



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:55 AM UTC

PDB ID : 5K85 / pdb_00005k85
Title : Crystal Structure of Acetyl-CoA Synthetase in Complex with Adenosine-5'-p
ropylphosphate and Coenzyme A from *Cryptococcus neoformans* H99
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SSGCID
Deposited on : 2016-05-27
Resolution : 2.30 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](#) ①) were used in the production of this report:

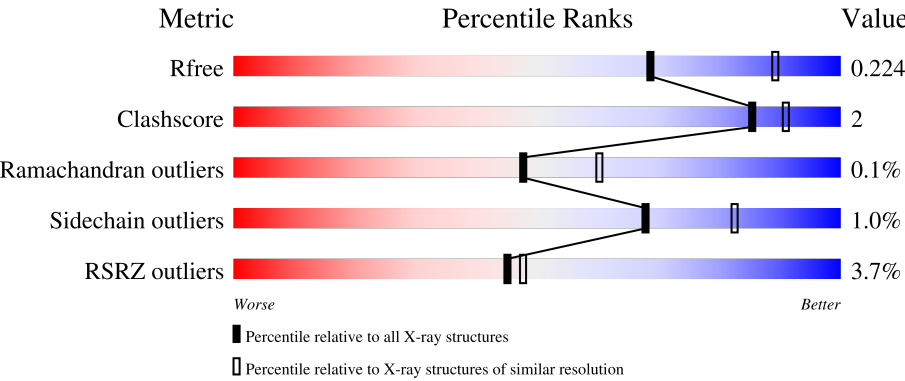
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	694	2% 89% 5% 6%
1	B	694	3% 87% 6% 7%
1	C	694	5% 79% 5% 16%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15536 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 Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	0	10	0
			5090	3252	864	947	27			
1	B	647	Total	C	N	O	S	0	15	0
			5121	3269	871	954	27			
1	C	584	Total	C	N	O	S	0	0	0
			4413	2824	749	816	24			

There are 45 discrepancies between the modelled and reference sequences:

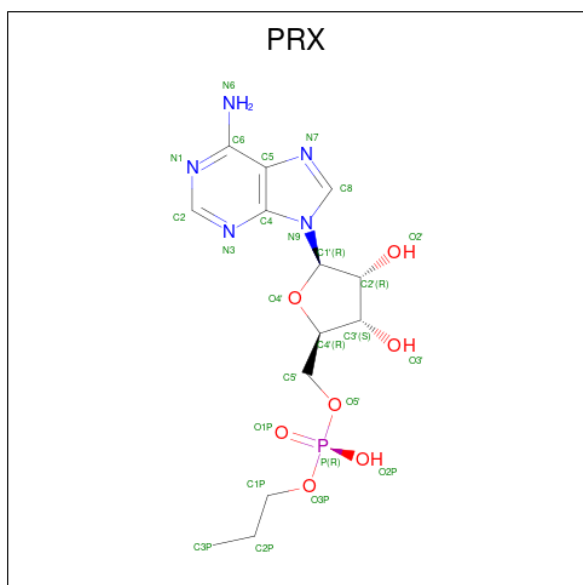
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression tag	UNP J9VFT1
A	-6	HIS	-	expression tag	UNP J9VFT1
A	-5	HIS	-	expression tag	UNP J9VFT1
A	-4	GLU	-	expression tag	UNP J9VFT1
A	-3	ASN	-	expression tag	UNP J9VFT1
A	-2	LEU	-	expression tag	UNP J9VFT1
A	-1	TYR	-	expression tag	UNP J9VFT1
A	0	PHE	-	expression tag	UNP J9VFT1
A	1	GLN	-	expression tag	UNP J9VFT1
B	-13	MET	-	initiating methionine	UNP J9VFT1
B	-12	HIS	-	expression tag	UNP J9VFT1
B	-11	HIS	-	expression tag	UNP J9VFT1
B	-10	HIS	-	expression tag	UNP J9VFT1
B	-9	HIS	-	expression tag	UNP J9VFT1
B	-8	HIS	-	expression tag	UNP J9VFT1
B	-7	HIS	-	expression tag	UNP J9VFT1
B	-6	HIS	-	expression tag	UNP J9VFT1

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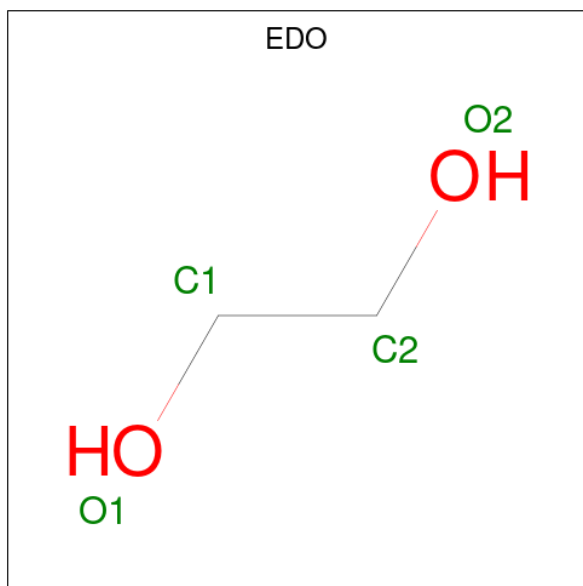
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
C	-13	MET	-	initiating methionine	UNP J9VFT1
C	-12	HIS	-	expression tag	UNP J9VFT1
C	-11	HIS	-	expression tag	UNP J9VFT1
C	-10	HIS	-	expression tag	UNP J9VFT1
C	-9	HIS	-	expression tag	UNP J9VFT1
C	-8	HIS	-	expression tag	UNP J9VFT1
C	-7	HIS	-	expression tag	UNP J9VFT1
C	-6	HIS	-	expression tag	UNP J9VFT1
C	-5	HIS	-	expression tag	UNP J9VFT1
C	-4	GLU	-	expression tag	UNP J9VFT1
C	-3	ASN	-	expression tag	UNP J9VFT1
C	-2	LEU	-	expression tag	UNP J9VFT1
C	-1	TYR	-	expression tag	UNP J9VFT1
C	0	PHE	-	expression tag	UNP J9VFT1
C	1	GLN	-	expression tag	UNP J9VFT1

- Molecule 2 is ADENOSINE-5'-MONOPHOSPHATE-PROPYL ESTER (CCD ID: PRX) (formula: $C_{13}H_{20}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			26	13	5	7	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



