



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:24 AM UTC

PDB ID : 5HQM / pdb_00005hqm
Title : Structure function studies of R. palustris RubisCO (R. palustris/R. rubrum chimera)
Authors : Arbing, M.A.; Shin, A.; Cascio, D.; Satagopan, S.; Tabita, F.R.
Deposited on : 2016-01-21
Resolution : 1.95 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

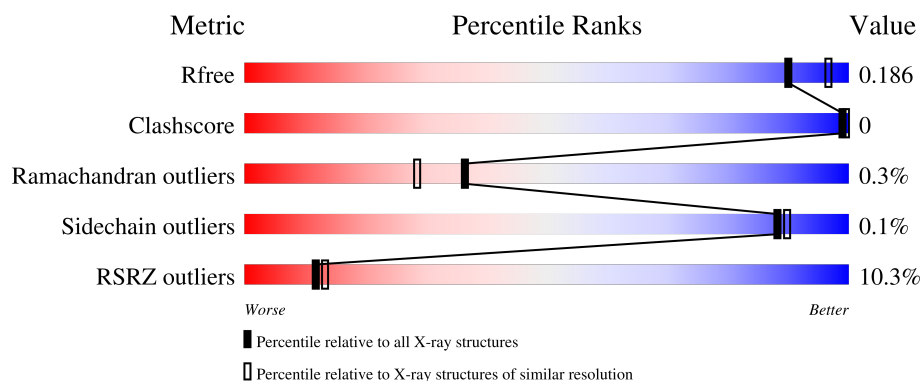
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	487	3% 92% 6%
1	B	487	16% 91% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13945 atoms, of which 6536 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 biphosphate carboxylase (R. palustris/R. rubrum chimera), Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	459	Total	C	H	N	O	S	0	0	0
			6857	2242	3331	612	654	18			
1	B	454	Total	C	H	N	O	S	0	0	0
			6606	2163	3187	596	641	19			

There are 40 discrepancies between the modelled and reference sequences:

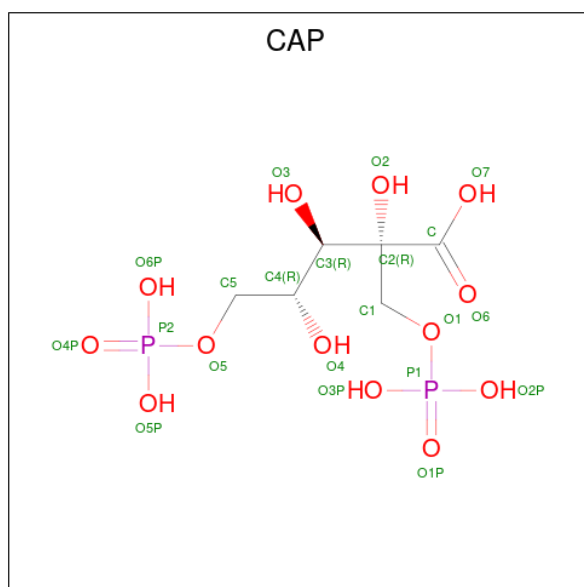
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q6N0W9
A	-18	GLY	-	expression tag	UNP Q6N0W9
A	-17	SER	-	expression tag	UNP Q6N0W9
A	-16	SER	-	expression tag	UNP Q6N0W9
A	-15	HIS	-	expression tag	UNP Q6N0W9
A	-14	HIS	-	expression tag	UNP Q6N0W9
A	-13	HIS	-	expression tag	UNP Q6N0W9
A	-12	HIS	-	expression tag	UNP Q6N0W9
A	-11	HIS	-	expression tag	UNP Q6N0W9
A	-10	HIS	-	expression tag	UNP Q6N0W9
A	-9	SER	-	expression tag	UNP Q6N0W9
A	-8	SER	-	expression tag	UNP Q6N0W9
A	-7	GLY	-	expression tag	UNP Q6N0W9
A	-6	LEU	-	expression tag	UNP Q6N0W9
A	-5	VAL	-	expression tag	UNP Q6N0W9
A	-4	PRO	-	expression tag	UNP Q6N0W9
A	-3	ARG	-	expression tag	UNP Q6N0W9
A	-2	GLY	-	expression tag	UNP Q6N0W9
A	-1	SER	-	expression tag	UNP Q6N0W9
A	0	HIS	-	expression tag	UNP Q6N0W9
B	-19	MET	-	initiating methionine	UNP Q6N0W9
B	-18	GLY	-	expression tag	UNP Q6N0W9
B	-17	SER	-	expression tag	UNP Q6N0W9
B	-16	SER	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q6N0W9
B	-14	HIS	-	expression tag	UNP Q6N0W9
B	-13	HIS	-	expression tag	UNP Q6N0W9
B	-12	HIS	-	expression tag	UNP Q6N0W9
B	-11	HIS	-	expression tag	UNP Q6N0W9
B	-10	HIS	-	expression tag	UNP Q6N0W9
B	-9	SER	-	expression tag	UNP Q6N0W9
B	-8	SER	-	expression tag	UNP Q6N0W9
B	-7	GLY	-	expression tag	UNP Q6N0W9
B	-6	LEU	-	expression tag	UNP Q6N0W9
B	-5	VAL	-	expression tag	UNP Q6N0W9
B	-4	PRO	-	expression tag	UNP Q6N0W9
B	-3	ARG	-	expression tag	UNP Q6N0W9
B	-2	GLY	-	expression tag	UNP Q6N0W9
B	-1	SER	-	expression tag	UNP Q6N0W9
B	0	HIS	-	expression tag	UNP Q6N0W9

