



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:01 AM UTC

PDB ID : 5IFI / pdb_00005ifi
Title : CRYSTAL STRUCTURE OF ACETYL-COA SYNTHETASE IN COMPLEX
WITH ADENOSINE-5'-PROPYLPHOSPHATE FROM CRYPTOCOCCUS
NEOFORMANS H99
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID); SSGCID;
Fox III, D.; Edwards, T.E.; Lorimer, D.D.; Mutz, M.W.
Deposited on : 2016-02-26
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) 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

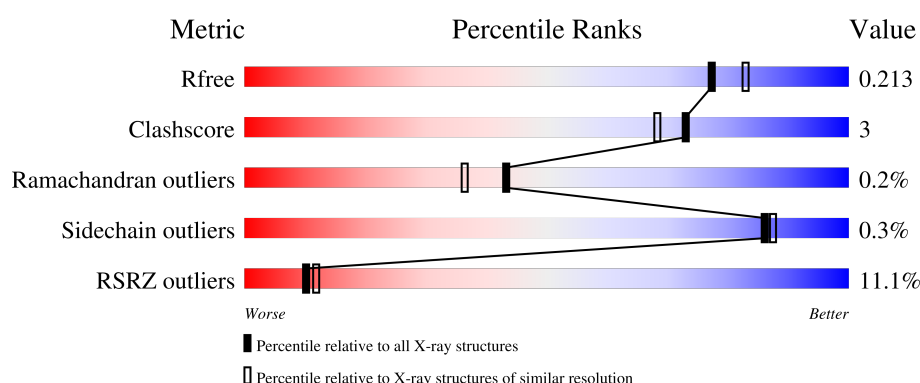
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	694	5% 87% 6% 6%
1	B	694	6% 86% 6% 7%
1	C	694	19% 74% 7% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PRX	C	701	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15384 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	650	Total	C	N	O	S	0	7	0
			5045	3221	858	939	27			
1	B	642	Total	C	N	O	S	0	11	0
			5010	3190	858	936	26			
1	C	567	Total	C	N	O	S	0	1	0
			4187	2668	712	784	23			

There are 45 discrepancies between the modelled and reference sequences:

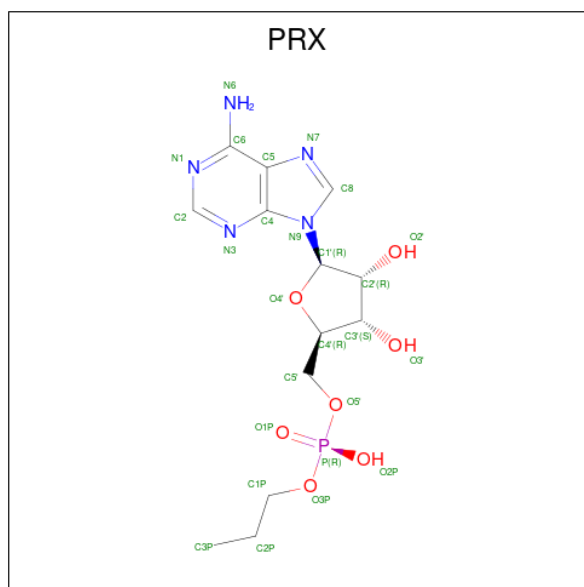
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression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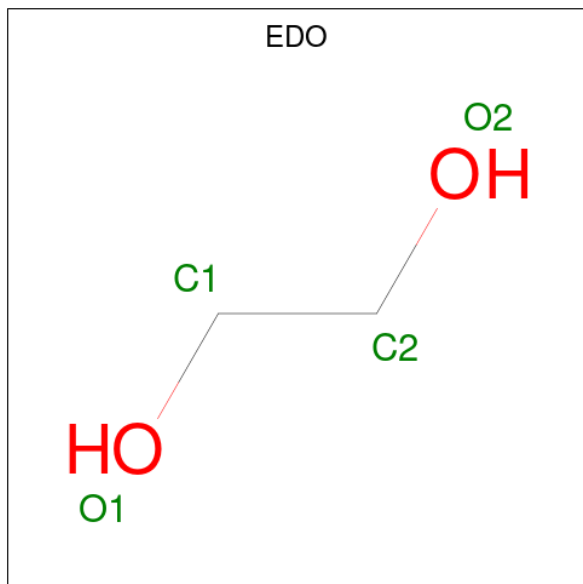
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1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



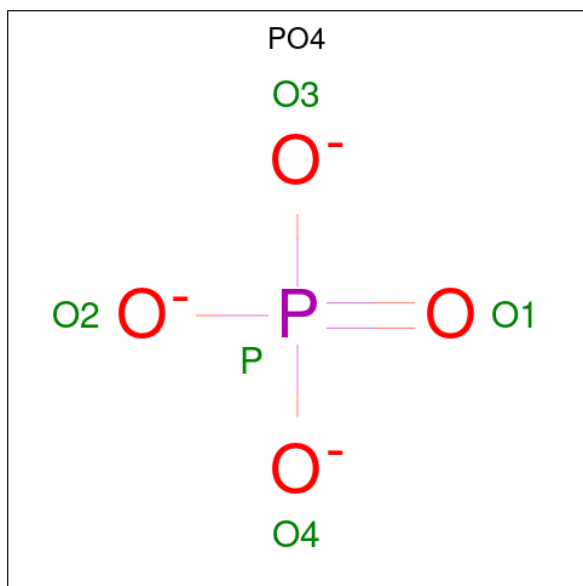
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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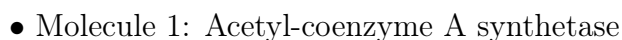
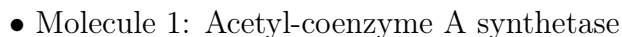
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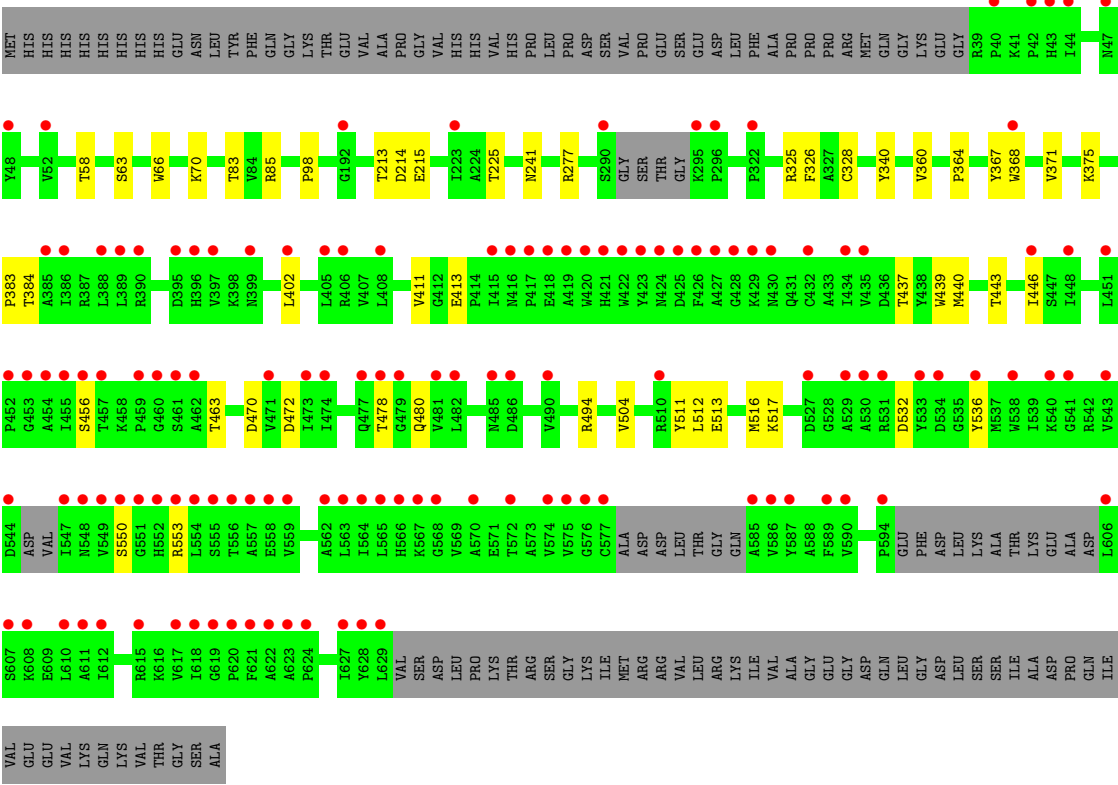
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	398	Total	O	0	1
			399	399		
5	B	385	Total	O	0	2
			386	386		
5	C	186	Total	O	0	1
			187	187		

