



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2020 – 12:09 PM EST

PDB ID : 7KQ6  
Title : Crystal Structure of Acetyl-coenzyme A synthetase from *Coccidioides immitis* in complex with PRX  
Authors : Seattle Structural Genomics Center for Infectious Disease; 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

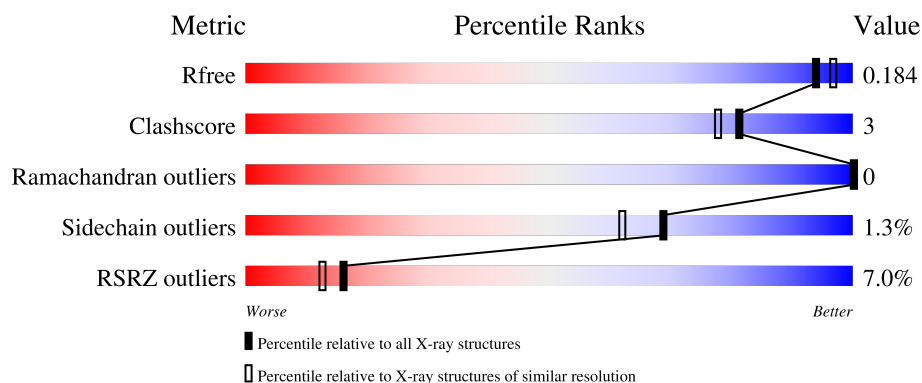
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	706	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>5%</div> <div>16%</div> </div> </div>
1	C	706	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div>14%</div> </div> </div>

## 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:

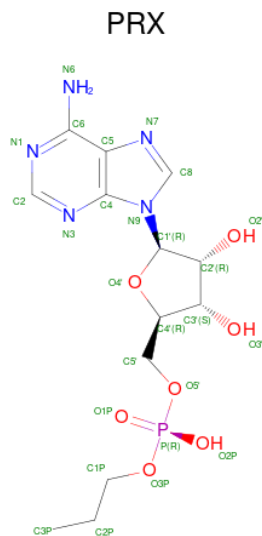
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP J3KJC6
A	-13	HIS	-	expression tag	UNP J3KJC6
A	-12	HIS	-	expression tag	UNP J3KJC6
A	-11	HIS	-	expression tag	UNP J3KJC6
A	-10	HIS	-	expression tag	UNP J3KJC6
A	-9	HIS	-	expression tag	UNP J3KJC6
A	-8	HIS	-	expression 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

*Continued on next page...*

*Continued from previous page...*

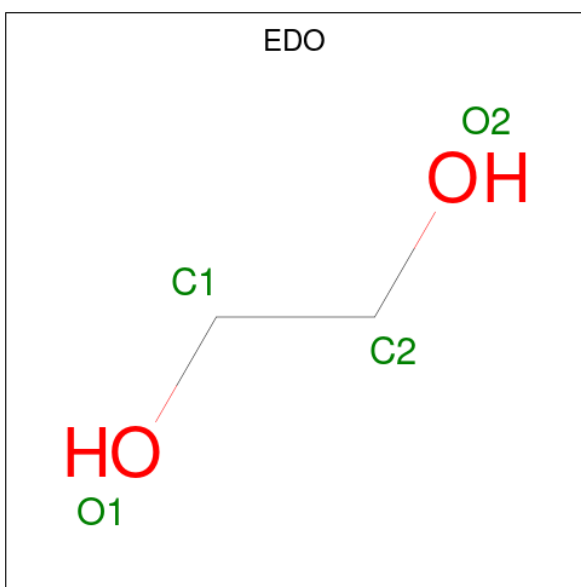
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP J3KJC6
B	-6	HIS	-	expression tag	UNP J3KJC6
B	-5	GLU	-	expression tag	UNP J3KJC6
B	-4	ASN	-	expression tag	UNP J3KJC6
B	-3	LEU	-	expression tag	UNP J3KJC6
B	-2	TYR	-	expression tag	UNP J3KJC6
B	-1	PHE	-	expression tag	UNP J3KJC6
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 (three-letter code: PRX) (formula:  $C_{13}H_{20}N_5O_7P$ ) (labeled as "Ligand of Interest" by author).