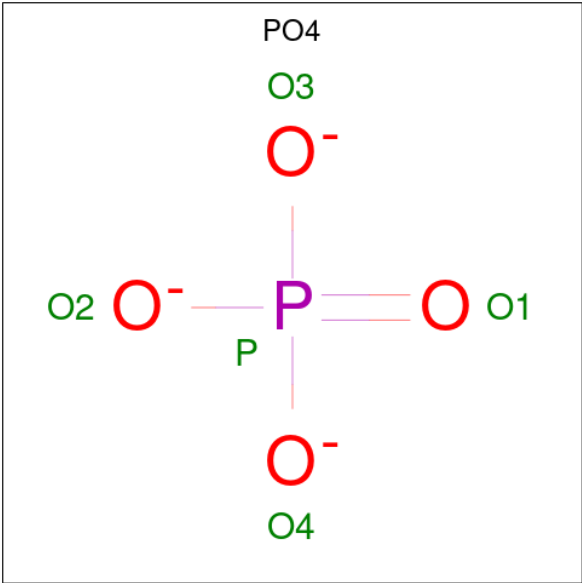
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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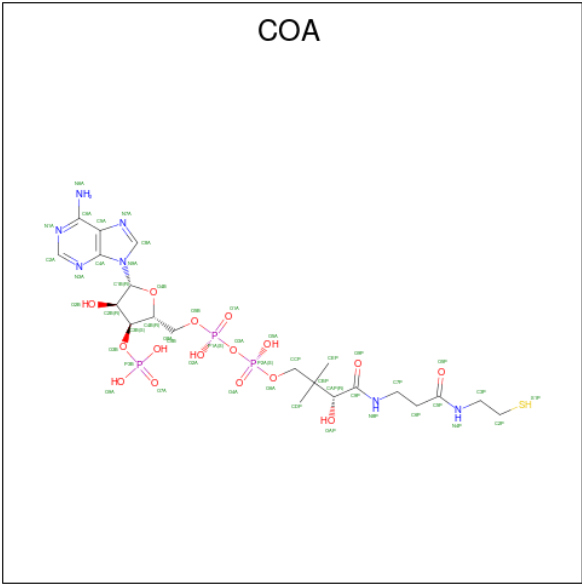
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

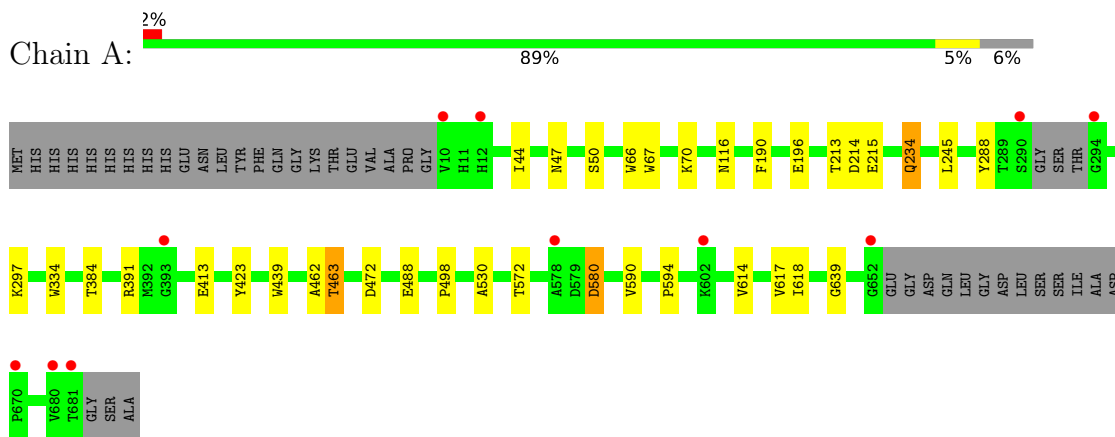
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	303	Total	O	0	0
			303	303		
6	B	280	Total	O	0	0
			280	280		
6	C	158	Total	O	0	0
			158	158		

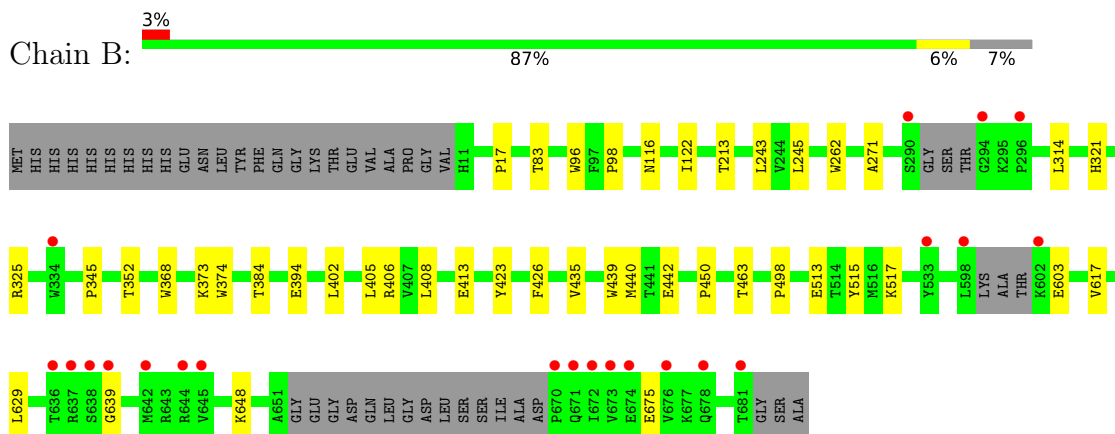
3 Residue-property plots [i](#)

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.

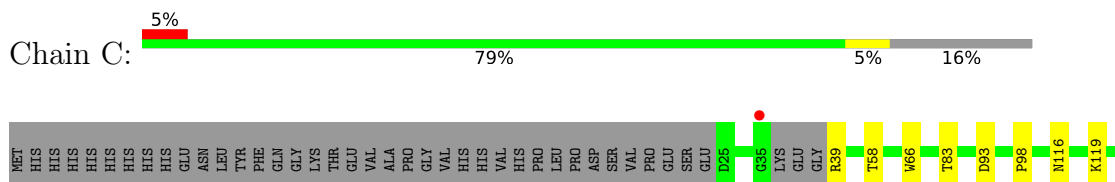
- Molecule 1: Acetyl-coenzyme A synthetase

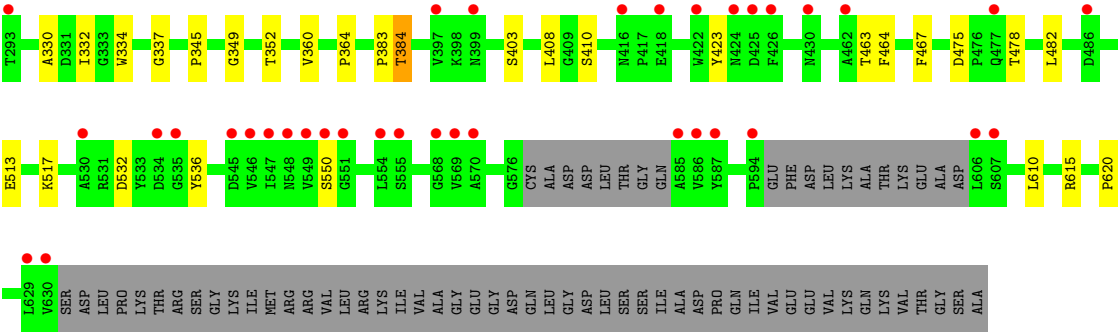


- Molecule 1: Acetyl-coenzyme A synthetase



- Molecule 1: Acetyl-coenzyme A synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.80Å 186.09Å 85.32Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	27.57 – 2.30 27.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (27.57-2.30) 97.5 (27.57-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.29Å)	Xtriage
Refinement program	PHENIX (DEV_2443: ???)	Depositor
R, R_{free}	0.179 , 0.217 0.189 , 0.224	Depositor DCC
R_{free} test set	1996 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15536	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: PO4, EDO, COA, PRX