- 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
2	A	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	B	1	Total	C	H	O	P	0	0
			30	6	9	13	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0

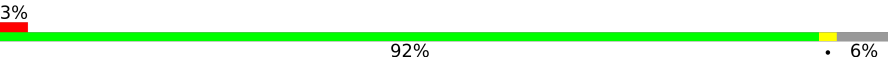
- Molecule 5 is water.

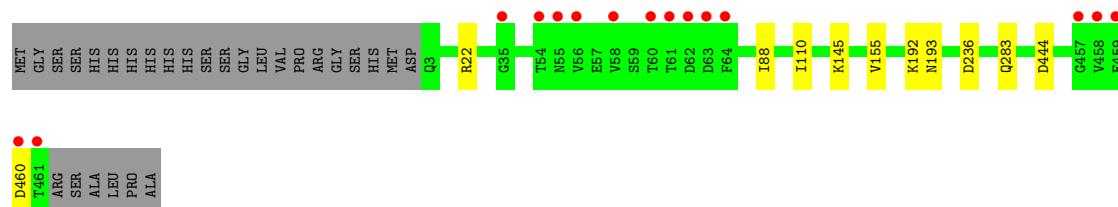
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	214	Total O 214 214	0	0
5	B	204	Total O 204 204	0	0

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.

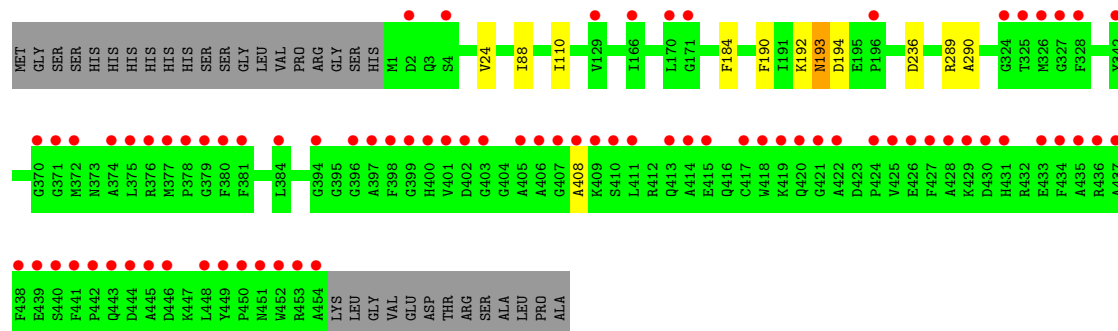
- Molecule 1: Ribulose biphosphate carboxylase (R. palustris/R. rubrum chimera), Ribulose biphosphate carboxylase

Chain A: 