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 (three-letter code: 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		

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

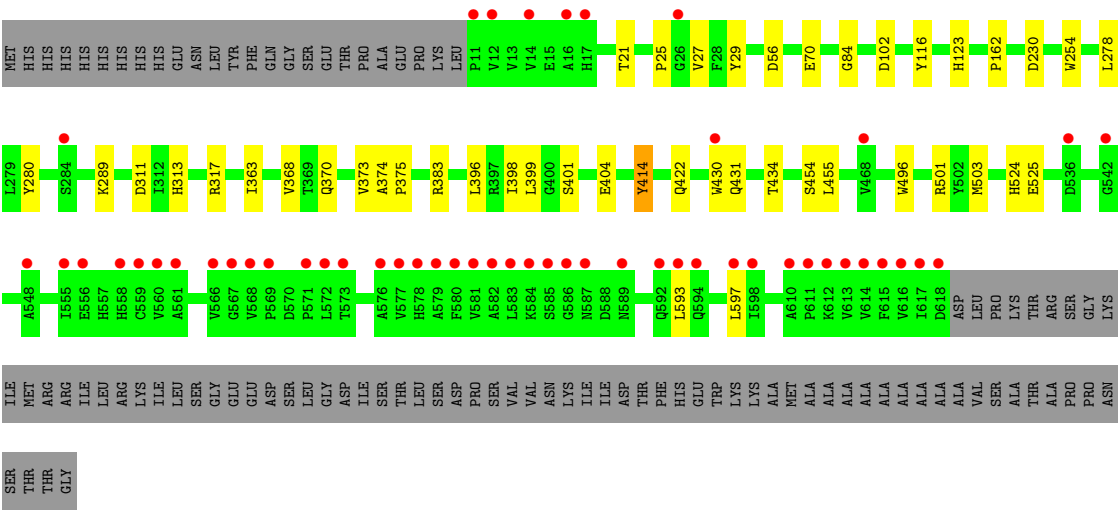
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19rc4-4035	Depositor
R, $R_{free}$	0.162 , 0.185 0.161 , 0.184	Depositor DCC
$R_{free}$ test set	2010 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, 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	0.37	0/4927	0.57	0/6715
1	B	0.37	0/4720	0.58	0/6431
1	C	0.35	0/4858	0.56	0/6626
All	All	0.36	0/14505	0.57	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 [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	4772	0	4593	19	1
1	B	4574	0	4382	23	0
1	C	4711	0	4484	31	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	542	0	0	1	0
4	C	472	0	0	4	0
All	All	15819	0	13708	72	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 (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: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: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: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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:399:LEU:HB3	1:C:414:TYR:CZ	2.53	0.43
1:C:289:LYS:HG2	1:C:501:ARG:CZ	2.47	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:373:VAL:O	1:C:401:SER:HA	2.20	0.42
1:C:278:LEU:HD21	1:C:496:TRP:CE3	2.55	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
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 [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	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 [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	494/584 (85%)	488 (99%)	6 (1%)	71	65
1	B	467/584 (80%)	460 (98%)	7 (2%)	65	56
1	C	481/584 (82%)	474 (98%)	7 (2%)	65	56
All	All	1442/1752 (82%)	1422 (99%)	20 (1%)	69	59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ASP
1	A	287	LYS
1	A	289	LYS
1	A	317	ARG
1	A	414	TYR
1	A	594	GLN
1	B	102	ASP
1	B	281	THR
1	B	317	ARG
1	B	414	TYR
1	B	431	GLN
1	B	468	VAL
1	B	531	ARG
1	C	21	THR
1	C	56[A]	ASP
1	C	56[B]	ASP
1	C	102	ASP
1	C	317	ARG
1	C	383	ARG
1	C	414	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

