



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:21 AM UTC

PDB ID : 7KQ6 / pdb_00007kq6
Title : Crystal Structure of Acetyl-coenzyme A synthetase from *Coccidioides immitis* in complex with PRX
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2020-11-13
Resolution : 1.80 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

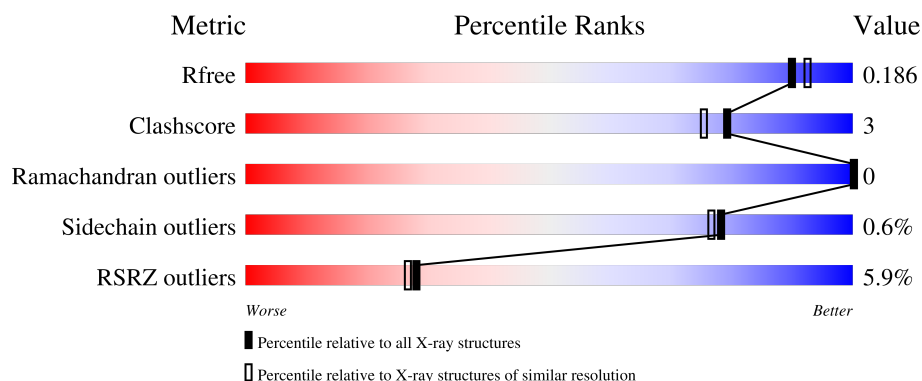
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	706	4% 82% 14%
1	B	706	5% 78% 5% 16%
1	C	706	7% 80% 6% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15819 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	610	Total	C	N	O	S	0	8	0
			4772	3061	817	875	19			
1	B	590	Total	C	N	O	S	0	6	0
			4574	2936	785	835	18			
1	C	608	Total	C	N	O	S	0	5	0
			4711	3013	810	870	18			

There are 48 discrepancies between the modelled and reference sequences:

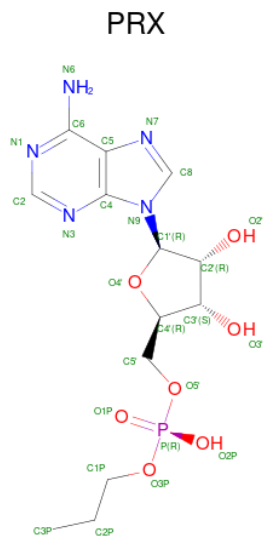
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP J3KJC6
A	-13	HIS	-	expression tag	UNP J3KJC6
A	-12	HIS	-	expression tag	UNP J3KJC6
A	-11	HIS	-	expression tag	UNP J3KJC6
A	-10	HIS	-	expression tag	UNP J3KJC6
A	-9	HIS	-	expression tag	UNP J3KJC6
A	-8	HIS	-	expression tag	UNP J3KJC6
A	-7	HIS	-	expression tag	UNP J3KJC6
A	-6	HIS	-	expression tag	UNP J3KJC6
A	-5	GLU	-	expression tag	UNP J3KJC6
A	-4	ASN	-	expression tag	UNP J3KJC6
A	-3	LEU	-	expression tag	UNP J3KJC6
A	-2	TYR	-	expression tag	UNP J3KJC6
A	-1	PHE	-	expression tag	UNP J3KJC6
A	0	GLN	-	expression tag	UNP J3KJC6
A	1	GLY	-	expression tag	UNP J3KJC6
B	-14	MET	-	initiating methionine	UNP J3KJC6
B	-13	HIS	-	expression tag	UNP J3KJC6
B	-12	HIS	-	expression tag	UNP J3KJC6
B	-11	HIS	-	expression tag	UNP J3KJC6
B	-10	HIS	-	expression tag	UNP J3KJC6
B	-9	HIS	-	expression tag	UNP J3KJC6
B	-8	HIS	-	expression tag	UNP J3KJC6

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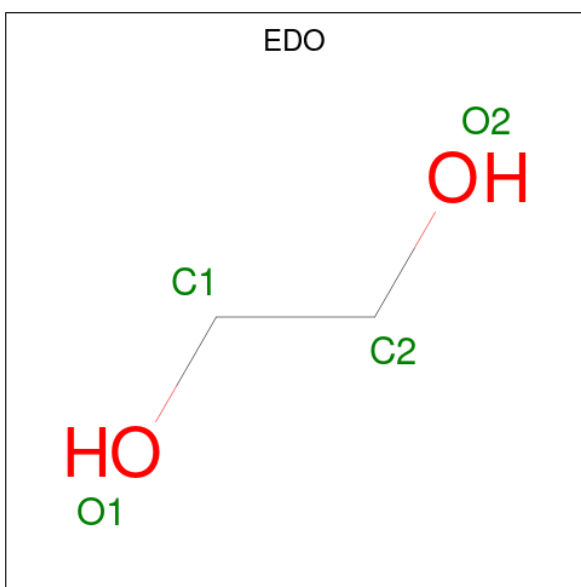
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP J3KJC6
B	-6	HIS	-	expression tag	UNP J3KJC6
B	-5	GLU	-	expression tag	UNP J3KJC6
B	-4	ASN	-	expression tag	UNP J3KJC6
B	-3	LEU	-	expression tag	UNP J3KJC6
B	-2	TYR	-	expression tag	UNP J3KJC6
B	-1	PHE	-	expression tag	UNP J3KJC6
B	0	GLN	-	expression tag	UNP J3KJC6
B	1	GLY	-	expression tag	UNP J3KJC6
C	-14	MET	-	initiating methionine	UNP J3KJC6
C	-13	HIS	-	expression tag	UNP J3KJC6
C	-12	HIS	-	expression tag	UNP J3KJC6
C	-11	HIS	-	expression tag	UNP J3KJC6
C	-10	HIS	-	expression tag	UNP J3KJC6
C	-9	HIS	-	expression tag	UNP J3KJC6
C	-8	HIS	-	expression tag	UNP J3KJC6
C	-7	HIS	-	expression tag	UNP J3KJC6
C	-6	HIS	-	expression tag	UNP J3KJC6
C	-5	GLU	-	expression tag	UNP J3KJC6
C	-4	ASN	-	expression tag	UNP J3KJC6
C	-3	LEU	-	expression tag	UNP J3KJC6
C	-2	TYR	-	expression tag	UNP J3KJC6
C	-1	PHE	-	expression tag	UNP J3KJC6
C	0	GLN	-	expression tag	UNP J3KJC6
C	1	GLY	-	expression tag	UNP J3KJC6