- Molecule 1: Ribulose biphosphate carboxylase (R. palustris/R. rubrum chimera), Ribulose biphosphate carboxylase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	165.12Å 165.12Å 95.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.56 – 1.95 82.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (82.56-1.95) 99.7 (82.56-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.95Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0	Depositor
R, R_{free}	0.167 , 0.192 0.163 , 0.186	Depositor DCC
R_{free} test set	7050 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13945	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, K, 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	0.84	0/3602	1.06	4/4877 (0.1%)
1	B	0.85	1/3490 (0.0%)	1.04	3/4733 (0.1%)
All	All	0.84	1/7092 (0.0%)	1.05	7/9610 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	ASP	CA-C	5.45	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	GLN	OE1-CD-NE2	-6.86	115.74	122.60
1	B	236	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	193	ASN	CA-CB-CG	5.89	118.49	112.60
1	A	444	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	236	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	190	PHE	CA-CB-CG	5.43	119.23	113.80
1	B	193	ASN	CA-CB-CG	5.26	117.86	112.60

There are no chirality outliers.

There are no planarity outliers.

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	3526	3331	3384	3	0
1	B	3419	3187	3223	3	0
2	A	21	9	7	0	0
2	B	21	9	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	214	0	0	0	0
5	B	204	0	0	0	0
All	All	7409	6536	6622	6	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 0.

All (6) 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:A:22:ARG:NH2	1:A:88:ILE:HD11	2.25	0.51
1:A:145:LYS:HG3	1:A:155:VAL:HB	1.95	0.48
1:B:24:VAL:HG23	1:B:88:ILE:HG22	1.99	0.45
1:A:22:ARG:CZ	1:A:88:ILE:HD11	2.48	0.44
1:B:184:PHE:CD1	1:B:408:ALA:HB2	2.56	0.41
1:B:289:ARG:O	1:B:290:ALA:C	2.64	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	456/487 (94%)	442 (97%)	12 (3%)	2 (0%)	30	21
1	B	451/487 (93%)	439 (97%)	11 (2%)	1 (0%)	43	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	907/974 (93%)	881 (97%)	23 (2%)	3 (0%)	36	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	ASP
1	A	110	ILE
1	B	110	ILE

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	348/377 (92%)	348 (100%)	0	100	100
1	B	328/377 (87%)	327 (100%)	1 (0%)	86	87
All	All	676/754 (90%)	675 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	B	283	GLN
1	B	316	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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	A	192	3,1	10,11,12	1.66	2 (20%)	6,12,14	2.41	2 (33%)
1	KCX	B	192	3,1	10,11,12	2.19	2 (20%)	6,12,14	3.75	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	192	3,1	-	0/9/10/12	-
1	KCX	B	192	3,1	-	0/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	KCX	OQ1-CX	5.53	1.31	1.21
1	A	192	KCX	OQ1-CX	3.73	1.28	1.21
1	B	192	KCX	CX-NZ	3.31	1.41	1.35
1	A	192	KCX	CX-NZ	3.03	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	KCX	OQ1-CX-NZ	-7.92	112.89	124.92
1	A	192	KCX	CE-NZ-CX	-5.33	112.94	121.98
1	B	192	KCX	CE-NZ-CX	-4.63	114.13	121.98
1	A	192	KCX	OQ1-CX-NZ	-2.20	121.59	124.92

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	A	501	3	18,20,20	1.28	2 (11%)	23,31,31	1.84	7 (30%)
2	CAP	B	501	3	18,20,20	1.02	0	23,31,31	1.84	7 (30%)

