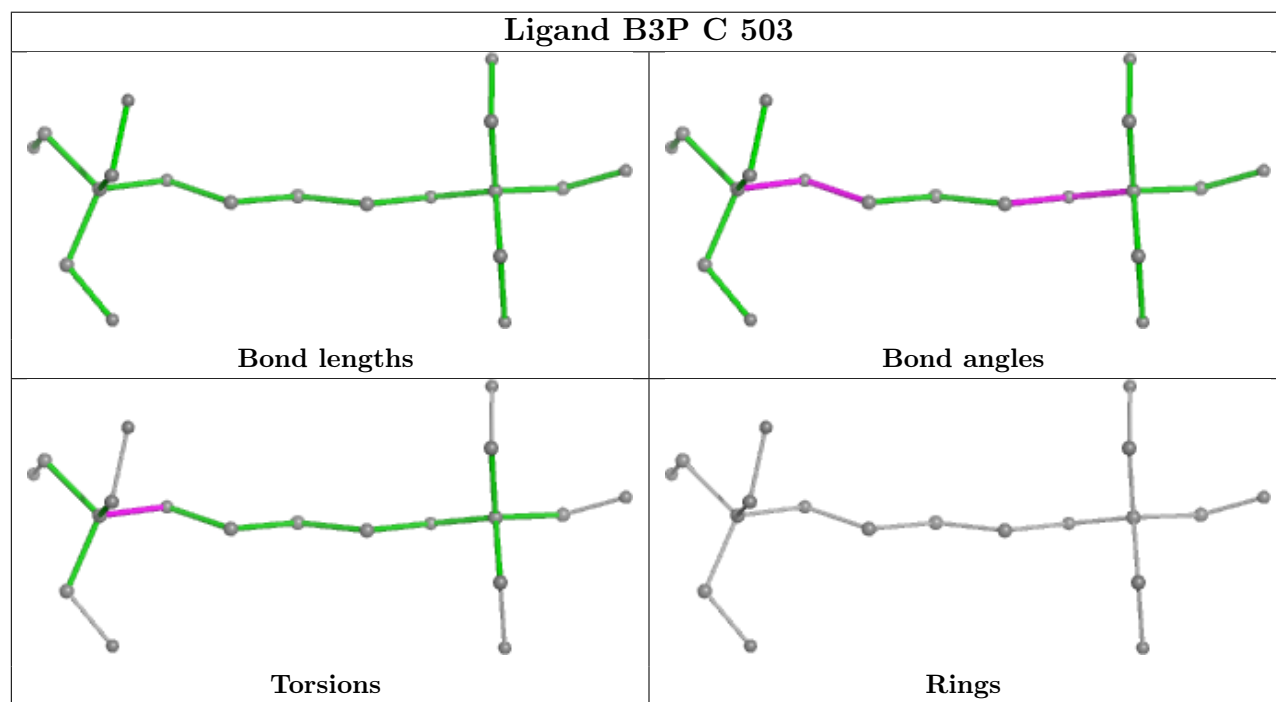| Mol	Chain	Res	Type	Atoms
3	A	501	CAP	O6-C-C2-C1
3	A	501	CAP	O7-C-C2-C1
3	A	501	CAP	O6-C-C2-O2
3	A	501	CAP	O7-C-C2-O2
3	A	501	CAP	C2-C3-C4-O4