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	705	-	3,3,3	0.54	0	2,2,2	0.20	0
3	EDO	C	711	-	3,3,3	0.46	0	2,2,2	0.49	0
3	EDO	C	710	-	3,3,3	0.43	0	2,2,2	0.10	0
3	EDO	A	708	-	3,3,3	0.38	0	2,2,2	0.23	0
3	EDO	A	710	-	3,3,3	0.45	0	2,2,2	0.41	0
3	EDO	B	714	-	3,3,3	0.51	0	2,2,2	0.25	0
3	EDO	B	703	-	3,3,3	0.51	0	2,2,2	0.32	0
3	EDO	B	708	-	3,3,3	0.55	0	2,2,2	0.18	0
3	EDO	A	706	-	3,3,3	0.44	0	2,2,2	0.40	0
3	EDO	B	702	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	A	707	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	B	712	-	3,3,3	0.55	0	2,2,2	0.26	0
3	EDO	C	704	-	3,3,3	0.44	0	2,2,2	0.53	0
3	EDO	A	704	-	3,3,3	0.41	0	2,2,2	0.42	0
3	EDO	B	704	-	3,3,3	0.55	0	2,2,2	0.16	0
3	EDO	B	709	-	3,3,3	0.38	0	2,2,2	0.27	0
2	PRX	C	702	-	25,28,28	0.63	0	27,41,41	0.73	1 (3%)
3	EDO	C	709	-	3,3,3	0.52	0	2,2,2	0.28	0
3	EDO	B	706	-	3,3,3	0.58	0	2,2,2	0.20	0
3	EDO	C	706	-	3,3,3	0.52	0	2,2,2	0.39	0
3	EDO	C	707	-	3,3,3	0.48	0	2,2,2	0.44	0
3	EDO	B	705	-	3,3,3	0.46	0	2,2,2	0.49	0
3	EDO	C	703	-	3,3,3	0.44	0	2,2,2	0.48	0
3	EDO	A	703	-	3,3,3	0.45	0	2,2,2	0.53	0
3	EDO	A	709	-	3,3,3	0.40	0	2,2,2	0.42	0
3	EDO	C	701	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	B	707	-	3,3,3	0.51	0	2,2,2	0.23	0
2	PRX	B	701	-	25,28,28	0.58	0	27,41,41	0.76	1 (3%)
3	EDO	B	710	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	B	711	-	3,3,3	0.43	0	2,2,2	0.51	0
3	EDO	A	702	-	3,3,3	0.48	0	2,2,2	0.48	0
2	PRX	A	701	-	25,28,28	0.63	0	27,41,41	0.72	1 (3%)
3	EDO	C	708	-	3,3,3	0.28	0	2,2,2	0.65	0
3	EDO	A	705	-	3,3,3	0.57	0	2,2,2	0.19	0
3	EDO	B	713	-	3,3,3	0.41	0	2,2,2	0.55	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	705	-	-	0/1/1/1	-
3	EDO	C	711	-	-	0/1/1/1	-
3	EDO	C	710	-	-	0/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
3	EDO	A	710	-	-	0/1/1/1	-
3	EDO	B	714	-	-	0/1/1/1	-
3	EDO	B	703	-	-	1/1/1/1	-
3	EDO	B	708	-	-	1/1/1/1	-
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	B	712	-	-	1/1/1/1	-
3	EDO	C	704	-	-	0/1/1/1	-
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	B	709	-	-	0/1/1/1	-
2	PRX	C	702	-	-	0/11/31/31	0/3/3/3
3	EDO	C	709	-	-	0/1/1/1	-
3	EDO	B	706	-	-	0/1/1/1	-
3	EDO	C	706	-	-	0/1/1/1	-
3	EDO	C	707	-	-	0/1/1/1	-
3	EDO	B	705	-	-	0/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	A	709	-	-	0/1/1/1	-
3	EDO	C	701	-	-	1/1/1/1	-
3	EDO	B	707	-	-	0/1/1/1	-
2	PRX	B	701	-	-	0/11/31/31	0/3/3/3
3	EDO	B	710	-	-	0/1/1/1	-
3	EDO	B	711	-	-	1/1/1/1	-
3	EDO	A	702	-	-	0/1/1/1	-
2	PRX	A	701	-	-	0/11/31/31	0/3/3/3
3	EDO	C	708	-	-	1/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	B	713	-	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	PRX	C5-C6-N6	2.37	123.96	120.35
2	C	702	PRX	C5-C6-N6	2.34	123.91	120.35
2	A	701	PRX	C5-C6-N6	2.19	123.68	120.35

There are no chirality outliers.