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	A	501	3	-	8/29/29/29	-
2	CAP	B	501	3	-	9/29/29/29	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CAP	P2-O6P	-2.92	1.44	1.54
2	A	501	CAP	C2-C	-2.44	1.51	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	CAP	O7-C-C2	5.09	122.59	114.06
2	B	501	CAP	O5-P2-O4P	4.64	118.99	106.44
2	A	501	CAP	O6P-P2-O5	3.45	115.66	106.67
2	A	501	CAP	O6-C-C2	-3.03	116.67	122.32
2	B	501	CAP	O6P-P2-O4P	-2.99	99.18	110.83
2	B	501	CAP	O5P-P2-O5	2.80	113.96	106.67
2	B	501	CAP	O6P-P2-O5	2.78	113.93	106.67
2	B	501	CAP	O7-C-C2	2.35	118.00	114.06
2	A	501	CAP	O5-P2-O4P	2.34	112.76	106.44
2	A	501	CAP	O2P-P1-O1	2.25	112.55	106.67
2	B	501	CAP	O2P-P1-O1	2.24	112.52	106.67
2	A	501	CAP	O1-P1-O1P	2.12	112.16	106.44
2	A	501	CAP	O3P-P1-O1	2.11	112.17	106.67
2	B	501	CAP	O1-P1-O1P	2.05	111.98	106.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

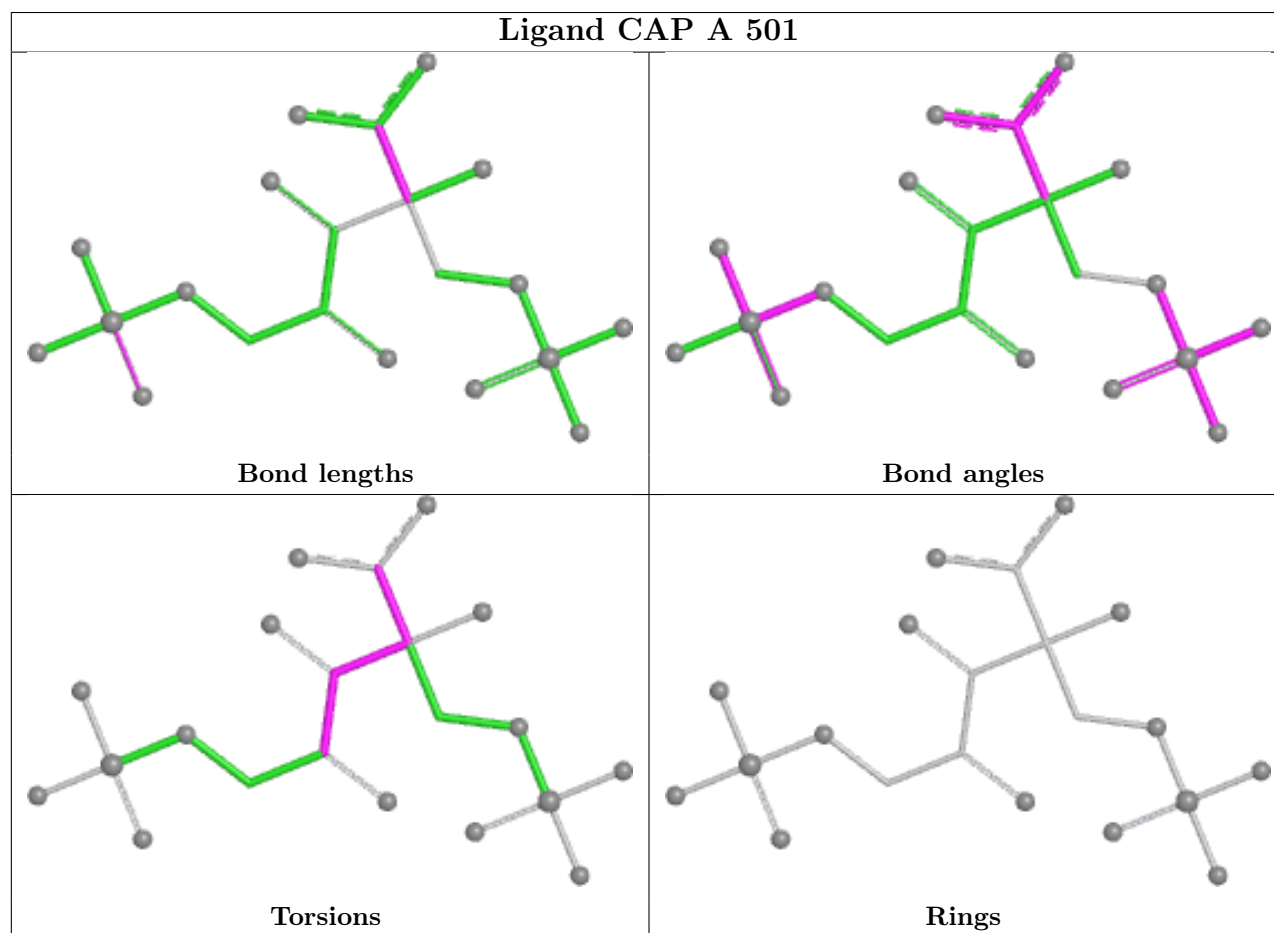
Mol	Chain	Res	Type	Atoms
2	A	501	CAP	O6-C-C2-O2
2	A	501	CAP	C2-C3-C4-O4
2	A	501	CAP	O3-C3-C4-O4
2	B	501	CAP	O6-C-C2-C3
2	B	501	CAP	O7-C-C2-C3
2	B	501	CAP	O6-C-C2-O2
2	B	501	CAP	O7-C-C2-O2
2	B	501	CAP	C2-C3-C4-O4
2	B	501	CAP	O3-C3-C4-O4
2	B	501	CAP	O6-C-C2-C1
2	B	501	CAP	O7-C-C2-C1
2	A	501	CAP	O6-C-C2-C3
2	A	501	CAP	O2-C2-C3-C4
2	B	501	CAP	O2-C2-C3-C4
2	A	501	CAP	O7-C-C2-C3
2	A	501	CAP	O7-C-C2-O2
2	A	501	CAP	O7-C-C2-C1