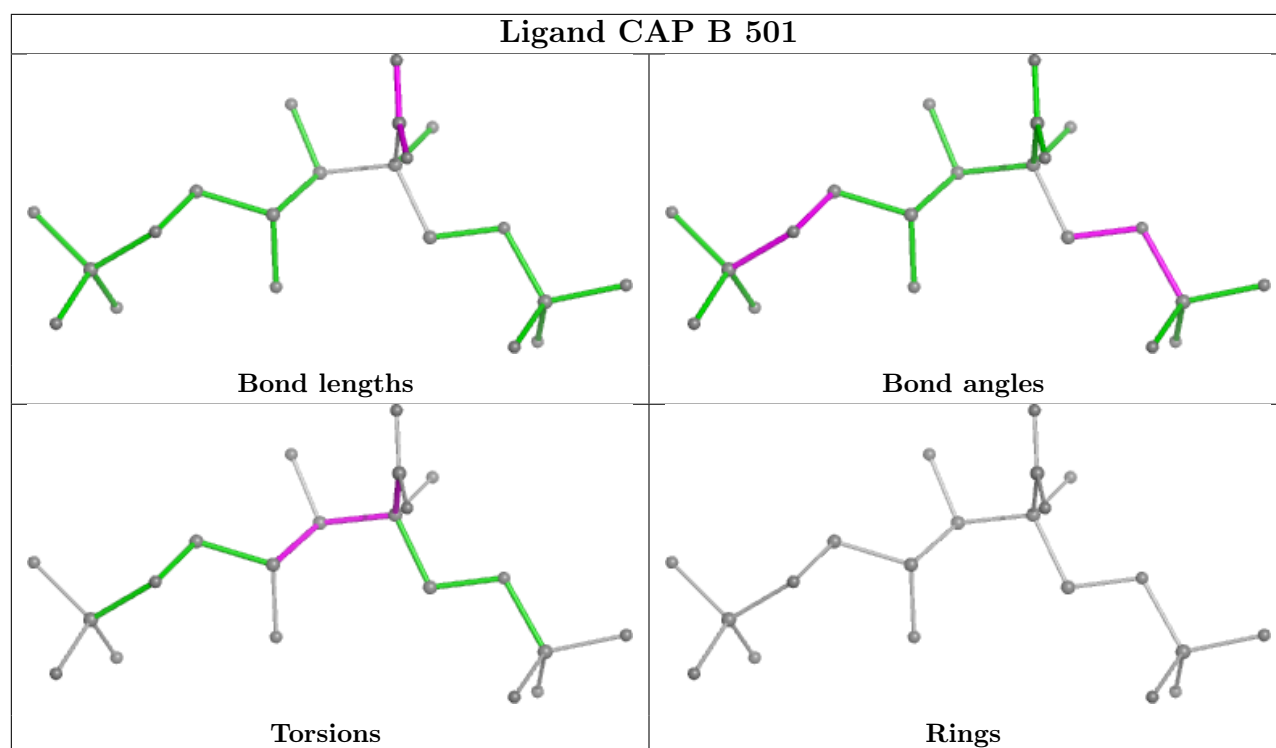There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	503	B3P	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 CAP A 501	
Bond lengths	Bond angles
Torsions	Rings