- 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	72.46Å 185.55Å 84.89Å 90.00° 93.67° 90.00°	Depositor
Resolution (Å)	41.84 – 1.95 41.84 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (41.84-1.95) 98.7 (41.84-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.95Å)	Xtriage
Refinement program	PHENIX (DEV_2328: ???)	Depositor
R, R_{free}	0.185 , 0.213 0.186 , 0.213	Depositor DCC
R_{free} test set	8031 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15384	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: PRX, PO4, 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	0/5198	0.49	0/7094
1	B	0.26	0/5156	0.46	0/7032
1	C	0.22	0/4301	0.42	0/5888
All	All	0.26	0/14655	0.46	0/20014

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	5045	0	4791	28	0
1	B	5010	0	4725	24	0
1	C	4187	0	3785	37	0
2	A	26	0	19	1	0
2	B	26	0	19	1	0
2	C	26	0	18	2	0
3	A	40	0	60	3	0
3	B	24	0	36	2	0
3	C	8	0	12	3	0
4	B	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	399	0	0	4	0
5	B	386	0	0	2	0
5	C	187	0	0	2	0
All	All	15384	0	13465	89	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 3.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ASN:HB3	3:C:703:EDO:H21	1.73	0.71
1:C:439:TRP:HB2	1:C:443:THR:HG21	1.73	0.70
1:C:513:GLU:HA	1:C:517:LYS:HG3	1.74	0.69
1:A:47:ASN:HA	3:A:707:EDO:H22	1.73	0.69
1:A:50:SER:HB2	3:A:702:EDO:H21	1.74	0.69
1:A:99:GLU:O	1:C:277:ARG:NH2	2.26	0.68
1:C:512:LEU:HA	1:C:516:MET:HG2	1.77	0.67
1:A:217:ARG:NH1	1:A:222:THR:OG1	2.29	0.66
1:B:405:LEU:HD13	1:B:408:LEU:HD21	1.80	0.64
1:B:384[A]:THR:HG21	1:B:639:GLY:HA3	1.83	0.61
1:C:368:TRP:HB3	1:C:402:LEU:HD21	1.83	0.59
1:A:545:ASP:OD1	1:A:647:ARG:NH2	2.36	0.58
1:B:495:ARG:NH1	5:B:801:HOH:O	2.28	0.58
1:C:532:ASP:OD1	1:C:536:TYR:N	2.36	0.58
1:B:603:GLU:HG3	1:B:629:LEU:HD12	1.85	0.58
1:C:472:ASP:OD1	1:C:494:ARG:NH1	2.39	0.56
1:C:325:ARG:NH2	1:C:375:LYS:O	2.37	0.55