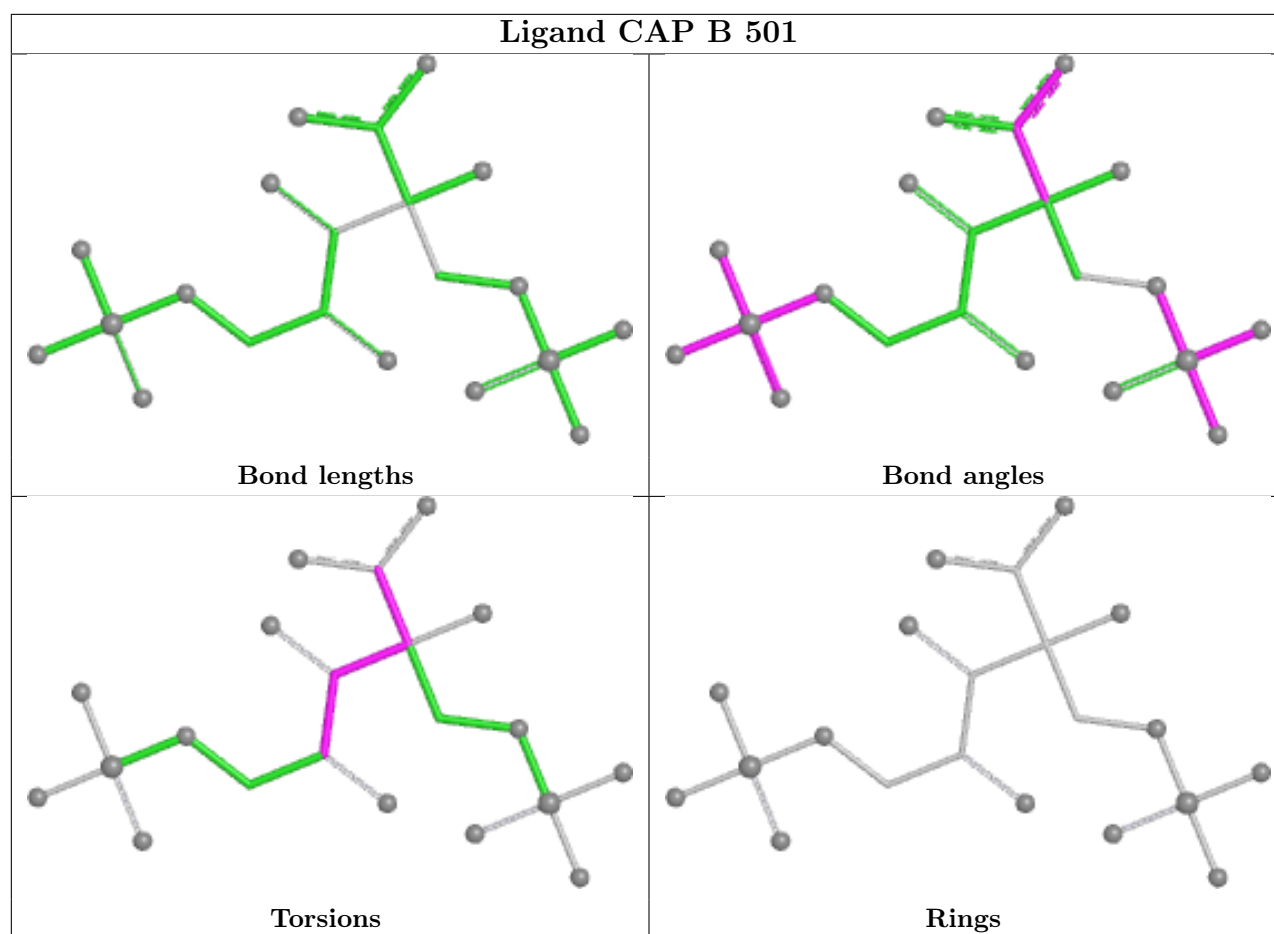
There are no ring outliers.