Ligand B3P C 503	
Bond lengths	Bond angles
Torsions	Rings

Ligand CAP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP B 501

Bond lengths

Bond angles

Torsions

Rings
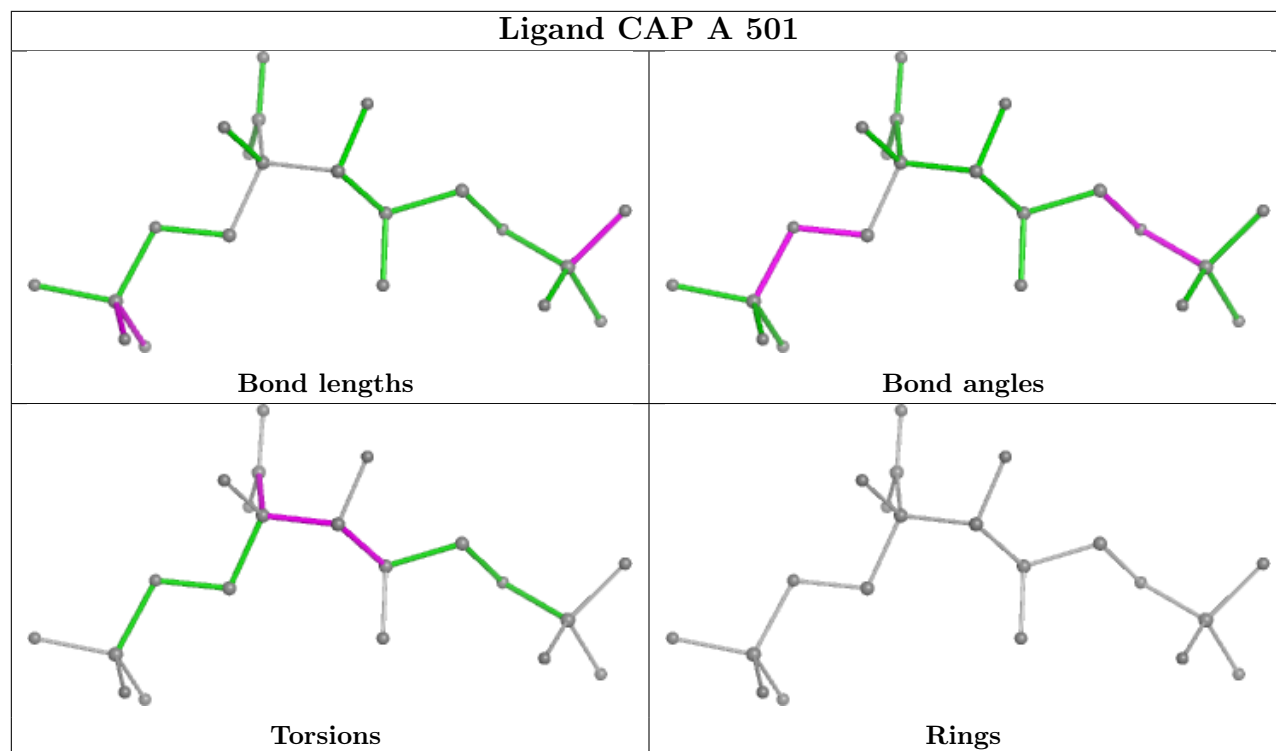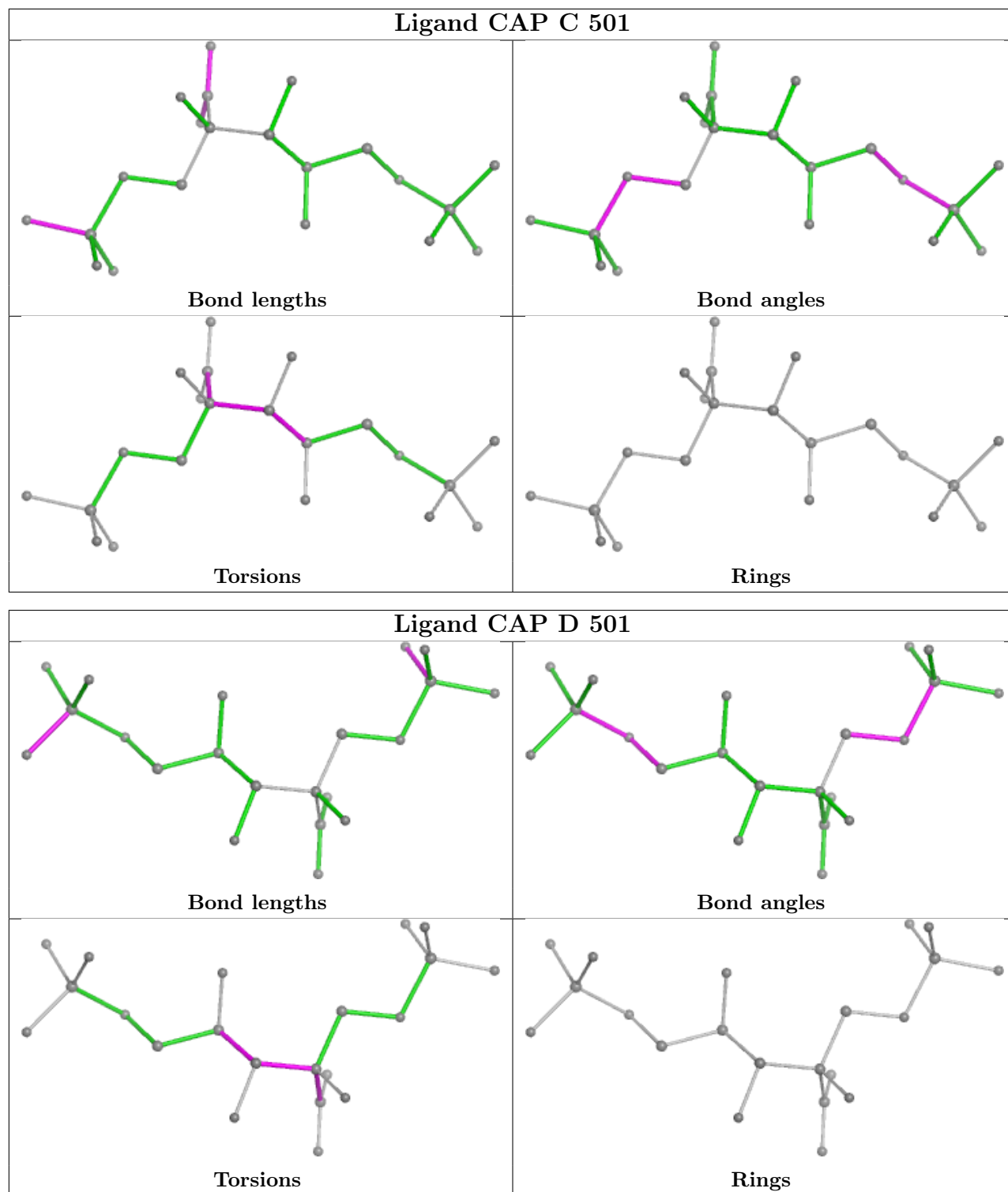
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	449/457 (98%)	-0.68	0	100	100	12, 15, 23, 42	0
1	B	450/457 (98%)	-0.67	2 (0%)	89	92	12, 15, 24, 35	0
1	C	448/457 (98%)	-0.66	3 (0%)	84	88	12, 15, 25, 46	0
1	D	450/457 (98%)	-0.66	1 (0%)	92	94	12, 15, 24, 46	0
2	E	99/105 (94%)	-0.26	0	100	100	16, 21, 31, 40	0
2	F	99/105 (94%)	-0.38	0	100	100	15, 19, 28, 36	0
2	G	102/105 (97%)	-0.17	2 (1%)	64	71	16, 22, 35, 72	0
2	H	105/105 (100%)	-0.26	1 (0%)	79	84	15, 20, 30, 42	0
All	All	2202/2248 (97%)	-0.59	9 (0%)	89	92	12, 16, 27, 72	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	GLN	2.6
2	G	101	HIS	2.6
2	G	100	HIS	2.5
1	B	206	TYR	2.5
2	H	103	HIS	2.4