All (6) 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

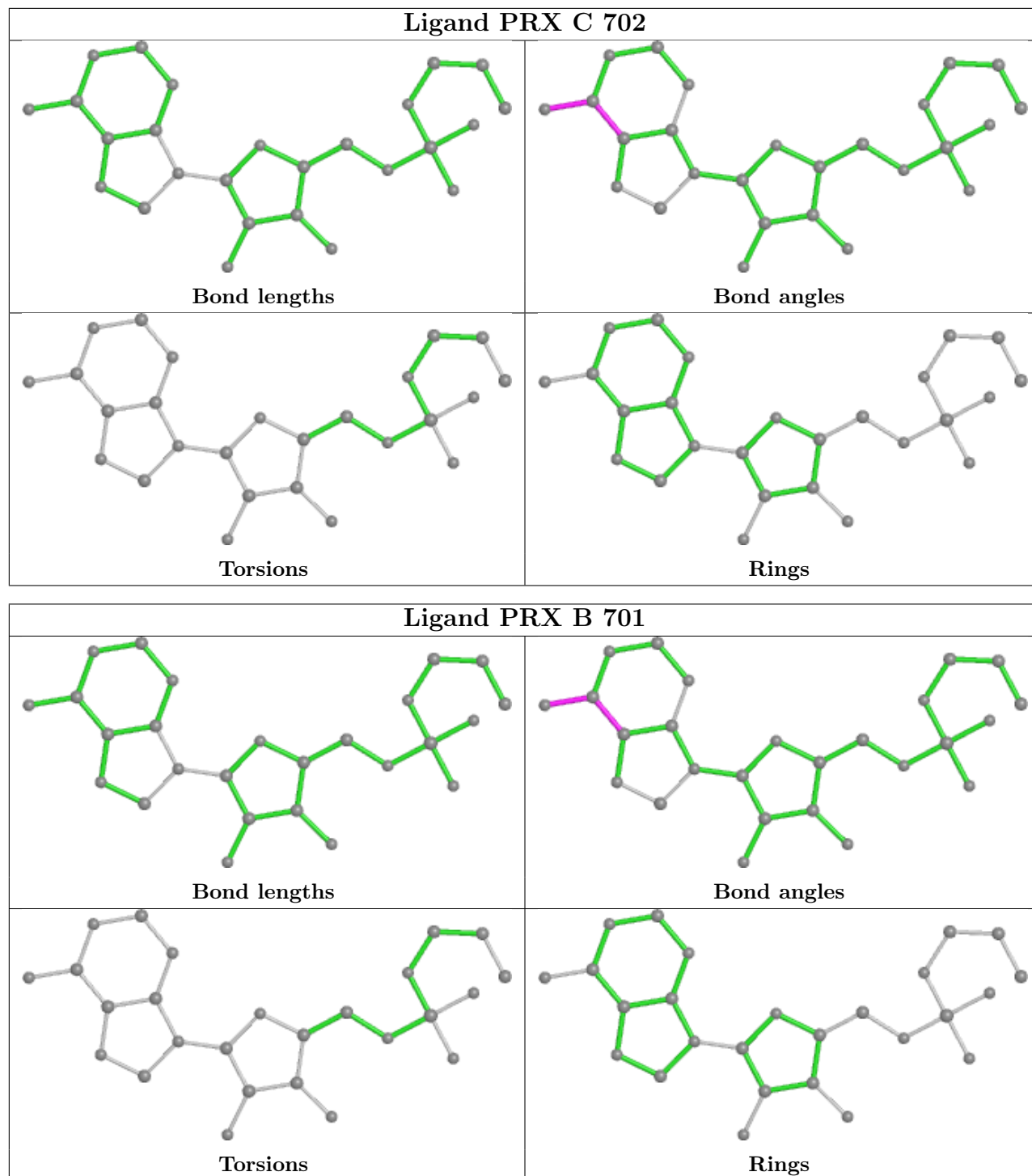
There are no ring outliers.