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	458/487 (94%)	0.06	15 (3%)	49	55	25, 42, 66, 111	0
1	B	453/487 (93%)	0.64	79 (17%)	4	4	24, 43, 78, 127	0
All	All	911/974 (93%)	0.35	94 (10%)	12	13	24, 42, 73, 127	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	454	ALA	8.6
1	A	461	THR	7.8
1	B	425	VAL	7.5
1	B	418	TRP	6.5
1	B	401	VAL	6.2
1	B	398	PHE	6.0
1	B	438	PHE	5.9
1	B	452	TRP	5.9
1	B	449	TYR	5.3
1	B	441	PHE	5.2
1	B	424	PRO	4.9
1	B	437	ALA	4.7
1	B	434	PHE	4.5
1	B	417	CYS	4.5
1	B	448	LEU	4.5
1	B	427	PHE	4.3
1	B	378	PRO	4.3
1	B	422	ALA	4.2
1	B	435	ALA	4.1
1	B	403	GLY	4.1
1	B	407	GLY	4.1
1	B	166	ILE	4.0
1	B	381	PHE	3.9
1	B	444	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	411	LEU	3.8
1	B	396	GLY	3.8
1	A	35	GLY	3.7
1	B	170	LEU	3.7
1	B	420	GLN	3.7
1	A	459	GLU	3.6
1	B	400	HIS	3.6
1	B	429	LYS	3.6
1	B	428	ALA	3.5
1	B	419	LYS	3.5
1	A	458	VAL	3.5
1	B	431	HIS	3.5
1	B	451	ASN	3.4
1	B	375	LEU	3.4
1	B	442	PRO	3.3
1	B	374	ALA	3.3
1	B	171	GLY	3.2
1	B	402	ASP	3.2
1	A	61	THR	3.1
1	A	63	ASP	3.1
1	B	325	THR	3.1
1	A	460	ASP	3.1
1	B	408	ALA	3.0
1	B	445	ALA	3.0
1	B	371	GLY	3.0
1	B	406	ALA	3.0
1	B	377	MET	2.9
1	B	433	GLU	2.9
1	B	430	ASP	2.9
1	B	439	GLU	2.8
1	B	397	ALA	2.8
1	B	443	GLN	2.8
1	B	450	PRO	2.8
1	B	410	SER	2.7
1	B	328	PHE	2.7
1	B	384	LEU	2.7
1	A	60	THR	2.7
1	A	457	GLY	2.7
1	A	64	PHE	2.6
1	B	372	MET	2.6
1	B	413	GLN	2.6
1	B	426	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	380	PHE	2.6
1	B	370	GLY	2.6
1	B	4	SER	2.6
1	B	196	PRO	2.6
1	B	405	ALA	2.6
1	B	324	GLY	2.5
1	B	399	GLY	2.5
1	A	54	THR	2.5
1	B	394	GLY	2.5
1	A	56	VAL	2.5
1	B	414	ALA	2.4
1	B	342	TYR	2.4
1	B	453	ARG	2.3
1	B	436	ARG	2.3
1	B	440	SER	2.3
1	B	376	ARG	2.3
1	B	421	GLY	2.2
1	B	409	LYS	2.2
1	B	446	ASP	2.2
1	B	379	GLY	2.2
1	B	327	GLY	2.2
1	A	58	VAL	2.1
1	B	415	GLU	2.1
1	A	55	ASN	2.1
1	B	2	ASP	2.1
1	A	62	ASP	2.1
1	B	129	VAL	2.0
1	B	326	MET	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	B	192	12/13	0.91	0.12	39,44,50,51	0
1	KCX	A	192	12/13	0.96	0.09	30,32,36,38	0