- Molecule 2 is ADENOSINE-5'-MONOPHOSPHATE-PROPYL ESTER (CCD ID: PRX) (formula: $C_{13}H_{20}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

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

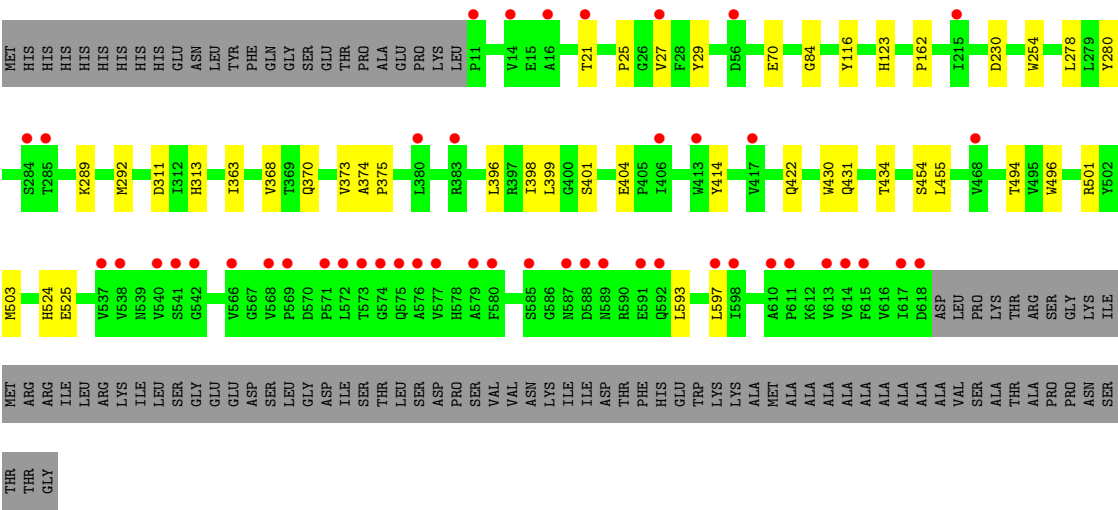
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	541	Total O 542 542	0	1
4	B	542	Total O 542 542	0	0
4	C	471	Total O 472 472	0	1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.98Å 116.08Å 107.33Å 90.00° 119.75° 90.00°	Depositor
Resolution (Å)	46.59 – 1.80 46.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.59-1.80) 96.0 (46.59-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19rc4-4035	Depositor
R, R_{free}	0.162 , 0.185 (Not available) , 0.186	Depositor DCC
R_{free} test set	2010 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.127 for -h-l,k,h 0.127 for l,k,-h-l 0.015 for h,-k,-h-l 0.016 for -h-l,-k,l 0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15819	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: PRX, EDO

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	0/4927	0.47	0/6715
1	B	0.29	0/4720	0.48	0/6431
1	C	0.27	0/4858	0.47	0/6626
All	All	0.28	0/14505	0.48	0/19772