1:C:340:TYR:OH	1:C:446:ILE:HG12	2.06	0.55
1:C:440:MET:H	1:C:443:THR:HG22	1.72	0.54
1:B:368:TRP:HB3	1:B:402:LEU:HD21	1.90	0.54
1:A:384:THR:HG21	1:A:639:GLY:HA3	1.90	0.53
1:B:439:TRP:CE2	2:B:701:PRX:H3P1	2.45	0.52
1:A:99:GLU:HG2	3:C:702:EDO:H11	1.91	0.52
1:A:617:VAL:HG23	1:A:618:ILE:HG13	1.91	0.52
1:C:411:VAL:HG21	1:C:439:TRP:HE1	1.74	0.52
1:C:437:THR:HB	1:C:446:ILE:HD12	1.91	0.52
1:A:439:TRP:CE2	2:A:701:PRX:H3P1	2.45	0.52
1:A:542:ARG:NH1	5:A:815:HOH:O	2.43	0.52
1:B:413:GLU:HG2	1:B:414:PRO:HD2	1.93	0.51
3:C:703:EDO:O1	5:C:801:HOH:O	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:MET:H	1:C:443:THR:CG2	2.24	0.51
1:C:440:MET:O	1:C:443:THR:HG22	2.10	0.51
1:A:218:ARG:NH1	5:A:816:HOH:O	2.45	0.50
1:C:383:PRO:HG2	1:C:413:GLU:HG2	1.94	0.50
1:B:58:THR:HG22	1:B:66:TRP:CD2	2.47	0.49
1:B:17:PRO:HB3	1:B:617:VAL:HG11	1.95	0.49
1:C:63:SER:OG	1:C:85:ARG:NH2	2.46	0.49
1:A:134:GLU:OE1	5:A:801:HOH:O	2.20	0.48
1:C:241:ASN:ND2	5:C:813:HOH:O	2.46	0.48
1:A:17:PRO:HD2	1:A:561:SER:HB2	1.96	0.48
1:B:314:LEU:HD22	1:B:345:PRO:HA	1.97	0.47
1:A:127:ASP:HA	1:A:357:SER:HB2	1.97	0.46
1:A:442:GLU:HG2	1:A:515:TYR:CZ	2.50	0.46
1:B:442:GLU:HG2	1:B:515:TYR:CZ	2.49	0.46
1:C:439:TRP:HB2	1:C:443:THR:CG2	2.41	0.46
1:A:193:PHE:CZ	1:A:334[B]:TRP:HH2	2.34	0.46
1:B:590:VAL:HB	1:B:629:LEU:HD23	1.96	0.46
1:C:214:ASP:OD1	1:C:215:GLU:N	2.48	0.46
1:C:553:ARG:NH1	2:C:701:PRX:O2P	2.49	0.46
1:A:67:TRP:CZ3	1:A:498:PRO:HG2	2.51	0.45
1:C:58:THR:HG22	1:C:66:TRP:CD2	2.52	0.45
1:C:384:THR:OG1	1:C:550:SER:HA	2.16	0.45
1:C:383:PRO:HG2	1:C:413:GLU:CG	2.48	0.44
1:A:613:GLN:O	1:A:617:VAL:HG22	2.17	0.44
1:C:83:THR:O	1:C:98:PRO:HD2	2.17	0.44
1:B:48:TYR:O	1:B:52:VAL:HG23	2.17	0.44
1:A:224:ALA:O	1:A:228:ILE:HG12	2.16	0.44
1:A:472:ASP:OD2	1:A:494[B]:ARG:HD2	2.17	0.44
1:A:462:ALA:O	1:A:463:THR:OG1	2.33	0.44
1:C:213:THR:HG23	1:C:225:THR:OG1	2.18	0.44
1:A:171:GLN:HE22	3:A:710:EDO:H22	1.82	0.43