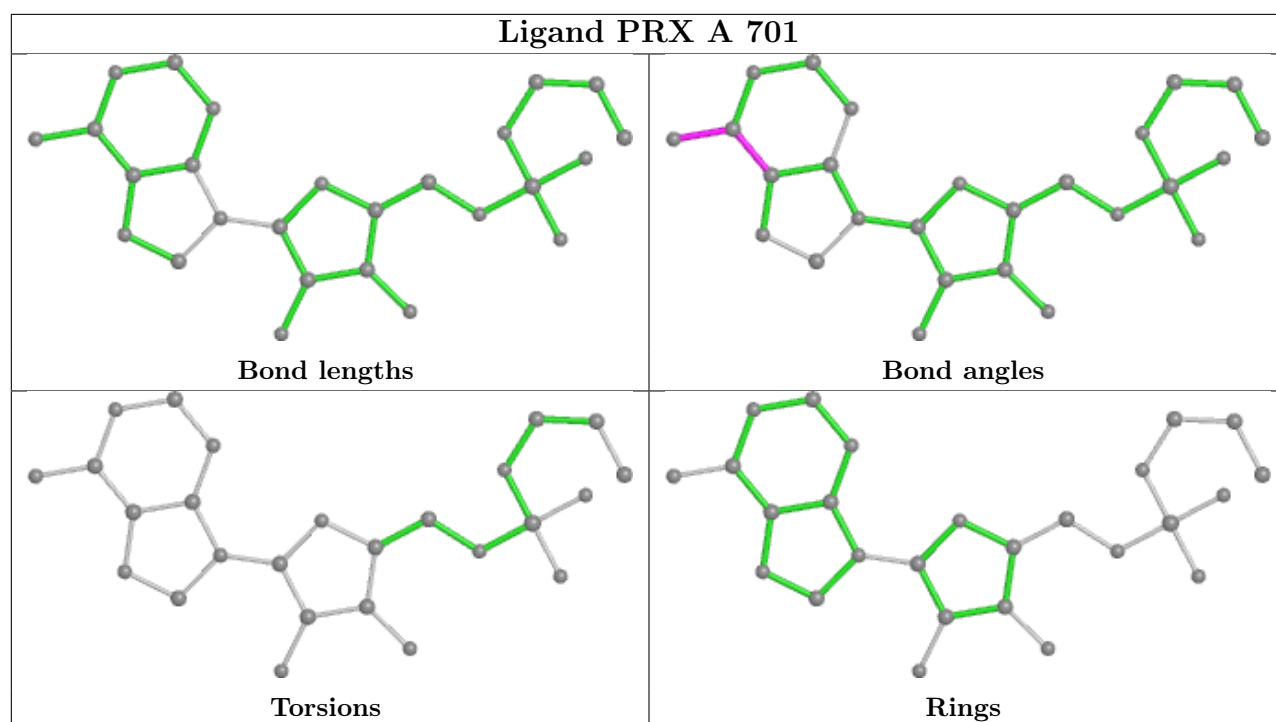
12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	710	EDO	2	0
3	A	708	EDO	3	0
3	B	708	EDO	1	0
3	B	709	EDO	2	0
2	C	702	PRX	1	0
3	C	703	EDO	2	0
3	C	701	EDO	1	0
2	B	701	PRX	2	0
3	A	702	EDO	1	0
2	A	701	PRX	1	0
3	C	708	EDO	2	0
3	B	713	EDO	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	610/706 (86%)	-0.08	31 (5%)	28	22	15, 25, 66, 106	0
1	B	590/706 (83%)	-0.00	44 (7%)	14	11	14, 25, 76, 102	0
1	C	608/706 (86%)	0.17	52 (8%)	10	8	15, 31, 81, 113	0
All	All	1808/2118 (85%)	0.03	127 (7%)	16	13	14, 27, 73, 113	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	613	VAL	8.7
1	A	580	PHE	7.4
1	B	580	PHE	7.1
1	B	561	ALA	6.4
1	C	615	PHE	6.3
1	C	577	VAL	6.3
1	B	579	ALA	6.0
1	B	615	PHE	6.0
1	C	568	VAL	5.9
1	B	593	LEU	5.9
1	C	580	PHE	5.8
1	C	617	ILE	5.8
1	B	583	LEU	5.8
1	B	558	HIS	5.8
1	B	581	VAL	5.7
1	C	542	GLY	5.7
1	B	613	VAL	5.4
1	A	615	PHE	5.4
1	B	559	CYS	5.2
1	C	585	SER	5.2
1	C	573	THR	5.2
1	B	614	VAL	4.9
1	A	614	VAL	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	563	ALA	4.7
1	A	613	VAL	4.7
1	B	592	GLN	4.7
1	C	581	VAL	4.6
1	B	560	VAL	4.5
1	C	14	VAL	4.5
1	C	614	VAL	4.4
1	A	617	ILE	4.4
1	C	572	LEU	4.4
1	C	582	ALA	4.4
1	C	576	ALA	4.3
1	C	566	VAL	4.3
1	C	611	PRO	4.3
1	B	582	ALA	4.2
1	B	542	GLY	4.2
1	B	591	GLU	4.2
1	C	589	ASN	4.1
1	A	585	SER	4.1
1	A	611	PRO	4.1
1	B	567	GLY	4.1
1	C	579	ALA	4.1
1	C	597	LEU	4.0
1	C	616	VAL	4.0
1	C	561	ALA	4.0
1	B	599	MET	3.9
1	C	610	ALA	3.9
1	A	468	VAL	3.9
1	B	597	LEU	3.8