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

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	4772	0	4593	20	1
1	B	4574	0	4382	26	0
1	C	4711	0	4484	32	0
2	A	26	0	19	1	0
2	B	26	0	19	2	0
2	C	26	0	19	1	0
3	A	36	0	54	4	0
3	B	52	0	78	4	0
3	C	40	0	60	7	0
4	A	542	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	542	0	0	2	0
4	C	472	0	0	4	0
All	All	15819	0	13708	76	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (76) 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:B:472:GLU:OE2	1:B:485:ARG:NH1	2.17	0.77
1:B:281:THR:HG21	1:B:432:THR:HG21	1.68	0.75
1:A:281[B]:THR:HG21	1:A:432:THR:HG21	1.69	0.74
1:A:287:LYS:HG2	1:A:288:PRO:HD2	1.76	0.67
1:A:71:LYS:HE3	1:B:70:GLU:HG3	1.78	0.65
1:B:153:THR:HG23	3:B:708:EDO:H12	1.83	0.60
1:A:70:GLU:HG2	3:C:701:EDO:H12	1.85	0.58
1:C:496:TRP:CZ3	3:C:710:EDO:H21	2.38	0.58
1:B:496:TRP:CZ3	3:B:709:EDO:H21	2.41	0.55
1:C:254:TRP:NE1	3:C:708:EDO:H22	2.23	0.53
1:B:111:LYS:NZ	4:B:807:HOH:O	2.39	0.53
1:C:292[B]:MET:HE3	1:C:494:THR:HG22	1.90	0.53
1:B:292[A]:MET:HE3	1:B:494:THR:HG22	1.91	0.53
1:C:254:TRP:HE1	3:C:708:EDO:H22	1.73	0.53
1:A:496:TRP:CZ3	3:A:708:EDO:H21	2.44	0.52
1:B:144:LYS:HG2	4:B:813:HOH:O	2.12	0.50
1:B:524:HIS:CE1	1:B:525:GLU:HG3	2.46	0.49
1:A:75:LYS:HB2	1:B:106:MET:HE3	1.95	0.48
1:A:454[B]:SER:OG	1:A:455:LEU:N	2.47	0.48
1:C:373:VAL:HG22	1:C:374:ALA:H	1.79	0.48
1:A:363:ILE:HG23	1:A:368:VAL:HB	1.94	0.48
1:A:597:LEU:HD13	1:A:614:VAL:HG11	1.97	0.47
1:A:281[B]:THR:CG2	1:A:432:THR:HG21	2.40	0.47
1:A:496:TRP:CE3	3:A:708:EDO:H21	2.50	0.47
1:C:29:TYR:CE1	3:C:703:EDO:H11	2.50	0.47
1:C:116:TYR:CD1	1:C:162:PRO:HD3	2.50	0.46
1:B:373:VAL:HG11	1:B:378:LEU:HD21	1.98	0.46
1:B:540:VAL:HG21	1:B:545:LEU:HD12	1.97	0.46
1:A:396:LEU:HD21	1:A:399:LEU:HD21	1.98	0.46
1:C:313:HIS:HD2	4:C:1226:HOH:O	1.99	0.45
1:A:116:TYR:CD1	1:A:162:PRO:HD3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:TYR:HA	1:B:289:LYS:O	2.15	0.45
1:C:84:GLY:HA3	1:C:503:MET:SD	2.57	0.45
1:C:123:HIS:HB3	4:C:804:HOH:O	2.15	0.45
1:C:29:TYR:CZ	3:C:703:EDO:H11	2.52	0.45
1:B:351:PRO:HB3	1:B:359:TYR:CE2	2.52	0.45
1:B:116:TYR:CD1	1:B:162:PRO:HD3	2.52	0.45
1:C:280:TYR:HA	1:C:289:LYS:O	2.17	0.45
1:C:593:LEU:O	1:C:597:LEU:HG	2.17	0.45
1:C:431:GLN:HG2	1:C:434:THR:HG23	1.99	0.45
1:C:524:HIS:CD2	1:C:525:GLU:HG3	2.51	0.45
1:A:399:LEU:HB3	1:A:414:TYR:CZ	2.52	0.44
1:B:399:LEU:HD12	1:B:425[B]:ILE:HD11	1.99	0.44
1:B:281:THR:CG2	1:B:432:THR:HG21	2.42	0.44
1:B:524:HIS:ND1	1:B:525:GLU:HG3	2.32	0.44
1:B:376[B]:THR:HG21	1:B:541:SER:HA	2.00	0.43
1:C:430:TRP:CE2	2:C:702:PRX:H3P1	2.52	0.43
1:C:496:TRP:CE3	3:C:710:EDO:H21	2.52	0.43
1:A:430:TRP:CE2	2:A:701:PRX:H3P1	2.53	0.43
1:C:363:ILE:HG23	1:C:368:VAL:HB	2.00	0.43
3:B:713:EDO:H21	1:C:70:GLU:HG2	2.00	0.43
1:C:289:LYS:HG2	1:C:501:ARG:CZ	2.47	0.43
1:C:399:LEU:HB3	1:C:414:TYR:CZ	2.53	0.43
1:A:238:LYS:NZ	4:A:831:HOH:O	2.51	0.43
1:C:230:ASP:OD2	4:C:801:HOH:O	2.22	0.43
1:C:311:ASP:OD1	1:C:313:HIS:HE1	2.02	0.43
1:B:496:TRP:CE3	3:B:709:EDO:H21	2.54	0.43
1:C:399:LEU:HB3	1:C:414:TYR:CE2	2.54	0.43
1:A:123:HIS:HB3	4:A:802:HOH:O	2.18	0.42
1:A:289:LYS:HG2	1:A:501:ARG:CZ	2.50	0.42
1:C:27:VAL:HG21	1:C:422:GLN:HG2	2.02	0.42
3:A:708:EDO:H22	1:B:141:TRP:CZ3	2.54	0.42
1:C:25:PRO:HD3	4:C:1064:HOH:O	2.19	0.42
1:C:370:GLN:HG3	1:C:398:ILE:HB	2.02	0.42
1:B:430:TRP:CE2	2:B:701:PRX:H3P1	2.55	0.42
1:C:278:LEU:HD21	1:C:496:TRP:CE3	2.55	0.42
1:C:373:VAL:O	1:C:401:SER:HA	2.20	0.42
1:C:396:LEU:HD21	1:C:399:LEU:HD21	2.01	0.41
1:A:29:TYR:CE1	3:A:702:EDO:H22	2.56	0.41
1:B:399:LEU:HB3	1:B:414:TYR:CZ	2.55	0.41
1:C:375:PRO:HG2	1:C:404:GLU:HG3	2.03	0.41
1:A:10:LEU:N	1:A:11:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:VAL:HG11	1:B:422:GLN:HG2	2.03	0.41
1:B:431:GLN:HB3	2:B:701:PRX:H5'2	2.02	0.41
1:B:178:HIS:CE1	1:B:277:PHE:HB3	2.56	0.40
1:C:454:SER:OG	1:C:455:LEU:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:O	1:A:226:LYS:NZ[2_646]	2.19	0.01

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	616/706 (87%)	591 (96%)	25 (4%)	0	100	100
1	B	588/706 (83%)	564 (96%)	24 (4%)	0	100	100
1	C	611/706 (86%)	584 (96%)	27 (4%)	0	100	100
All	All	1815/2118 (86%)	1739 (96%)	76 (4%)	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	494/584 (85%)	491 (99%)	3 (1%)	78	77
1	B	467/584 (80%)	463 (99%)	4 (1%)	70	67
1	C	481/584 (82%)	480 (100%)	1 (0%)	87	87
All	All	1442/1752 (82%)	1434 (99%)	8 (1%)	78	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	LYS
1	A	289	LYS
1	A	594	GLN
1	B	46	GLN
1	B	281	THR
1	B	431	GLN
1	B	468	VAL
1	C	21	THR