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	0.29	0/5250	0.47	0/7164
1	B	0.27	0/5282	0.45	0/7196
1	C	0.24	0/4541	0.42	0/6209
All	All	0.27	0/15073	0.45	0/20569

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5090	0	4836	21	0
1	B	5121	0	4902	20	0
1	C	4413	0	4084	23	0
2	A	26	0	19	1	0
2	B	26	0	19	1	0
2	C	26	0	19	0	0
3	A	28	0	42	3	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	48	0	32	5	0
6	A	303	0	0	1	0
6	B	280	0	0	0	0
6	C	158	0	0	0	0
All	All	15536	0	13971	64	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 (64) 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:50:SER:HB2	3:A:702:EDO:H21	1.70	0.74
1:C:39:ARG:NH2	1:C:403:SER:O	2.29	0.65
1:A:384:THR:HG21	1:A:639:GLY:HA3	1.79	0.63
1:B:513:GLU:HA	1:B:517:LYS:HG3	1.80	0.63
1:B:368:TRP:HB3	1:B:402:LEU:HD21	1.80	0.63
1:C:615:ARG:HG2	1:C:620:PRO:HA	1.80	0.62
1:B:384[A]:THR:HG21	1:B:639:GLY:HA3	1.81	0.61
1:A:234:GLN:NE2	6:A:805:HOH:O	2.36	0.58
1:A:617:VAL:HG23	1:A:618:ILE:HG13	1.86	0.58
1:A:439:TRP:CE2	2:A:701:PRX:H3P1	2.38	0.58
1:C:615:ARG:NH2	5:C:801:COA:O8A	2.35	0.56
1:C:334:TRP:CD1	5:C:801:COA:H31	2.41	0.56
1:A:47:ASN:HA	3:A:706:EDO:H22	1.86	0.55
1:B:439:TRP:CE2	2:B:702:PRX:H3P1	2.41	0.55
1:A:44:ILE:HG23	3:A:702:EDO:H22	1.91	0.53
1:A:196:GLU:OE1	1:A:196:GLU:N	2.41	0.50
1:C:332:ILE:HA	1:C:337:GLY:HA3	1.93	0.50
1:A:391:ARG:HH11	1:A:594:PRO:HD3	1.77	0.49
1:B:442:GLU:HG2	1:B:515:TYR:CZ	2.48	0.49
1:B:603:GLU:HG3	1:B:629:LEU:HD22	1.95	0.49
1:C:360:VAL:HA	1:C:364:PRO:HA	1.94	0.49
5:C:801:COA:HN8	5:C:801:COA:H131	1.77	0.49
1:B:405:LEU:HD13	1:B:408:LEU:HD21	1.93	0.49
1:C:408:LEU:HB3	1:C:423:TYR:CZ	2.48	0.49
1:A:190[A]:PHE:HZ	1:A:334[A]:TRP:HB2	1.77	0.49
1:C:475:ASP:HB3	1:C:478:THR:HB	1.93	0.49
1:B:17:PRO:HB3	1:B:617:VAL:HG11	1.94	0.48
1:B:314:LEU:HD22	1:B:345:PRO:HA	1.96	0.48
1:C:334:TRP:HD1	5:C:801:COA:H31	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ALA:HB1	5:C:801:COA:H32	1.97	0.47
1:C:463:THR:OG1	1:C:464:PHE:N	2.47	0.47
1:B:373:LYS:HE3	1:B:374:TRP:NE1	2.29	0.47
1:A:190[A]:PHE:CZ	1:A:334[A]:TRP:HB2	2.50	0.47
1:C:58:THR:HG21	1:C:467:PHE:HB3	1.95	0.47
1:C:83:THR:O	1:C:98:PRO:HD2	2.15	0.47
1:A:288:TYR:HA	1:A:297:LYS:O	2.16	0.46
1:A:66:TRP:CZ2	1:A:70:LYS:HE3	2.52	0.45
1:A:67:TRP:CZ3	1:A:498:PRO:HG2	2.52	0.45
1:B:440:MET:HE3	1:B:442:GLU:HB2	1.98	0.45
1:A:462:ALA:O	1:A:463:THR:OG1	2.32	0.45
1:B:213:THR:HG22	1:B:245:LEU:HB3	1.99	0.44
1:A:614:VAL:HG13	1:A:618:ILE:HD12	2.00	0.44
1:C:532:ASP:OD2	1:C:536:TYR:HB2	2.18	0.44
1:C:345:PRO:HB2	1:C:352:THR:HB	1.99	0.43
1:C:513:GLU:HA	1:C:517:LYS:HG3	2.00	0.43
1:B:243:LEU:HD11	1:B:262:TRP:HA	2.01	0.43
1:C:384:THR:OG1	1:C:550:SER:HA	2.18	0.43
1:B:83:THR:O	1:B:98:PRO:HD2	2.20	0.42
1:C:58:THR:HG22	1:C:66:TRP:CD2	2.54	0.42
1:A:580:ASP:OD1	1:A:580:ASP:N	2.42	0.42
1:B:271:ALA:HB3	1:C:93:ASP:HB3	2.01	0.42
1:B:321:HIS:HD2	1:B:406[B]:ARG:HH22	1.68	0.42
1:B:435:VAL:HG12	1:B:450:PRO:HG2	2.02	0.42
1:B:122:ILE:HA	1:B:352:THR:O	2.20	0.42
1:A:488[A]:GLU:HG3	1:A:530:ALA:HB2	2.01	0.42
1:C:119:LYS:NZ	1:C:349:GLY:O	2.51	0.41
1:A:214:ASP:OD1	1:A:215:GLU:N	2.52	0.41
1:B:96:TRP:CD1	1:B:498:PRO:HA	2.54	0.41
1:A:213:THR:HG22	1:A:245:LEU:HB3	2.02	0.41
1:C:383:PRO:HG3	1:C:410:SER:OG	2.21	0.40
1:C:475:ASP:HB2	1:C:482:LEU:HD21	2.02	0.40
1:B:394:GLU:HG2	1:B:426:PHE:CZ	2.57	0.40
1:C:408:LEU:HB3	1:C:423:TYR:CE2	2.56	0.40
1:A:572:THR:HG22	1:A:590:VAL:HA	2.03	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	656/694 (94%)	637 (97%)	18 (3%)	1 (0%)	43	55
1	B	654/694 (94%)	634 (97%)	19 (3%)	1 (0%)	43	55
1	C	576/694 (83%)	555 (96%)	21 (4%)	0	100	100
All	All	1886/2082 (91%)	1826 (97%)	58 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	THR
1	B	463	THR