1	C	583	LEU	3.8
1	B	284	SER	3.8
1	C	468	VAL	3.8
1	B	577	VAL	3.7
1	C	284	SER	3.7
1	A	583	LEU	3.6
1	A	616	VAL	3.5
1	C	569	PRO	3.5
1	B	566	VAL	3.5
1	C	11	PRO	3.5
1	A	618	ASP	3.5
1	C	592	GLN	3.4
1	B	468	VAL	3.4
1	B	565	VAL	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	581	VAL	3.4
1	C	12	VAL	3.4
1	C	567	GLY	3.4
1	C	586	GLY	3.3
1	A	568	VAL	3.3
1	A	589	ASN	3.3
1	B	594	GLN	3.2
1	B	598	ILE	3.2
1	B	589	ASN	3.1
1	B	595	LYS	3.1
1	B	14	VAL	3.1
1	C	560	VAL	3.0
1	B	555	ILE	2.9
1	B	557	HIS	2.9
1	A	559	CYS	2.9
1	A	619	ASP	2.9
1	A	10	LEU	2.8
1	A	571	PRO	2.7
1	C	555	ILE	2.7
1	C	558	HIS	2.7
1	B	556	GLU	2.7
1	A	18	GLN	2.7
1	C	594	GLN	2.7
1	B	590	ARG	2.7
1	B	616	VAL	2.6
1	C	16	ALA	2.6
1	B	469	THR	2.6
1	A	584	LYS	2.6
1	A	577	VAL	2.6
1	B	578	HIS	2.6
1	B	610	ALA	2.5
1	C	584	LYS	2.5
1	C	612	LYS	2.5
1	B	564	ALA	2.5
1	C	598	ILE	2.5
1	A	561	ALA	2.5
1	C	618	ASP	2.5
1	C	430	TRP	2.5
1	A	582	ALA	2.5
1	B	17	HIS	2.5
1	C	556	GLU	2.4
1	C	587	ASN	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	558	HIS	2.4
1	A	594	GLN	2.4
1	B	562	GLU	2.3
1	C	559	CYS	2.3
1	C	548	ALA	2.3
1	A	36	PRO	2.3
1	C	571	PRO	2.3
1	A	592	GLN	2.3
1	C	578	HIS	2.3
1	A	593	LEU	2.2
1	A	564	ALA	2.2
1	B	601	VAL	2.2
1	B	541	SER	2.2
1	C	17	HIS	2.1
1	A	430	TRP	2.1
1	C	26	GLY	2.1
1	C	593	LEU	2.0
1	C	536	ASP	2.0
1	A	560	VAL	2.0
1	B	550	ILE	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	B	712	4/4	0.83	0.17	30,32,38,47	0
3	EDO	C	711	4/4	0.88	0.15	35,36,39,54	0
3	EDO	B	708	4/4	0.89	0.14	30,36,37,39	0