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

Mol	Chain	Res	Type
1	A	17	HIS
1	A	575	GLN
1	B	34	HIS
1	B	146	GLN
1	B	415	HIS
1	B	524	HIS
1	C	17	HIS
1	C	46	GLN
1	C	600	GLN

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](#)

35 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	C	704	-	3,3,3	0.42	0	2,2,2	0.56	0
3	EDO	C	706	-	3,3,3	0.50	0	2,2,2	0.42	0
3	EDO	A	710	-	3,3,3	0.43	0	2,2,2	0.45	0
3	EDO	C	711	-	3,3,3	0.43	0	2,2,2	0.53	0
3	EDO	B	707	-	3,3,3	0.48	0	2,2,2	0.28	0
2	PRX	B	701	-	28,28,28	0.30	0	40,41,41	0.44	0
3	EDO	B	702	-	3,3,3	0.39	0	2,2,2	0.48	0
3	EDO	A	705	-	3,3,3	0.54	0	2,2,2	0.24	0
3	EDO	C	701	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	A	707	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	A	708	-	3,3,3	0.34	0	2,2,2	0.28	0
3	EDO	B	708	-	3,3,3	0.52	0	2,2,2	0.23	0
3	EDO	B	706	-	3,3,3	0.55	0	2,2,2	0.25	0
2	PRX	C	702	-	28,28,28	0.35	0	40,41,41	0.40	0
3	EDO	C	707	-	3,3,3	0.45	0	2,2,2	0.48	0
3	EDO	A	709	-	3,3,3	0.38	0	2,2,2	0.45	0
3	EDO	B	709	-	3,3,3	0.35	0	2,2,2	0.32	0
3	EDO	C	709	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	C	710	-	3,3,3	0.39	0	2,2,2	0.16	0
3	EDO	A	703	-	3,3,3	0.42	0	2,2,2	0.56	0
3	EDO	B	713	-	3,3,3	0.38	0	2,2,2	0.58	0
3	EDO	B	703	-	3,3,3	0.48	0	2,2,2	0.36	0
3	EDO	B	711	-	3,3,3	0.40	0	2,2,2	0.54	0
2	PRX	A	701	-	28,28,28	0.32	0	40,41,41	0.43	0
3	EDO	A	702	-	3,3,3	0.46	0	2,2,2	0.52	0
3	EDO	B	714	-	3,3,3	0.48	0	2,2,2	0.30	0
3	EDO	B	704	-	3,3,3	0.52	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	712	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	B	705	-	3,3,3	0.42	0	2,2,2	0.52	0
3	EDO	A	704	-	3,3,3	0.39	0	2,2,2	0.46	0
3	EDO	A	706	-	3,3,3	0.41	0	2,2,2	0.43	0
3	EDO	C	703	-	3,3,3	0.41	0	2,2,2	0.51	0
3	EDO	C	708	-	3,3,3	0.26	0	2,2,2	0.68	0
3	EDO	C	705	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	B	710	-	3,3,3	0.41	0	2,2,2	0.39	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	C	704	-	-	0/1/1/1	-
3	EDO	C	706	-	-	0/1/1/1	-
3	EDO	A	710	-	-	0/1/1/1	-
3	EDO	C	711	-	-	0/1/1/1	-
3	EDO	B	707	-	-	0/1/1/1	-
2	PRX	B	701	-	-	0/15/31/31	0/3/3/3
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	C	701	-	-	1/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
3	EDO	B	708	-	-	1/1/1/1	-
3	EDO	B	706	-	-	0/1/1/1	-
2	PRX	C	702	-	-	0/15/31/31	0/3/3/3
3	EDO	C	707	-	-	0/1/1/1	-
3	EDO	A	709	-	-	0/1/1/1	-
3	EDO	B	709	-	-	0/1/1/1	-
3	EDO	C	709	-	-	0/1/1/1	-
3	EDO	C	710	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	B	713	-	-	0/1/1/1	-
3	EDO	B	703	-	-	1/1/1/1	-
3	EDO	B	711	-	-	1/1/1/1	-
2	PRX	A	701	-	-	0/15/31/31	0/3/3/3
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	B	714	-	-	0/1/1/1	-
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	B	712	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	705	-	-	1/1/1/1	-
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
3	EDO	C	708	-	-	1/1/1/1	-
3	EDO	C	705	-	-	0/1/1/1	-
3	EDO	B	710	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	708	EDO	O1-C1-C2-O2
3	B	703	EDO	O1-C1-C2-O2
3	B	711	EDO	O1-C1-C2-O2
3	C	708	EDO	O1-C1-C2-O2
3	B	712	EDO	O1-C1-C2-O2
3	C	701	EDO	O1-C1-C2-O2
3	B	705	EDO	O1-C1-C2-O2