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	518/576 (90%)	512 (99%)	6 (1%)	63	79
1	B	528/576 (92%)	520 (98%)	8 (2%)	57	75
1	C	427/576 (74%)	424 (99%)	3 (1%)	76	87
All	All	1473/1728 (85%)	1456 (99%)	17 (1%)	68	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	234	GLN
1	A	413	GLU
1	A	423	TYR
1	A	472	ASP
1	A	580	ASP
1	B	116	ASN
1	B	325[A]	ARG
1	B	325[B]	ARG
1	B	413[A]	GLU
1	B	413[B]	GLU
1	B	423	TYR
1	B	648	LYS
1	B	675	GLU
1	C	116	ASN
1	C	384	THR
1	C	610	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	548	ASN
1	B	321	HIS
1	B	348	ASN
1	C	91	HIS
1	C	95	GLN
1	C	227	GLN
1	C	241	ASN
1	C	396	HIS
1	C	424	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands 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
3	EDO	B	703	-	3,3,3	0.44	0	2,2,2	0.62	0
2	PRX	C	802	-	28,28,28	2.91	8 (28%)	40,41,41	3.79	12 (30%)
3	EDO	C	803	-	3,3,3	0.40	0	2,2,2	0.50	0
3	EDO	A	707	-	3,3,3	0.38	0	2,2,2	0.49	0
3	EDO	A	702	-	3,3,3	0.56	0	2,2,2	0.08	0
3	EDO	A	706	-	3,3,3	0.38	0	2,2,2	0.40	0
3	EDO	B	704	-	3,3,3	0.42	0	2,2,2	0.41	0
2	PRX	B	702	-	28,28,28	2.85	8 (28%)	40,41,41	3.76	12 (30%)
2	PRX	A	701	-	28,28,28	2.85	8 (28%)	40,41,41	3.75	12 (30%)
3	EDO	A	705	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	A	708	-	3,3,3	0.44	0	2,2,2	0.48	0
3	EDO	A	703	-	3,3,3	0.47	0	2,2,2	0.28	0
5	COA	C	801	-	47,50,50	3.27	19 (40%)	69,75,75	1.54	12 (17%)
3	EDO	A	704	-	3,3,3	0.49	0	2,2,2	0.34	0
4	PO4	B	701	-	4,4,4	0.97	0	6,6,6	0.44	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
3	EDO	B	703	-	-	0/1/1/1	-
2	PRX	C	802	-	-	1/15/31/31	0/3/3/3
3	EDO	C	803	-	-	0/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	702	-	-	1/1/1/1	-
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	B	704	-	-	0/1/1/1	-
2	PRX	B	702	-	-	1/15/31/31	0/3/3/3
2	PRX	A	701	-	-	0/15/31/31	0/3/3/3
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
5	COA	C	801	-	-	15/48/64/64	0/3/3/3
3	EDO	A	704	-	-	0/1/1/1	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	801	COA	C2B-C3B	-11.99	1.26	1.53
2	C	802	PRX	C5-C4	7.95	1.53	1.39
2	A	701	PRX	C5-C4	7.77	1.52	1.39
2	B	702	PRX	C5-C4	7.64	1.52	1.39
2	C	802	PRX	C8-N9	-7.51	1.24	1.37
2	A	701	PRX	C8-N9	-7.27	1.25	1.37
2	B	702	PRX	C8-N9	-7.27	1.25	1.37
5	C	801	COA	C9P-N8P	7.09	1.50	1.33
5	C	801	COA	C5P-N4P	6.97	1.49	1.33
5	C	801	COA	P2A-O3A	6.92	1.67	1.59
5	C	801	COA	O4B-C1B	-5.85	1.28	1.42
2	C	802	PRX	C8-N7	-5.07	1.22	1.31
2	B	702	PRX	C8-N7	-4.94	1.22	1.31
2	C	802	PRX	C2-N3	4.72	1.42	1.33
2	A	701	PRX	C2-N3	4.71	1.42	1.33
5	C	801	COA	O4B-C4B	4.50	1.55	1.45
2	A	701	PRX	C6-N6	4.50	1.45	1.34
2	A	701	PRX	C8-N7	-4.49	1.23	1.31
2	B	702	PRX	C6-N6	4.48	1.45	1.34
5	C	801	COA	C2B-C1B	4.48	1.67	1.53
2	B	702	PRX	C2-N3	4.47	1.41	1.33
2	C	802	PRX	C6-N6	4.37	1.45	1.34
5	C	801	COA	C5B-C4B	-4.33	1.38	1.51
2	A	701	PRX	C5-N7	4.14	1.46	1.39
2	C	802	PRX	C5-C6	-4.01	1.29	1.41
2	B	702	PRX	C5-C6	-3.98	1.29	1.41
5	C	801	COA	C6A-N6A	3.97	1.44	1.34
5	C	801	COA	P3B-O3B	3.89	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	801	COA	P1A-O3A	3.79	1.63	1.59
2	A	701	PRX	C5-C6	-3.60	1.31	1.41
2	B	702	PRX	C5-N7	3.52	1.45	1.39
2	C	802	PRX	C5-N7	3.34	1.45	1.39
5	C	801	COA	C8A-N9A	-3.03	1.32	1.37
2	A	701	PRX	C6-N1	-2.93	1.27	1.35
2	B	702	PRX	C6-N1	-2.86	1.27	1.35
2	C	802	PRX	C6-N1	-2.80	1.27	1.35
5	C	801	COA	OAP-CAP	-2.75	1.37	1.42
5	C	801	COA	CCP-CBP	2.66	1.56	1.52
5	C	801	COA	O3B-C3B	2.41	1.52	1.44
5	C	801	COA	O9P-C9P	-2.35	1.18	1.23
5	C	801	COA	P1A-O5B	2.22	1.68	1.59
5	C	801	COA	C5A-N7A	-2.20	1.35	1.39
5	C	801	COA	C6P-C5P	2.15	1.55	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	PRX	N3-C4-N9	11.57	146.85	127.17
2	B	702	PRX	N3-C4-N9	11.17	146.16	127.17
2	A	701	PRX	N3-C4-N9	11.10	146.04	127.17
2	B	702	PRX	C4-N9-C8	9.93	116.16	105.74
2	C	802	PRX	C4-N9-C8	9.76	115.98	105.74
2	A	701	PRX	C4-N9-C8	9.64	115.86	105.74
2	A	701	PRX	C5-C4-N3	-9.43	113.73	126.72
2	C	802	PRX	C5-C4-N3	-9.42	113.75	126.72
2	B	702	PRX	C5-C4-N3	-9.16	114.11	126.72
2	A	701	PRX	C4-C5-N7	-8.90	100.41	110.58
2	B	702	PRX	C4-C5-N7	-8.59	100.77	110.58
2	C	802	PRX	C4-C5-N7	-8.58	100.77	110.58
2	C	802	PRX	C5-N7-C8	5.94	112.79	103.45
2	C	802	PRX	C5-C4-N9	-5.88	99.40	105.81
2	A	701	PRX	C5-N7-C8	5.86	112.66	103.45
2	B	702	PRX	C5-N7-C8	5.82	112.60	103.45
2	B	702	PRX	N1-C2-N3	-5.81	119.79	128.58
2	C	802	PRX	C6-C5-C4	5.69	124.95	117.18
2	A	701	PRX	N1-C2-N3	-5.66	120.02	128.58
2	B	702	PRX	C6-C5-C4	5.61	124.84	117.18
2	B	702	PRX	C5-C4-N9	-5.58	99.73	105.81
2	C	802	PRX	N1-C2-N3	-5.58	120.13	128.58
2	A	701	PRX	C6-C5-C4	5.55	124.75	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	801	COA	C5A-C4A-N3A	-5.54	119.09	126.72
2	A	701	PRX	C5-C4-N9	-5.17	100.18	105.81
2	B	702	PRX	C2-N1-C6	4.48	126.10	118.73
2	A	701	PRX	C2-N1-C6	4.44	126.03	118.73
2	C	802	PRX	C2-N1-C6	4.34	125.87	118.73
5	C	801	COA	N3A-C4A-N9A	4.14	134.21	127.17
5	C	801	COA	N3A-C2A-N1A	-4.05	122.45	128.58
5	C	801	COA	C2A-N3A-C4A	3.49	120.36	111.83
5	C	801	COA	C5A-N7A-C8A	2.88	107.97	103.45
5	C	801	COA	N9A-C8A-N7A	-2.77	110.01	113.94
2	A	701	PRX	C2-N3-C4	2.76	118.58	111.83
5	C	801	COA	C4A-C5A-N7A	-2.76	107.42	110.58
2	B	702	PRX	C4-N9-C1'	-2.71	120.28	126.63
2	A	701	PRX	C4-N9-C1'	-2.70	120.32	126.63
2	B	702	PRX	C2-N3-C4	2.66	118.32	111.83
5	C	801	COA	C3B-C2B-C1B	2.65	105.72	99.89
2	C	802	PRX	C2-N3-C4	2.62	118.24	111.83
5	C	801	COA	CAP-C9P-N8P	2.41	121.06	116.48
2	C	802	PRX	C4-N9-C1'	-2.27	121.33	126.63
2	B	702	PRX	N9-C8-N7	-2.25	110.74	113.94
5	C	801	COA	P3B-O3B-C3B	-2.22	117.50	123.43
2	A	701	PRX	N9-C8-N7	-2.18	110.84	113.94
5	C	801	COA	C4A-N9A-C8A	2.05	107.89	105.74
2	C	802	PRX	N9-C8-N7	-2.03	111.05	113.94
5	C	801	COA	CDP-CBP-CAP	2.03	112.23	108.77