6.3 Carbohydrates [i](#)

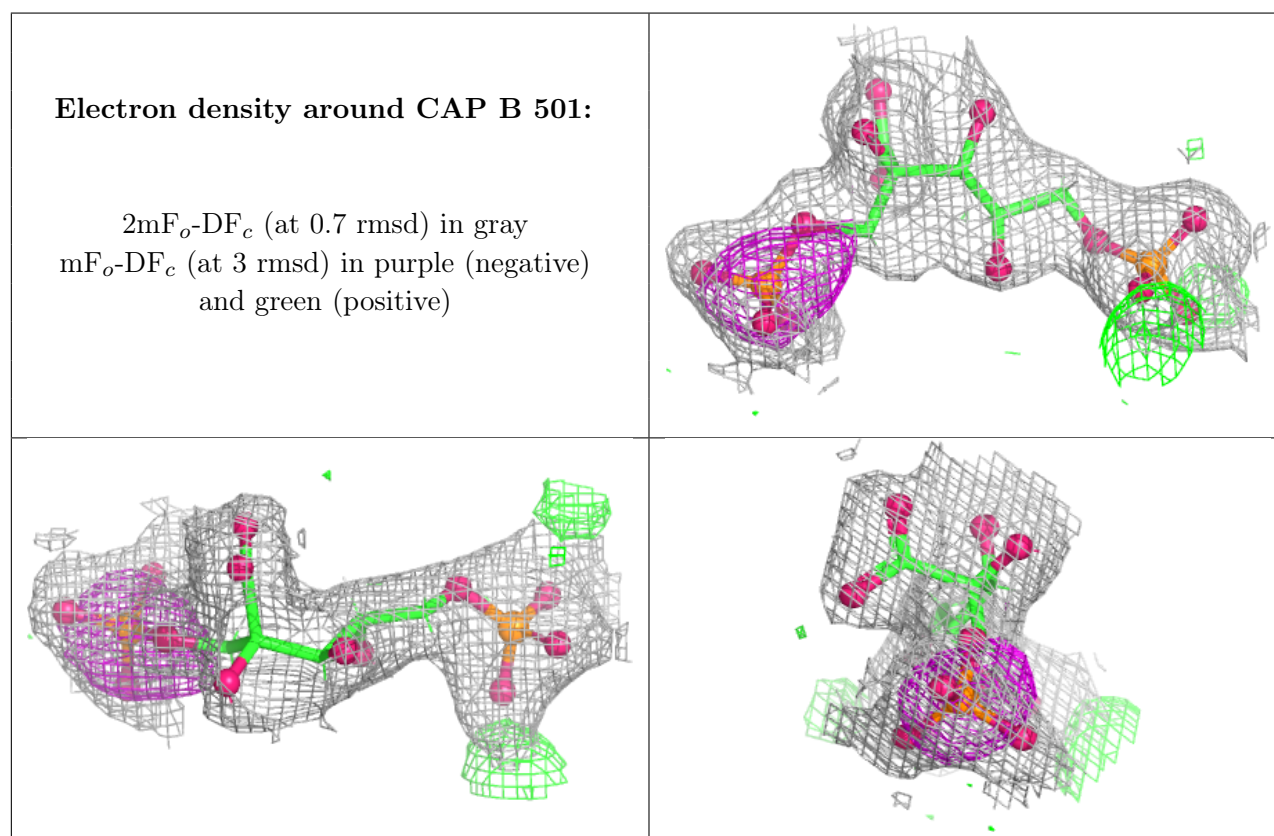
There are no oligosaccharides in this entry.