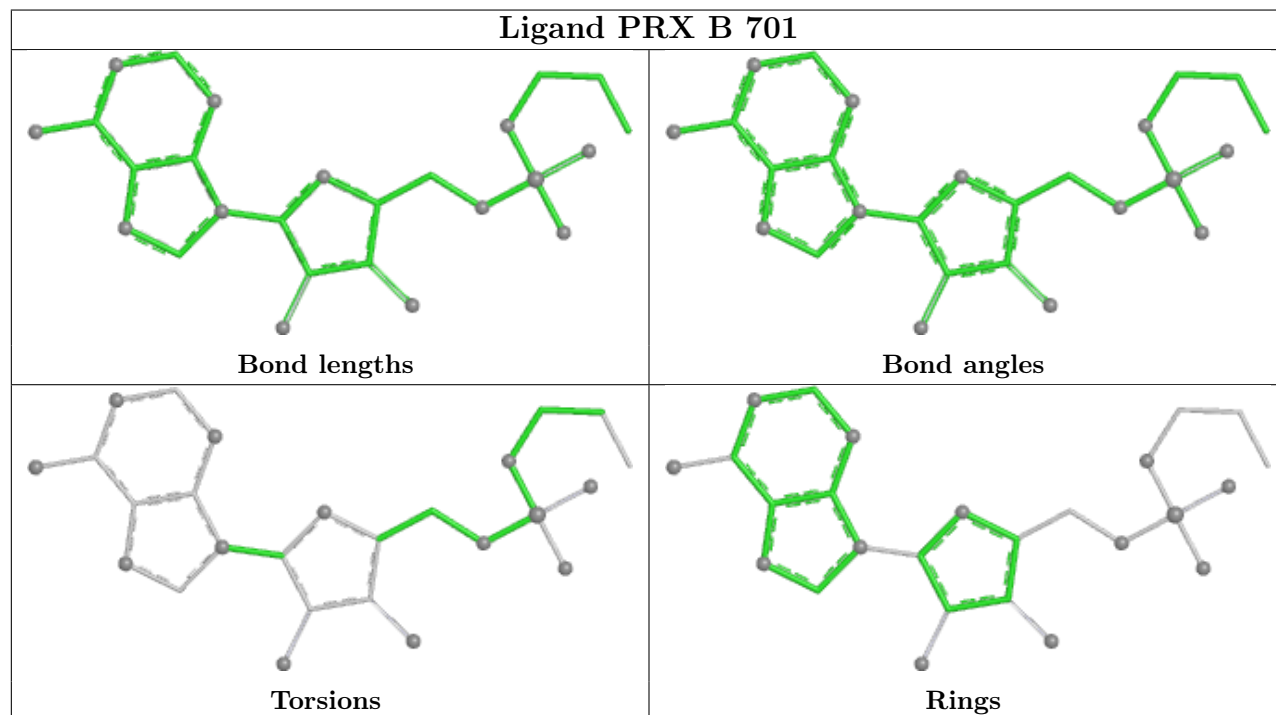
There are no ring outliers.

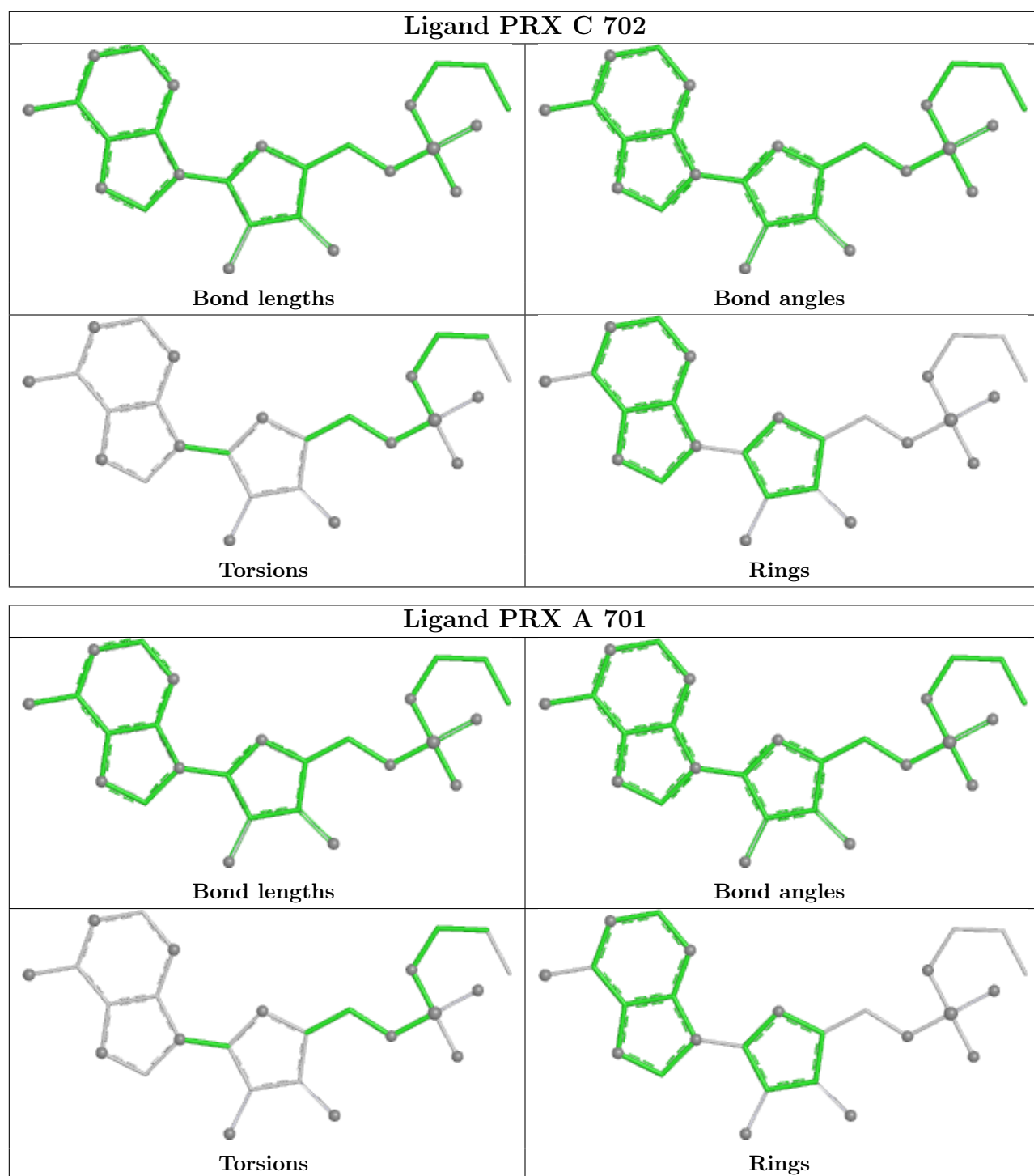
12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	PRX	2	0
3	C	701	EDO	1	0
3	A	708	EDO	3	0
3	B	708	EDO	1	0
2	C	702	PRX	1	0
3	B	709	EDO	2	0
3	C	710	EDO	2	0
3	B	713	EDO	1	0
2	A	701	PRX	1	0
3	A	702	EDO	1	0
3	C	703	EDO	2	0
3	C	708	EDO	2	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 ⓘ