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

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(Å²)	Q<0.9
1	KCX	D	187	12/13	0.97	0.05	12,12,12,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	B	187	12/13	0.98	0.04	12,12,12,13	0
1	KCX	C	187	12/13	0.98	0.04	12,12,12,12	0
1	KCX	A	187	12/13	0.98	0.04	12,12,12,12	0

6.3   Carbohydrates (i)

There are no monosaccharides in this entry.

6.4   Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

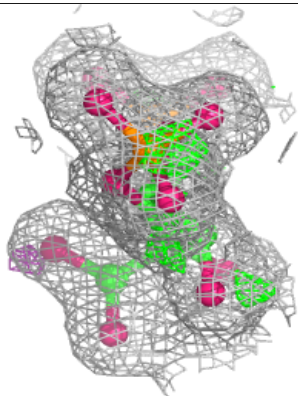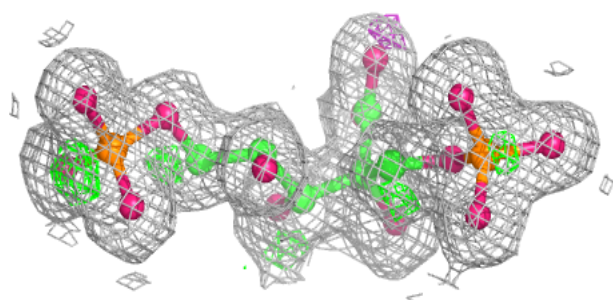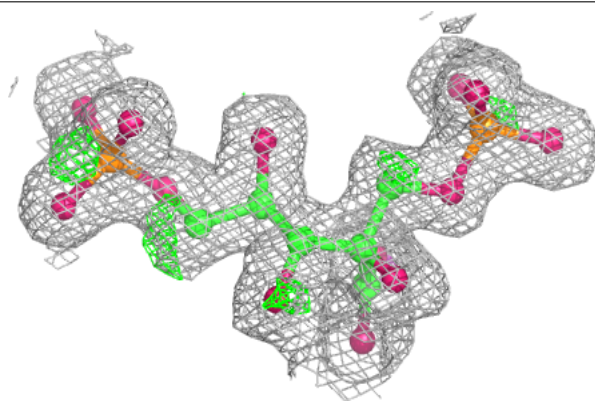| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	