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	801	COA	C5B-O5B-P1A-O1A
5	C	801	COA	C5B-O5B-P1A-O3A
5	C	801	COA	CCP-O6A-P2A-O5A
5	C	801	COA	O9P-C9P-CAP-CBP
5	C	801	COA	N8P-C9P-CAP-CBP
5	C	801	COA	O9P-C9P-CAP-OAP
5	C	801	COA	N8P-C9P-CAP-OAP
5	C	801	COA	C5P-C6P-C7P-N8P
5	C	801	COA	C6P-C7P-N8P-C9P
5	C	801	COA	CEP-CBP-CCP-O6A
3	A	702	EDO	O1-C1-C2-O2
2	B	702	PRX	C5'-O5'-P-O1P

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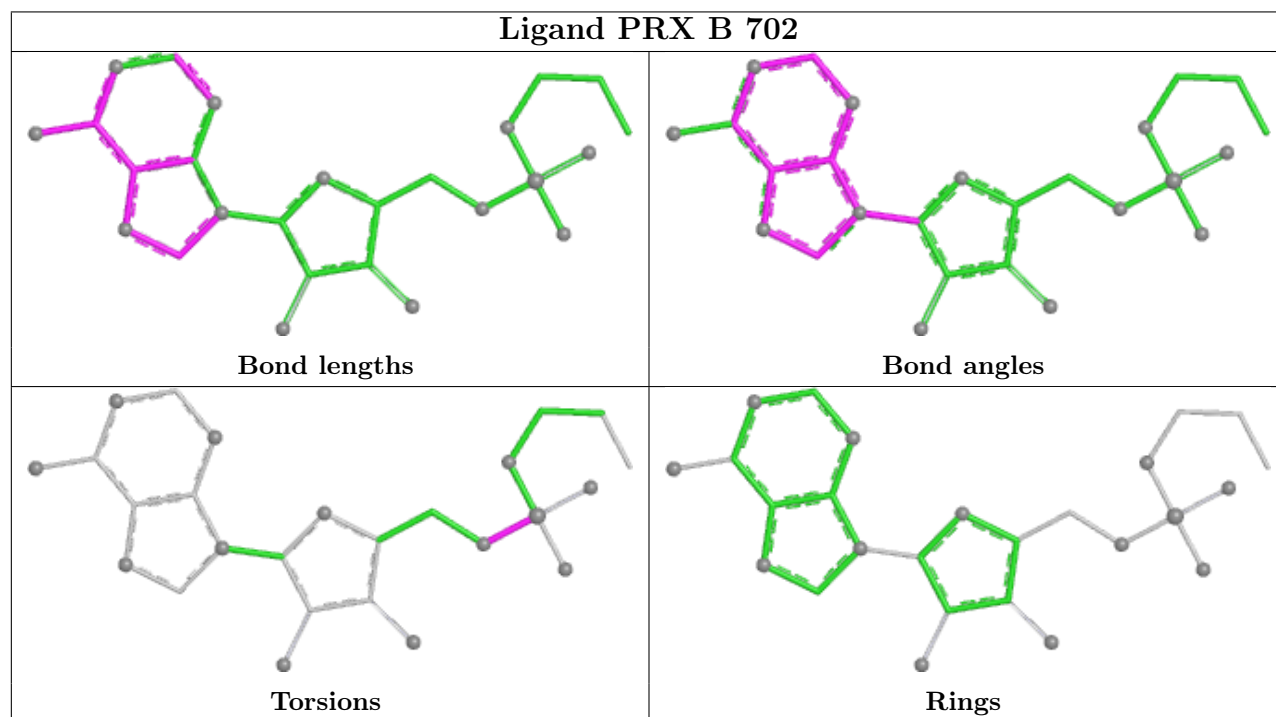
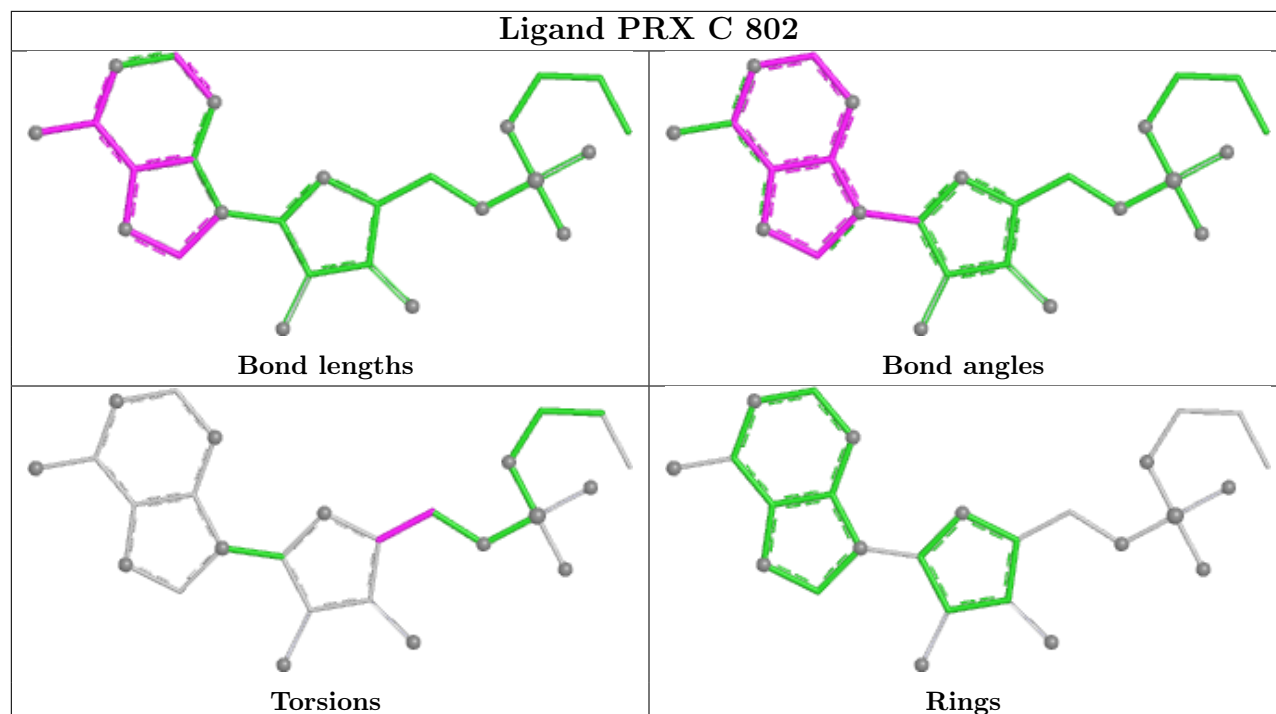
Mol	Chain	Res	Type	Atoms
5	C	801	COA	CCP-O6A-P2A-O3A
5	C	801	COA	CCP-O6A-P2A-O4A
5	C	801	COA	C3B-O3B-P3B-O9A
5	C	801	COA	CDP-CBP-CCP-O6A
5	C	801	COA	S1P-C2P-C3P-N4P
2	C	802	PRX	C3'-C4'-C5'-O5'