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	610/706 (86%)	-0.22	27 (4%)	39	38	11, 24, 66, 106	8 (1%)
1	B	590/706 (83%)	-0.20	32 (5%)	31	30	10, 24, 76, 102	6 (1%)
1	C	608/706 (86%)	0.12	47 (7%)	19	17	11, 31, 81, 113	5 (0%)
All	All	1808/2118 (85%)	-0.10	106 (5%)	28	27	10, 26, 73, 113	19 (1%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	PRO	5.2
1	C	568	VAL	5.1
1	C	613	VAL	4.8
1	B	616	VAL	4.6
1	C	541	SER	4.6
1	A	613	VAL	4.5
1	B	613	VAL	4.5
1	C	589	ASN	4.4
1	C	577	VAL	4.3
1	C	588	ASP	4.3
1	A	10	LEU	4.2
1	A	589	ASN	4.1
1	C	573	THR	4.1
1	A	580	PHE	4.1
1	B	615	PHE	4.1
1	C	569	PRO	4.1
1	B	539	ASN	4.0
1	A	588	ASP	4.0
1	A	619	ASP	4.0
1	B	538	VAL	4.0
1	C	610	ALA	4.0
1	C	618	ASP	3.9
1	B	598	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	11	PRO	3.9
1	B	589	ASN	3.7
1	C	572	LEU	3.7
1	C	617	ILE	3.7
1	B	580	PHE	3.6
1	A	577	VAL	3.5
1	B	579	ALA	3.5
1	A	593	LEU	3.5
1	B	592	GLN	3.4
1	C	571	PRO	3.3
1	C	614	VAL	3.3
1	B	577	VAL	3.2
1	B	468	VAL	3.2
1	A	35	GLU	3.2
1	B	610	ALA	3.1
1	C	587	ASN	3.1
1	A	617	ILE	3.1
1	B	594	GLN	3.1
1	B	11	PRO	3.1
1	C	540	VAL	3.1
1	B	543	HIS	3.1
1	C	611	PRO	3.1
1	B	545	LEU	3.0
1	B	540	VAL	3.0
1	B	590	ARG	3.0
1	C	468	VAL	3.0
1	C	615	PHE	3.0
1	B	406	ILE	3.0
1	C	542	GLY	2.9
1	B	284	SER	2.9
1	C	576	ALA	2.9
1	B	581	VAL	2.8
1	C	591	GLU	2.8
1	C	575	GLN	2.8
1	C	406	ILE	2.8
1	A	571	PRO	2.8
1	A	587	ASN	2.7
1	B	537	VAL	2.7
1	A	615	PHE	2.7
1	C	597	LEU	2.7
1	A	616	VAL	2.6
1	B	542	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	580	PHE	2.5
1	B	536	ASP	2.5
1	A	22	PHE	2.5
1	C	579	ALA	2.5
1	C	27	VAL	2.5
1	C	284	SER	2.4
1	C	585	SER	2.4
1	C	537	VAL	2.4
1	B	582	ALA	2.4
1	C	574	GLY	2.4
1	A	572	LEU	2.3
1	A	591	GLU	2.3
1	A	611	PRO	2.3
1	B	565	VAL	2.3
1	C	14	VAL	2.3
1	B	583	LEU	2.3
1	C	413	TRP	2.3
1	A	568	VAL	2.3
1	C	417	VAL	2.3
1	A	590	ARG	2.2
1	C	383	ARG	2.2
1	A	284	SER	2.2
1	C	56[A]	ASP	2.2
1	A	583	LEU	2.2
1	C	21	THR	2.2
1	C	598	ILE	2.1
1	C	538	VAL	2.1
1	B	567	GLY	2.1
1	A	569	PRO	2.1
1	C	380	LEU	2.1
1	C	16	ALA	2.1
1	A	618	ASP	2.1
1	C	285	THR	2.1
1	B	541	SER	2.1
1	A	586	GLY	2.1
1	A	407	ALA	2.1
1	B	591	GLU	2.0
1	C	215	ILE	2.0
1	C	592	GLN	2.0
1	B	599	MET	2.0
1	C	566	VAL	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.