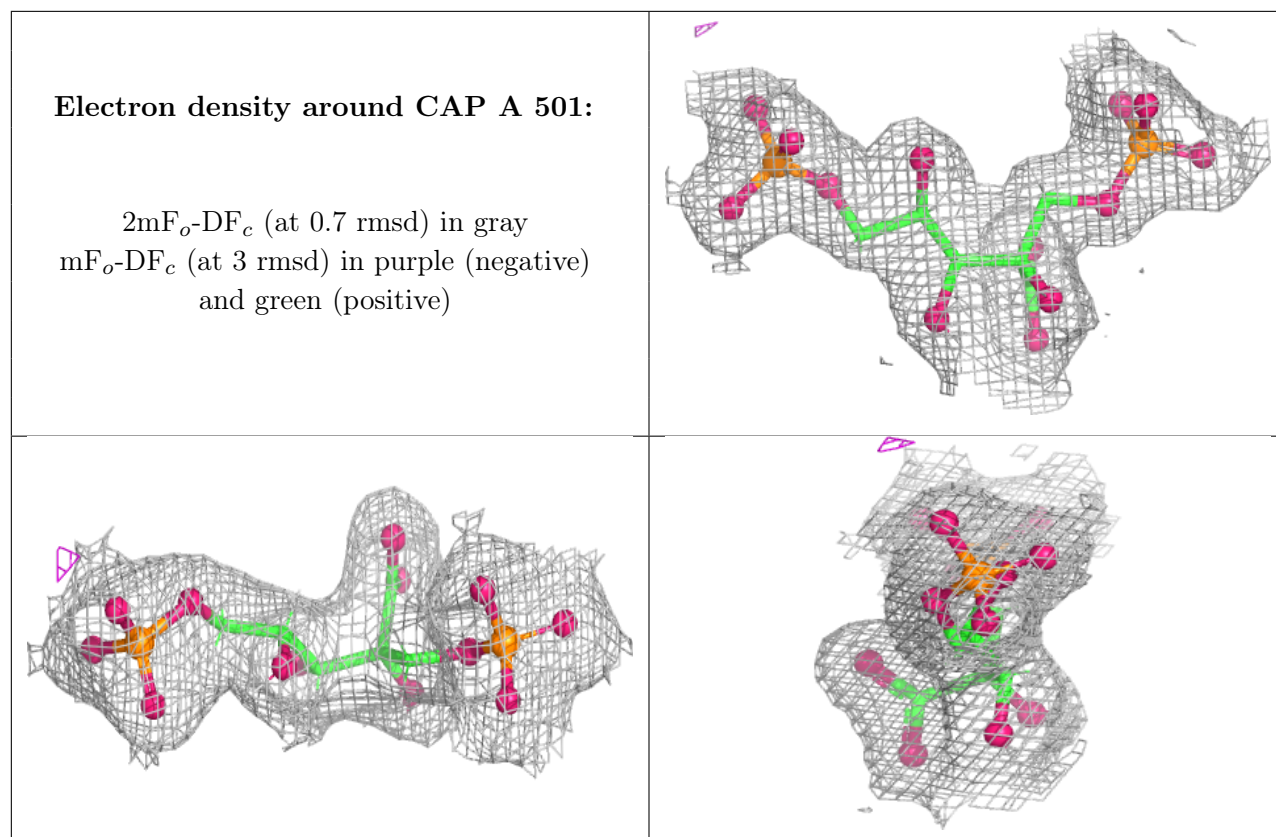
6.4 Ligands [i](#)

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
2	CAP	B	501	21/21	0.88	0.11	51,55,59,62	0
4	K	A	503	1/1	0.96	0.07	49,49,49,49	0
4	K	B	503	1/1	0.97	0.06	49,49,49,49	0
2	CAP	A	501	21/21	0.98	0.05	33,39,43,43	0
3	MG	A	502	1/1	0.99	0.03	36,36,36,36	0
3	MG	B	502	1/1	0.99	0.10	49,49,49,49	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.