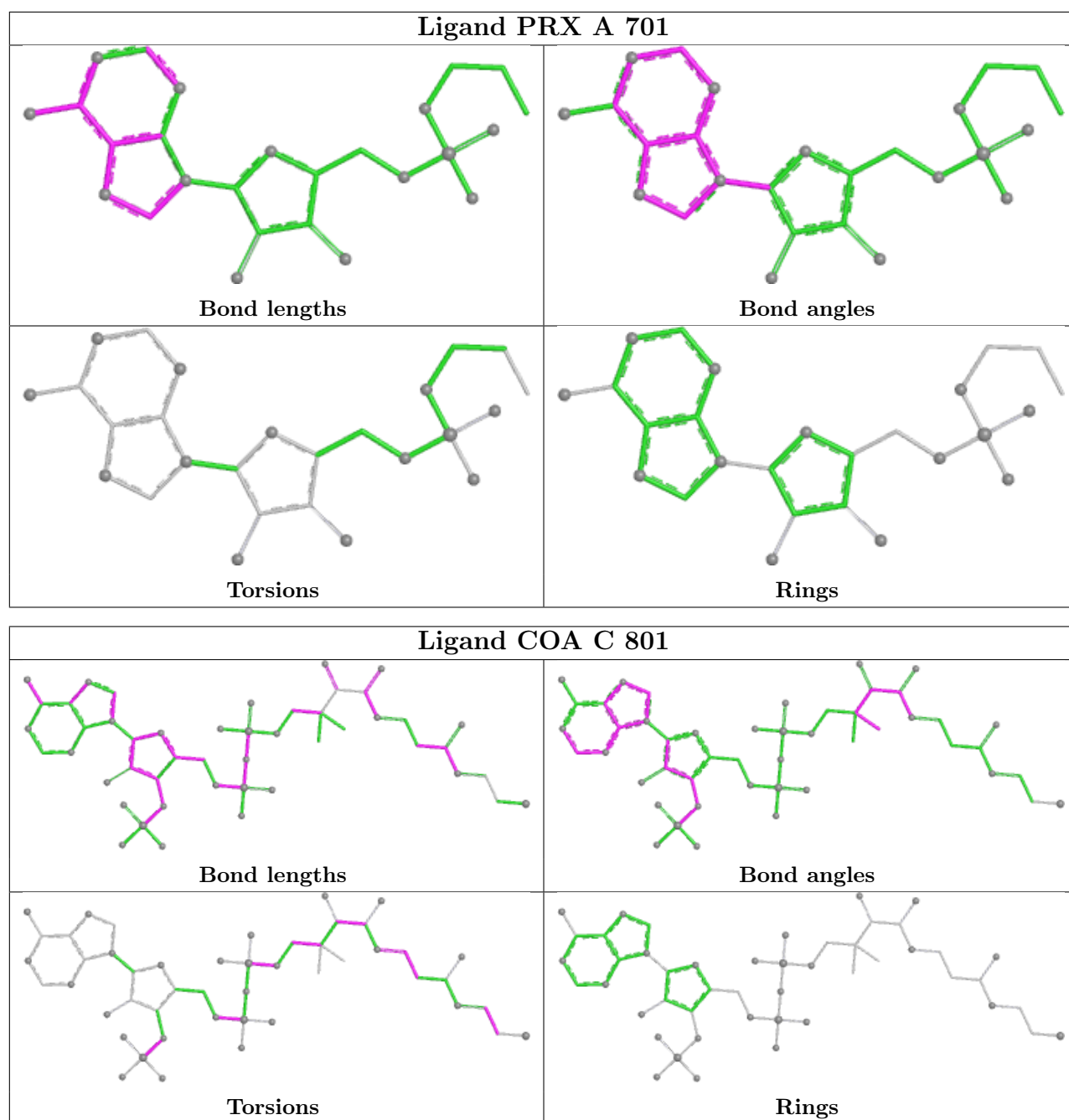
There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	EDO	2	0
3	A	706	EDO	1	0
2	B	702	PRX	1	0
2	A	701	PRX	1	0
5	C	801	COA	5	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 [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	652/694 (93%)	-0.16	11 (1%)	69 70	16, 41, 79, 97	10 (1%)
1	B	647/694 (93%)	-0.15	22 (3%)	48 50	16, 41, 71, 104	15 (2%)
1	C	584/694 (84%)	0.31	37 (6%)	26 28	27, 57, 100, 114	0
All	All	1883/2082 (90%)	-0.01	70 (3%)	45 48	16, 44, 88, 114	25 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	671	GLN	4.4
1	C	594	PRO	4.4
1	C	425	ASP	4.1
1	C	399	ASN	4.1
1	A	681	THR	4.0
1	B	681	THR	3.8
1	C	545	ASP	3.7
1	B	672	ILE	3.7
1	C	547	ILE	3.7
1	C	35	GLY	3.6
1	B	676	VAL	3.4
1	C	550	SER	3.4
1	B	639	GLY	3.4
1	C	607	SER	3.3
1	C	568	GLY	3.1
1	C	477	GLN	3.1
1	A	670	PRO	3.1
1	C	418	GLU	3.0
1	B	638	SER	3.0
1	C	486	ASP	3.0
1	C	534	ASP	3.0
1	C	585	ALA	2.9
1	C	549	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	533	TYR	2.8
1	B	670	PRO	2.8
1	C	555	SER	2.8
1	C	426	PHE	2.8
1	C	606	LEU	2.8
1	A	652	GLY	2.8
1	A	10	VAL	2.8
1	B	294	GLY	2.7
1	C	546	VAL	2.7
1	C	416	ASN	2.6
1	B	644	ARG	2.6
1	A	393	GLY	2.6
1	B	645	VAL	2.6
1	C	554	LEU	2.5
1	B	637	ARG	2.5
1	B	334[A]	TRP	2.5
1	C	462	ALA	2.5
1	A	602	LYS	2.5
1	C	569	VAL	2.5
1	C	424	ASN	2.4
1	B	642	MET	2.4
1	B	598	LEU	2.4
1	C	293	THR	2.4
1	A	290	SER	2.4
1	C	629	LEU	2.4
1	C	422	TRP	2.4
1	C	586	VAL	2.4
1	C	630	VAL	2.3
1	C	397	VAL	2.3
1	C	570	ALA	2.3
1	A	680	VAL	2.3
1	A	578	ALA	2.2
1	B	290	SER	2.2
1	B	296	PRO	2.2
1	C	548	ASN	2.2
1	B	602	LYS	2.2
1	B	636	THR	2.2
1	C	530	ALA	2.2
1	B	673	VAL	2.2
1	C	430	ASN	2.2
1	C	551	GLY	2.2
1	B	674	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	678	GLN	2.1
1	C	587	TYR	2.1
1	A	12	HIS	2.0
1	A	294	GLY	2.0
1	C	535	GLY	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.