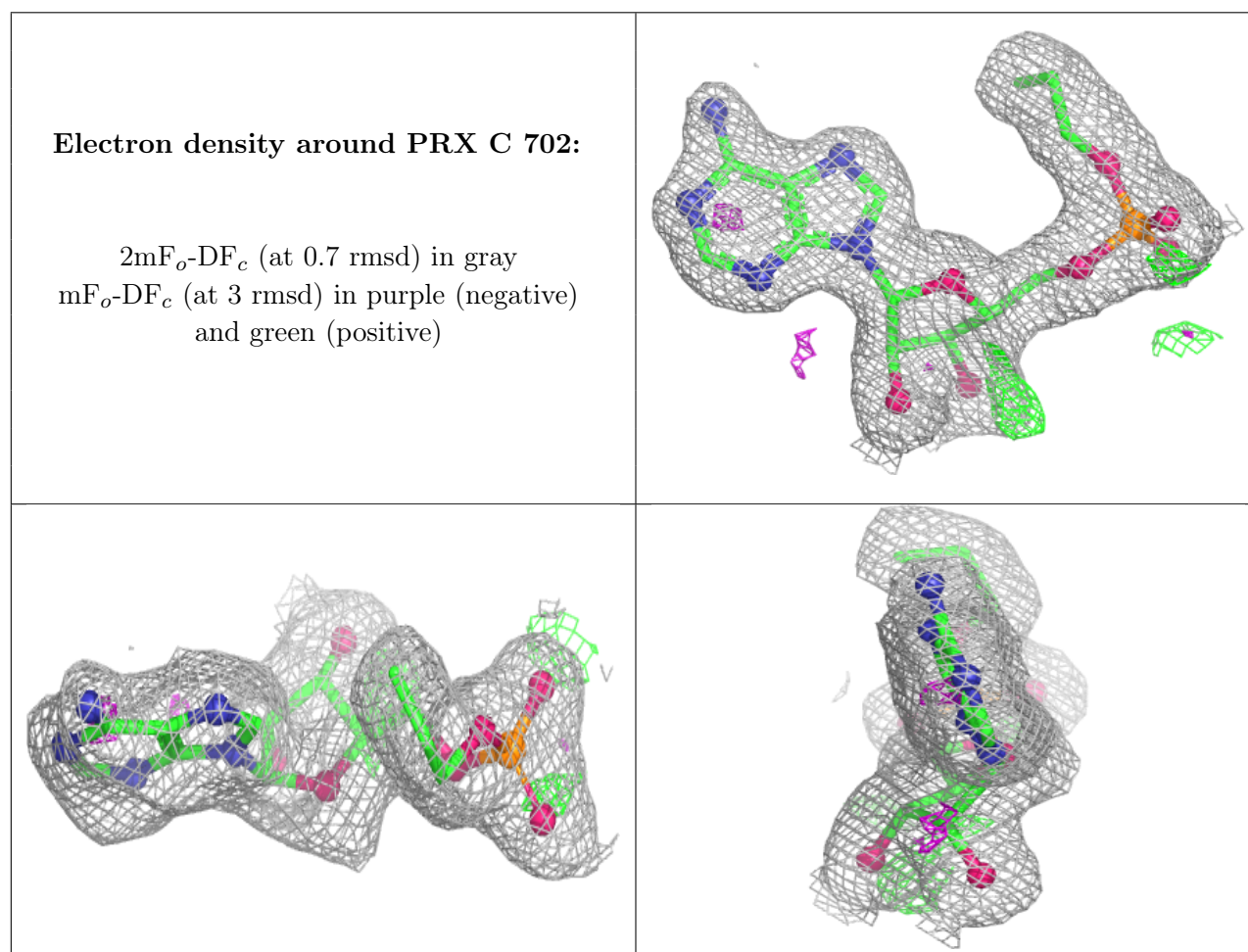
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	709	4/4	0.80	0.14	45,45,47,49	0
3	EDO	B	714	4/4	0.85	0.17	31,38,44,45	0
3	EDO	C	704	4/4	0.85	0.15	37,41,48,51	0
3	EDO	B	712	4/4	0.86	0.14	30,32,38,47	0
3	EDO	C	711	4/4	0.86	0.14	35,36,39,54	0
3	EDO	A	704	4/4	0.89	0.14	33,37,37,39	0
3	EDO	B	711	4/4	0.89	0.12	33,35,38,50	0
3	EDO	C	703	4/4	0.90	0.12	37,37,42,45	0
3	EDO	C	701	4/4	0.91	0.11	34,35,35,41	0
3	EDO	A	702	4/4	0.91	0.18	32,34,44,45	0
3	EDO	B	703	4/4	0.91	0.14	32,36,39,40	0
3	EDO	B	706	4/4	0.91	0.10	29,31,34,38	0
3	EDO	B	713	4/4	0.92	0.09	33,38,38,39	0
3	EDO	C	706	4/4	0.92	0.14	26,31,35,41	0
3	EDO	B	708	4/4	0.92	0.15	30,36,37,39	0
3	EDO	A	703	4/4	0.93	0.14	35,37,43,47	0
3	EDO	C	708	4/4	0.93	0.16	26,27,32,34	0
3	EDO	C	705	4/4	0.93	0.11	30,32,34,36	0
3	EDO	B	702	4/4	0.94	0.11	32,34,39,40	0
3	EDO	A	706	4/4	0.94	0.09	25,27,28,29	0
3	EDO	B	704	4/4	0.94	0.09	28,28,29,33	0
3	EDO	A	710	4/4	0.94	0.10	31,36,39,40	0
3	EDO	B	705	4/4	0.95	0.11	21,26,26,37	0
3	EDO	C	707	4/4	0.95	0.07	25,30,31,32	0
3	EDO	A	707	4/4	0.95	0.09	21,26,30,42	0
3	EDO	B	707	4/4	0.95	0.09	25,28,28,29	0
3	EDO	A	708	4/4	0.96	0.10	25,28,31,33	0