1:C:472:ASP:CG	1:C:494:ARG:HH11	2.26	0.43
1:C:360:VAL:HA	1:C:364:PRO:HA	2.00	0.43
1:C:66:TRP:O	1:C:70:LYS:HG2	2.19	0.43
1:B:315[A]:LYS:NZ	5:B:803:HOH:O	2.34	0.43
1:A:470:ASP:OD2	1:A:494[A]:ARG:HD3	2.19	0.42
1:B:83:THR:O	1:B:98:PRO:HD2	2.19	0.42
1:A:472:ASP:OD1	5:A:802:HOH:O	2.22	0.42
1:C:516:MET:N	1:C:516:MET:SD	2.93	0.42
1:C:504:VAL:HG23	1:C:511:TYR:HB2	2.02	0.41
1:A:368:TRP:HB3	1:A:402:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:TYR:HA	1:B:297:LYS:O	2.19	0.41
1:B:435:VAL:HA	1:B:450:PRO:HG2	2.03	0.41
1:C:440:MET:HG2	2:C:701:PRX:H3'	2.02	0.41
1:C:470:ASP:OD2	1:C:494:ARG:NE	2.54	0.41
1:C:478:THR:HG22	1:C:480:GLN:HB2	2.03	0.41
1:B:492:VAL:HB	1:B:522:TYR:HB3	2.03	0.41
1:B:161:ALA:H	3:B:708:EDO:H11	1.86	0.41
1:C:456:SER:O	1:C:536:TYR:OH	2.26	0.41
1:A:417:PRO:HB3	1:A:459:PRO:HB2	2.02	0.40
1:C:326:PHE:CE1	1:C:328:CYS:HB2	2.56	0.40
1:C:367:TYR:O	1:C:371:VAL:HG23	2.21	0.40
1:A:288:TYR:HA	1:A:297:LYS:O	2.20	0.40
1:B:24:GLU:O	3:B:706:EDO:H22	2.22	0.40
1:B:466:PHE:CG	1:B:467:PHE:N	2.88	0.40
1:A:572:THR:HG22	1:A:590:VAL:HG13	2.04	0.40
1:B:23:SER:OG	1:B:24:GLU:OE1	2.36	0.40
1:B:548:ASN:O	1:B:584:GLN:HB2	2.21	0.40
1:B:577:CYS:HB3	1:B:587:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	651/694 (94%)	628 (96%)	22 (3%)	1 (0%)	43	36
1	B	645/694 (93%)	625 (97%)	19 (3%)	1 (0%)	43	36
1	C	558/694 (80%)	537 (96%)	20 (4%)	1 (0%)	43	36
All	All	1854/2082 (89%)	1790 (96%)	61 (3%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	THR
1	C	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	513/576 (89%)	512 (100%)	1 (0%)	87	89
1	B	505/576 (88%)	501 (99%)	4 (1%)	73	74
1	C	390/576 (68%)	390 (100%)	0	100	100
All	All	1408/1728 (82%)	1403 (100%)	5 (0%)	86	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	B	217[A]	ARG
1	B	217[B]	ARG
1	B	262	TRP
1	B	595	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	396	HIS
1	A	431	GLN