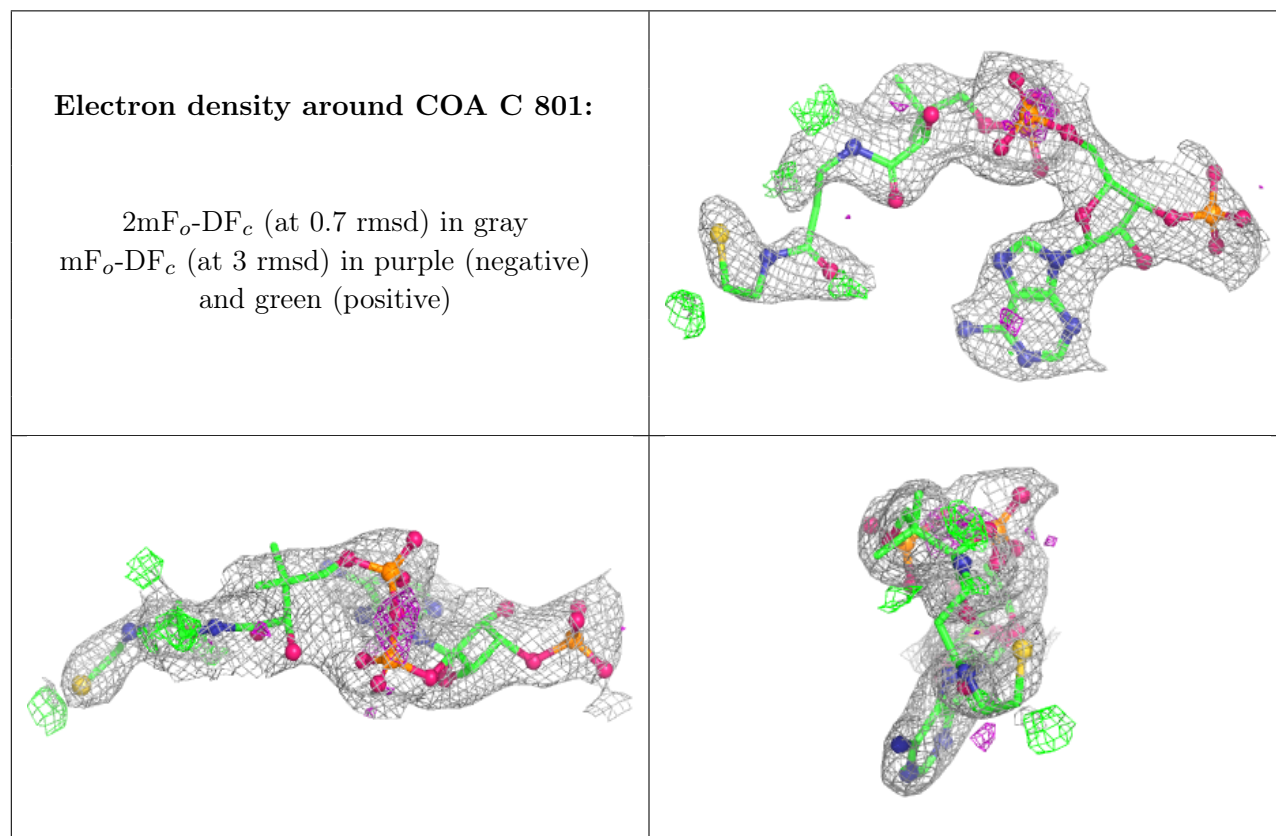
6.4 Ligands [i](#)

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
3	EDO	A	708	4/4	0.73	0.22	75,75,76,76	0
5	COA	C	801	48/48	0.80	0.17	96,101,104,104	0
3	EDO	A	704	4/4	0.84	0.15	58,58,59,59	0
3	EDO	A	702	4/4	0.84	0.14	55,56,56,57	0
3	EDO	A	703	4/4	0.84	0.14	58,58,58,58	0
4	PO4	B	701	5/5	0.85	0.11	93,94,94,94	0
3	EDO	A	706	4/4	0.88	0.19	58,58,59,59	0
3	EDO	B	703	4/4	0.91	0.13	42,43,43,43	0
2	PRX	C	802	26/26	0.92	0.10	55,60,62,62	0
3	EDO	A	707	4/4	0.92	0.11	46,46,46,46	0
3	EDO	B	704	4/4	0.93	0.09	57,57,57,57	0
3	EDO	A	705	4/4	0.94	0.15	63,63,63,63	0
3	EDO	C	803	4/4	0.97	0.07	45,45,45,46	0
2	PRX	A	701	26/26	0.97	0.06	30,32,32,32	0
2	PRX	B	702	26/26	0.97	0.06	29,31,35,35	0