*Continued on next page...*



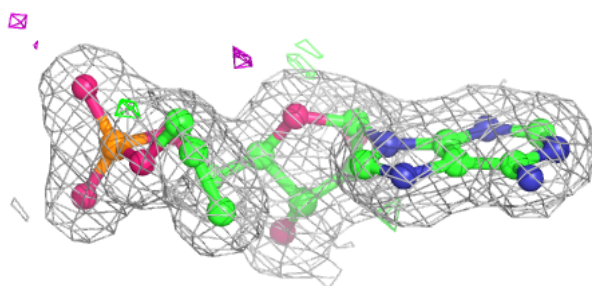
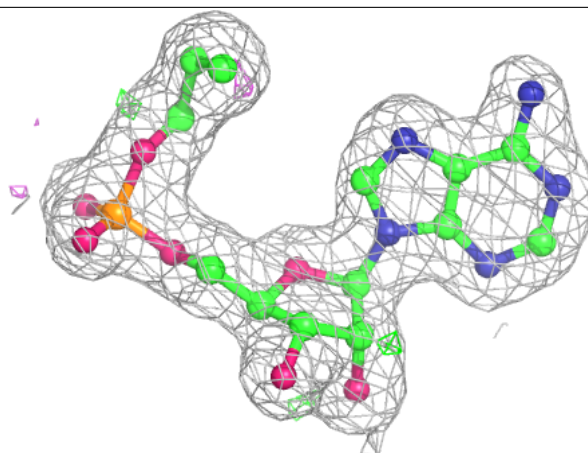
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	C	704	4/4	0.89	0.22	37,41,48,51	0
3	EDO	B	714	4/4	0.91	0.13	31,38,44,45	0
3	EDO	B	706	4/4	0.92	0.10	29,31,34,38	0
3	EDO	C	703	4/4	0.92	0.22	37,37,42,45	0
3	EDO	A	709	4/4	0.92	0.32	45,45,47,49	0
3	EDO	C	701	4/4	0.92	0.09	34,35,35,41	0
3	EDO	C	705	4/4	0.93	0.19	30,32,34,36	0
3	EDO	A	703	4/4	0.93	0.23	35,37,43,47	0
3	EDO	A	702	4/4	0.93	0.31	32,34,44,45	0
3	EDO	C	706	4/4	0.94	0.19	26,31,35,41	0
3	EDO	B	703	4/4	0.94	0.22	32,36,39,40	0
3	EDO	B	707	4/4	0.95	0.08	25,28,28,29	0
3	EDO	A	705	4/4	0.95	0.10	25,28,30,31	0
3	EDO	B	704	4/4	0.96	0.09	28,28,29,33	0
3	EDO	C	709	4/4	0.96	0.10	31,34,36,38	0
3	EDO	A	710	4/4	0.96	0.08	31,36,39,40	0
3	EDO	A	706	4/4	0.96	0.07	25,27,28,29	0
3	EDO	B	710	4/4	0.96	0.14	28,29,31,34	0
3	EDO	B	705	4/4	0.96	0.18	21,26,26,37	0
3	EDO	C	708	4/4	0.96	0.15	26,27,32,34	0
3	EDO	A	704	4/4	0.96	0.11	33,37,37,39	0
3	EDO	B	713	4/4	0.96	0.08	33,38,38,39	0
3	EDO	B	702	4/4	0.97	0.19	32,34,39,40	0
2	PRX	A	701	26/26	0.97	0.11	19,22,24,31	0
3	EDO	C	707	4/4	0.97	0.07	25,30,31,32	0
2	PRX	C	702	26/26	0.97	0.13	21,27,31,33	0
3	EDO	B	711	4/4	0.97	0.12	33,35,38,50	0
2	PRX	B	701	26/26	0.98	0.12	20,22,25,27	0
3	EDO	B	709	4/4	0.98	0.12	23,25,30,31	0
3	EDO	A	708	4/4	0.98	0.10	25,28,31,33	0
3	EDO	A	707	4/4	0.98	0.15	21,26,30,42	0
3	EDO	C	710	4/4	0.99	0.09	23,27,30,31	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.