1	B	34	GLN
1	B	91	HIS
1	B	95	GLN
1	B	116	ASN
1	B	235	GLN
1	B	396	HIS
1	B	399	ASN

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Mol	Chain	Res	Type
1	B	485	ASN
1	C	227	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 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$
4	PO4	B	702	-	4,4,4	1.01	0	6,6,6	0.43	0
3	EDO	A	705	-	3,3,3	0.44	0	2,2,2	0.36	0
2	PRX	A	701	-	28,28,28	2.73	8 (28%)	40,41,41	3.88	14 (35%)
3	EDO	A	707	-	3,3,3	0.38	0	2,2,2	0.41	0
2	PRX	C	701	-	28,28,28	2.98	8 (28%)	40,41,41	4.13	14 (35%)
3	EDO	A	703	-	3,3,3	0.35	0	2,2,2	0.63	0
3	EDO	A	711	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	C	702	-	3,3,3	0.36	0	2,2,2	0.58	0
3	EDO	A	709	-	3,3,3	0.46	0	2,2,2	0.24	0
3	EDO	B	710	-	3,3,3	0.45	0	2,2,2	0.29	0
3	EDO	B	706	-	3,3,3	0.47	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PRX	B	701	-	28,28,28	2.84	9 (32%)	40,41,41	3.91	14 (35%)
3	EDO	C	703	-	3,3,3	0.22	0	2,2,2	0.24	0
3	EDO	A	702	-	3,3,3	0.59	0	2,2,2	0.12	0
4	PO4	B	704	-	4,4,4	0.92	0	6,6,6	0.46	0
3	EDO	B	709	-	3,3,3	0.38	0	2,2,2	0.52	0
3	EDO	A	708	-	3,3,3	0.40	0	2,2,2	0.40	0
3	EDO	B	707	-	3,3,3	0.40	0	2,2,2	0.36	0
3	EDO	B	711	-	3,3,3	0.46	0	2,2,2	0.42	0
4	PO4	B	705	-	4,4,4	0.94	0	6,6,6	0.46	0
3	EDO	A	706	-	3,3,3	0.37	0	2,2,2	0.57	0
3	EDO	A	704	-	3,3,3	0.41	0	2,2,2	0.49	0
4	PO4	B	703	-	4,4,4	0.96	0	6,6,6	0.40	0
3	EDO	A	710	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	B	708	-	3,3,3	0.45	0	2,2,2	0.35	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	A	705	-	-	1/1/1/1	-
2	PRX	A	701	-	-	0/15/31/31	0/3/3/3
3	EDO	A	707	-	-	1/1/1/1	-
2	PRX	C	701	-	1/1/5/5	0/15/31/31	0/3/3/3
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	A	711	-	-	1/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
3	EDO	A	709	-	-	1/1/1/1	-
3	EDO	B	710	-	-	0/1/1/1	-
3	EDO	B	706	-	-	0/1/1/1	-
2	PRX	B	701	-	-	0/15/31/31	0/3/3/3
3	EDO	C	703	-	-	1/1/1/1	-