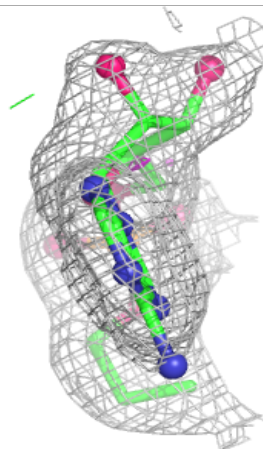
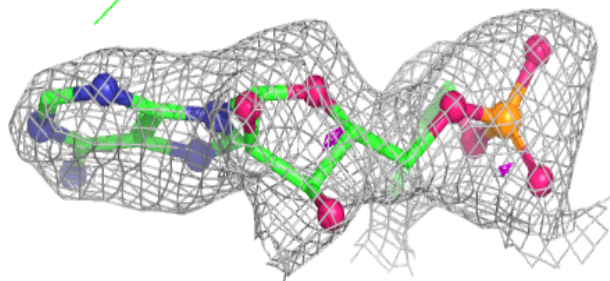
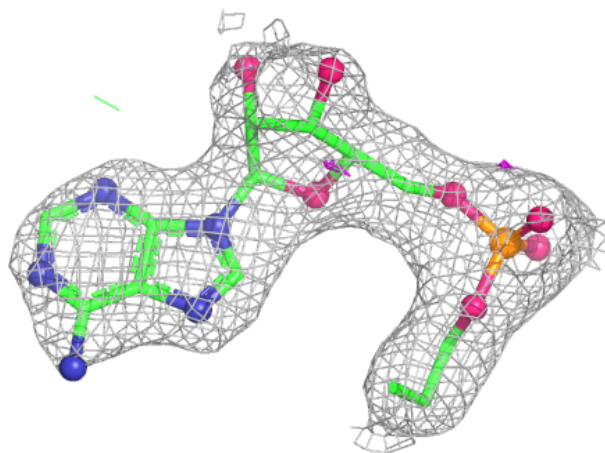
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



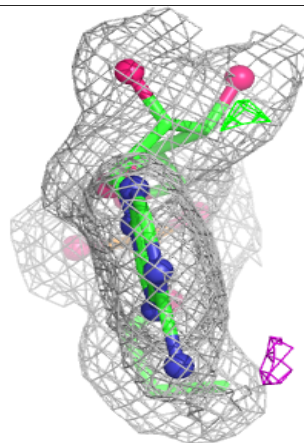
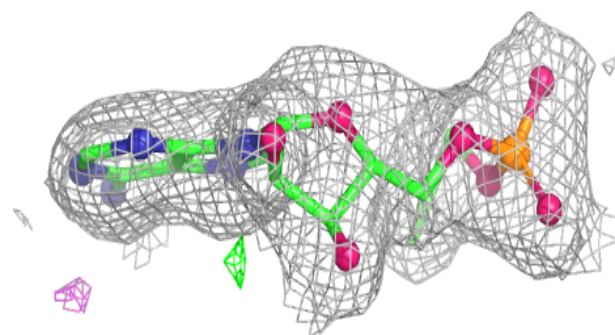
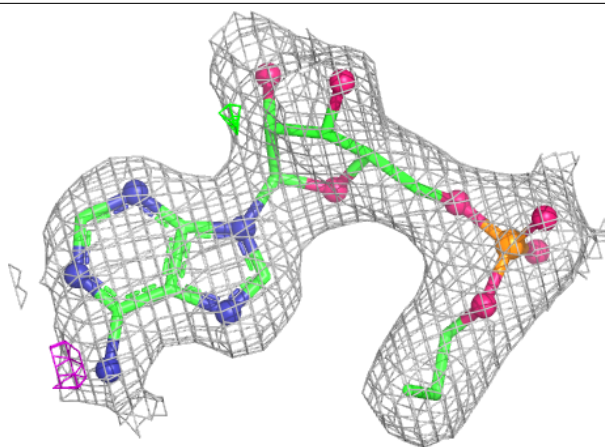
Electron density around PRX C 802:

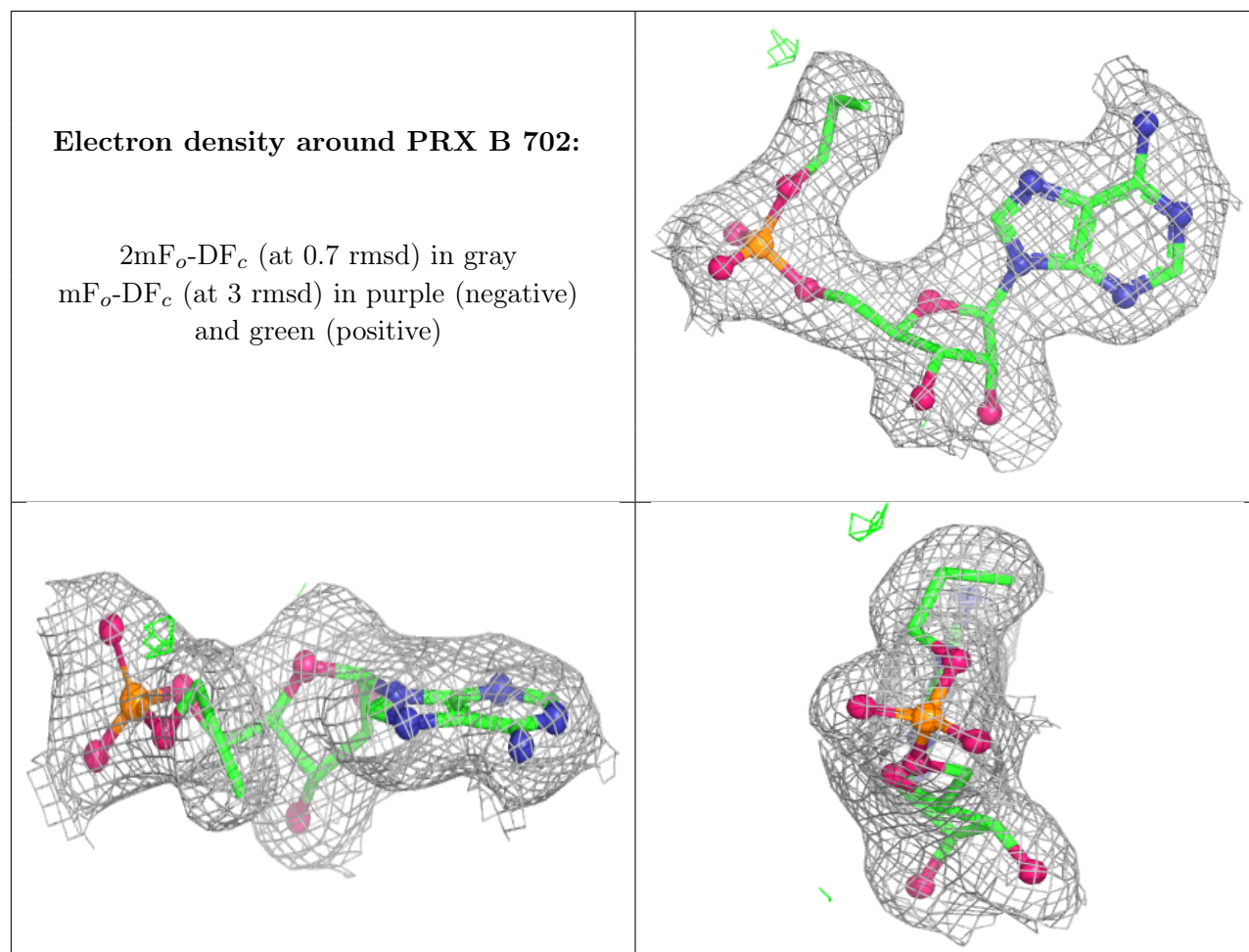
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PRX A 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 ⓘ

There are no such residues in this entry.