B3P	C	503	19/19	0.92	0.08	18,23,32,34	0
3	CAP	A	501	21/21	0.97	0.05	12,12,13,13	0
3	CAP	C	501	21/21	0.98	0.05	12,12,13,14	0
3	CAP	D	501	21/21	0.98	0.05	12,12,14,14	0
3	CAP	B	501	21/21	0.98	0.05	12,12,13,14	0
4	MG	B	502	1/1	0.99	0.02	13,13,13,13	0
4	MG	C	502	1/1	0.99	0.01	12,12,12,12	0
4	MG	D	502	1/1	0.99	0.02	12,12,12,12	0
4	MG	A	502	1/1	0.99	0.03	12,12,12,12	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.
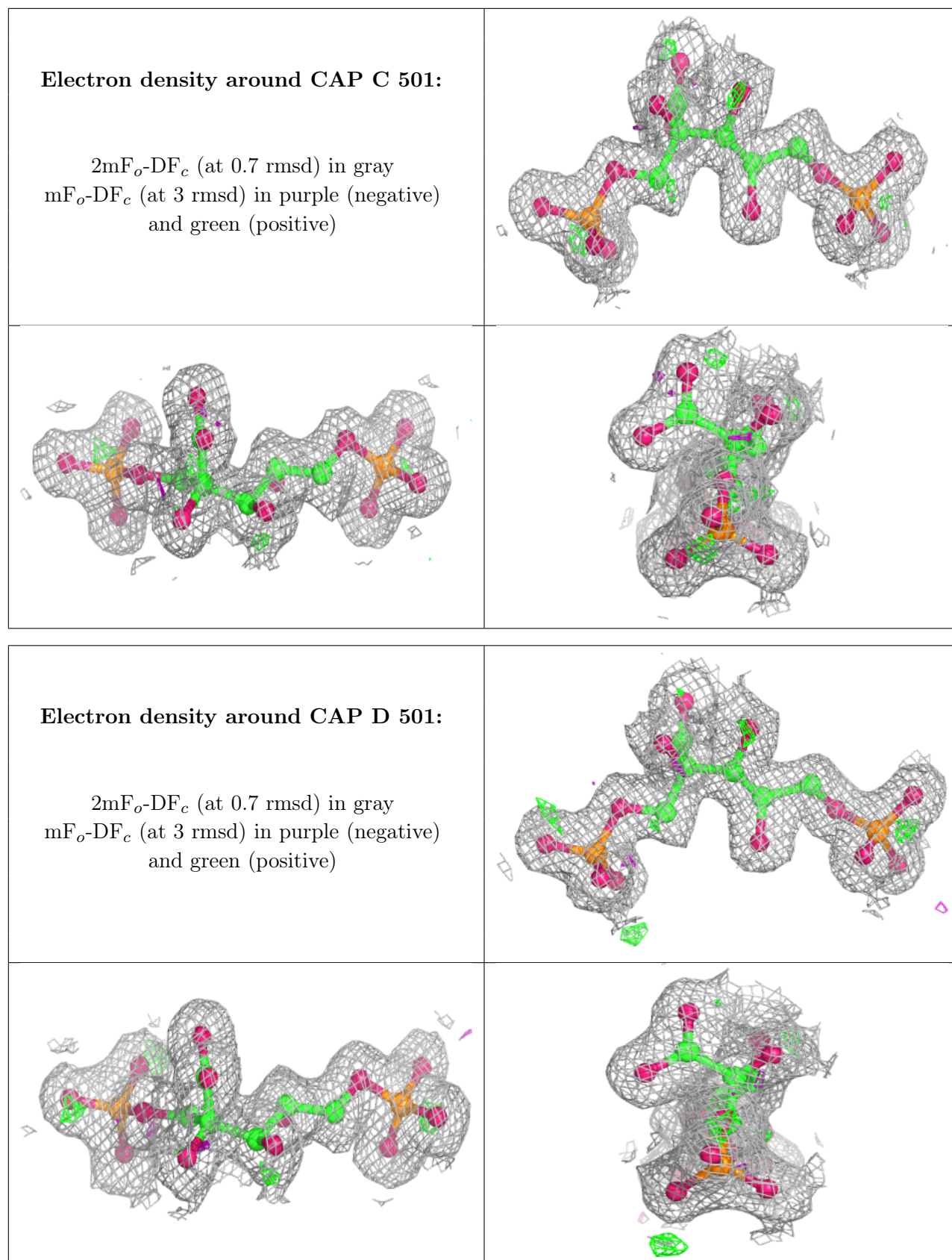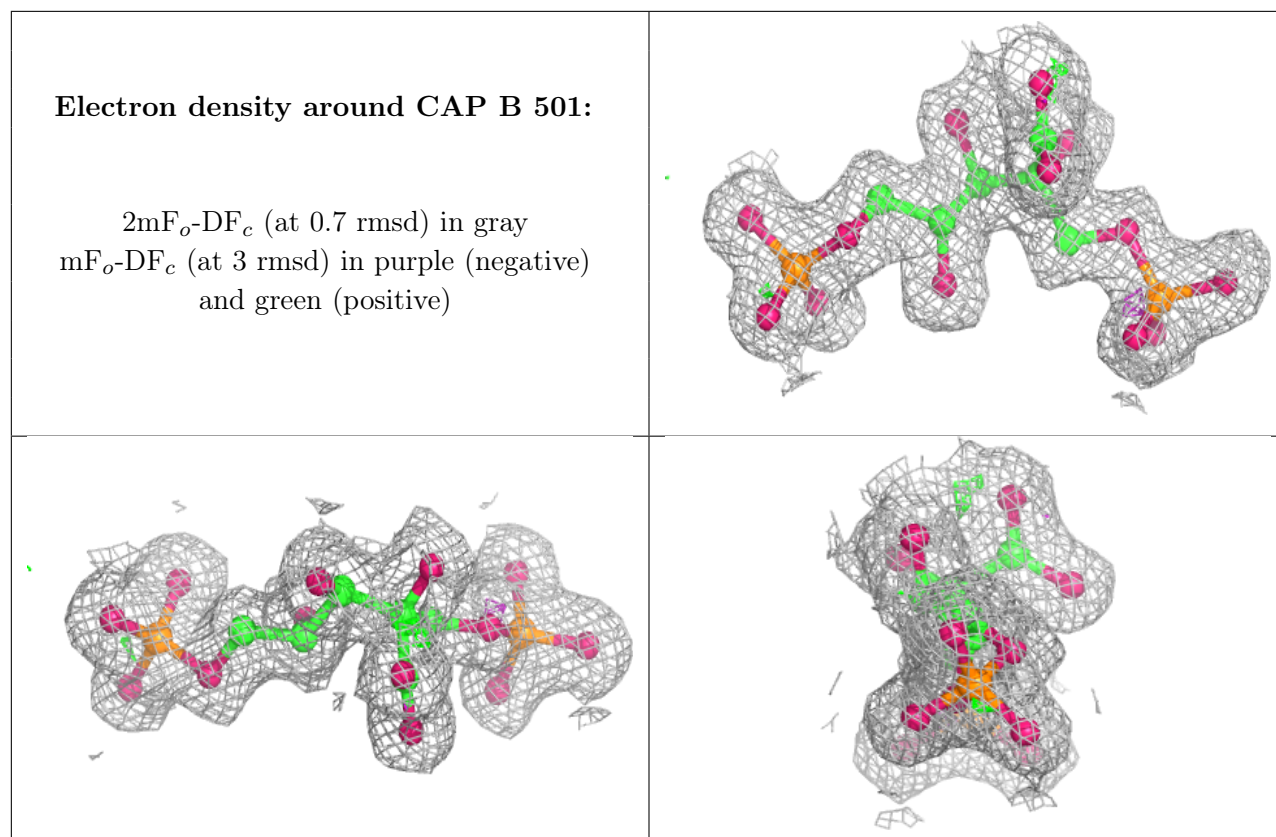