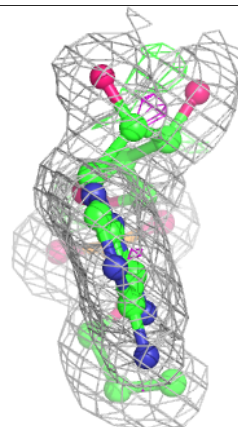
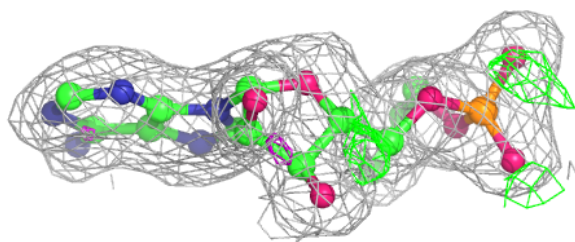
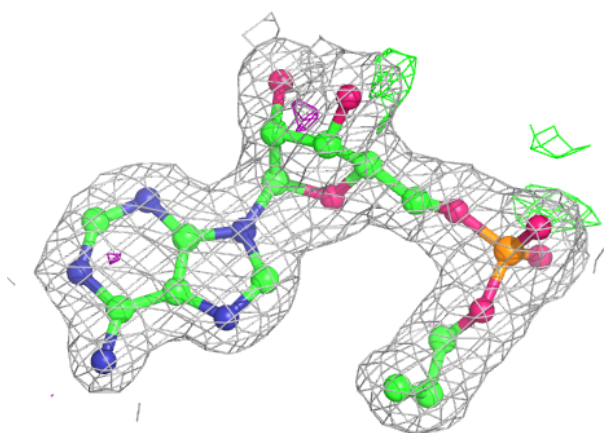
**Electron density around PRX A 701:**

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

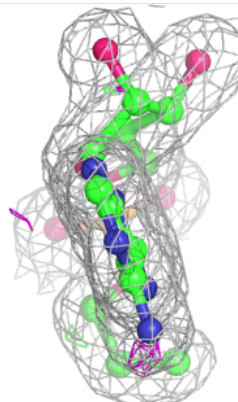
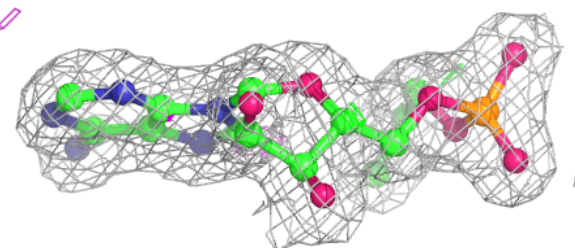
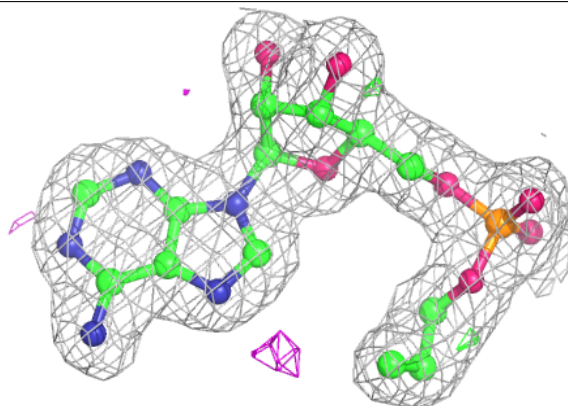


**Electron density around PRX C 702:**

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

**Electron density around PRX B 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.