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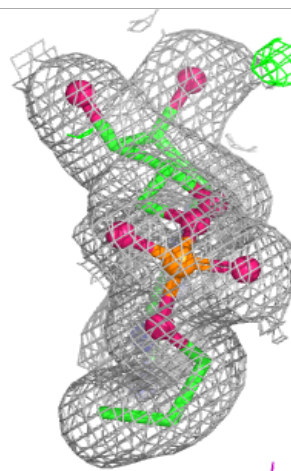
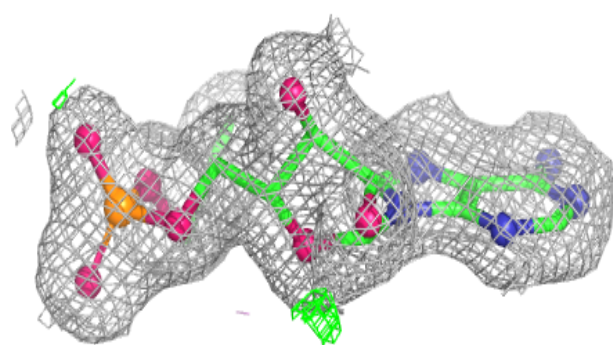
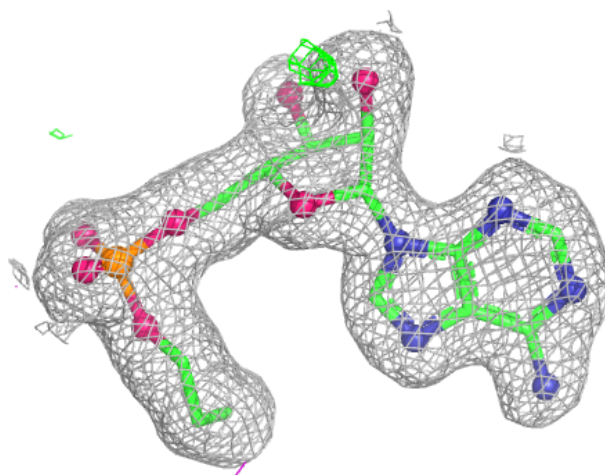
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	705	4/4	0.96	0.08	25,28,30,31	0
3	EDO	B	709	4/4	0.96	0.09	23,25,30,31	0
3	EDO	C	709	4/4	0.96	0.08	31,34,36,38	0
3	EDO	B	710	4/4	0.96	0.10	28,29,31,34	0
2	PRX	C	702	26/26	0.97	0.07	21,27,31,33	0
2	PRX	A	701	26/26	0.98	0.05	19,22,24,31	0
3	EDO	C	710	4/4	0.98	0.05	23,27,30,31	0
2	PRX	B	701	26/26	0.98	0.04	20,22,25,27	0

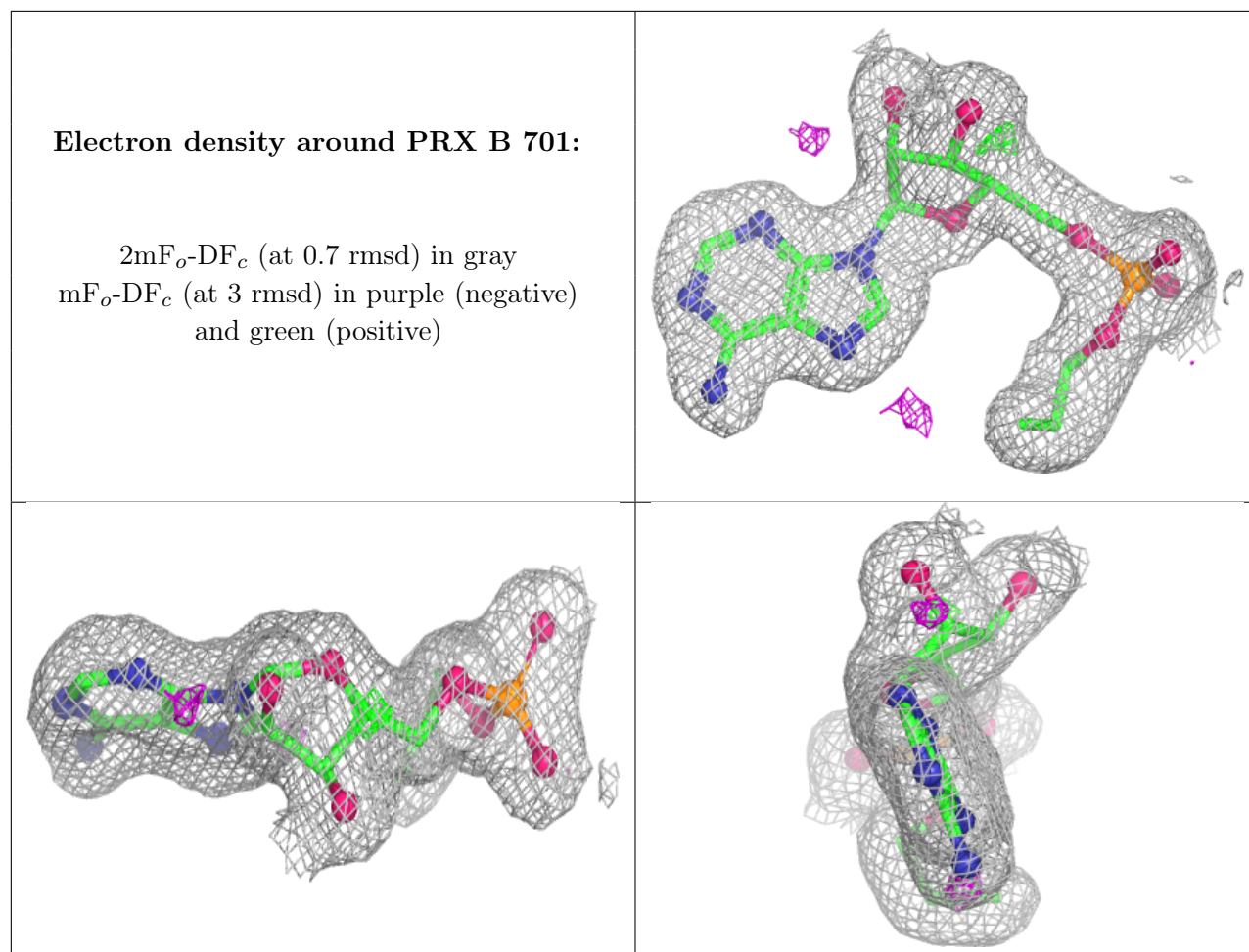
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around PRX 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 [i](#)

There are no such residues in this entry.