Electron density around B3P C 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
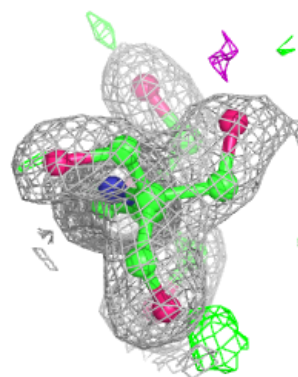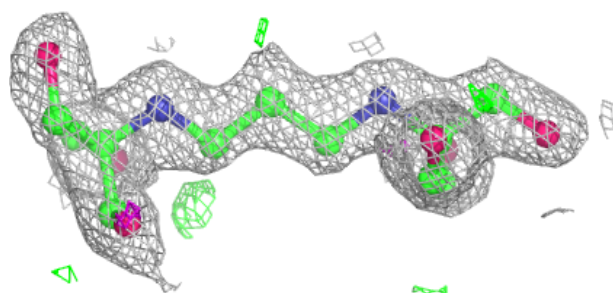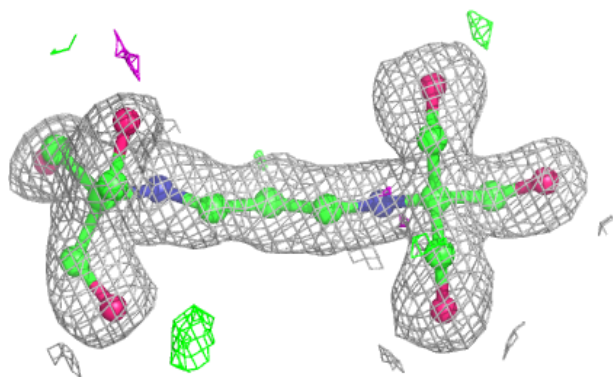
Electron density around CAP A 501:

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

Electron density around 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)

Electron density around CAP D 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 B 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 ⓘ

There are no such residues in this entry.