3	EDO	A	702	-	-	1/1/1/1	-
3	EDO	B	709	-	-	1/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
3	EDO	B	707	-	-	1/1/1/1	-
3	EDO	B	711	-	-	0/1/1/1	-
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	A	710	-	-	0/1/1/1	-
3	EDO	B	708	-	-	0/1/1/1	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	PRX	C5-C4	7.81	1.53	1.39
2	A	701	PRX	C5-C4	7.41	1.52	1.39
2	C	701	PRX	C8-N9	-7.32	1.25	1.37
2	B	701	PRX	C5-C4	7.20	1.51	1.39
2	B	701	PRX	C8-N9	-6.94	1.25	1.37
2	A	701	PRX	C8-N9	-6.41	1.26	1.37
2	C	701	PRX	C8-N7	-5.75	1.20	1.31
2	B	701	PRX	C8-N7	-5.58	1.21	1.31
2	A	701	PRX	C8-N7	-4.91	1.22	1.31
2	C	701	PRX	C2-N3	4.78	1.42	1.33
2	B	701	PRX	C2-N3	4.62	1.42	1.33
2	A	701	PRX	C2-N3	4.58	1.42	1.33
2	C	701	PRX	C6-N6	4.52	1.45	1.34
2	C	701	PRX	C5-C6	-4.36	1.28	1.41
2	A	701	PRX	C6-N6	4.27	1.45	1.34
2	B	701	PRX	C6-N6	4.20	1.44	1.34
2	B	701	PRX	C5-C6	-4.11	1.29	1.41
2	A	701	PRX	C5-C6	-4.01	1.29	1.41
2	B	701	PRX	C5-N7	3.07	1.44	1.39
2	A	701	PRX	C6-N1	-3.07	1.27	1.35
2	B	701	PRX	C6-N1	-3.00	1.27	1.35
2	A	701	PRX	C5-N7	2.88	1.44	1.39
2	C	701	PRX	C6-N1	-2.78	1.28	1.35
2	C	701	PRX	C5-N7	2.65	1.43	1.39
2	B	701	PRX	P-O2P	-2.13	1.45	1.55

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	PRX	N3-C4-N9	12.20	147.92	127.17
2	B	701	PRX	N3-C4-N9	11.38	146.53	127.17
2	A	701	PRX	N3-C4-N9	11.06	145.97	127.17
2	B	701	PRX	C4-N9-C8	10.46	116.72	105.74
2	A	701	PRX	C4-N9-C8	10.00	116.24	105.74
2	C	701	PRX	C4-N9-C8	9.92	116.15	105.74
2	C	701	PRX	C5-C4-N3	-9.21	114.04	126.72
2	A	701	PRX	C5-C4-N3	-8.77	114.65	126.72
2	B	701	PRX	C5-C4-N3	-8.37	115.19	126.72
2	A	701	PRX	C4-C5-N7	-7.96	101.48	110.58
2	C	701	PRX	C4-C5-N7	-7.59	101.91	110.58
2	C	701	PRX	O4'-C1'-N9	7.58	122.66	108.09
2	B	701	PRX	C4-C5-N7	-7.45	102.06	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	PRX	C5-C4-N9	-7.15	98.02	105.81
2	B	701	PRX	C5-C4-N9	-6.92	98.27	105.81
2	B	701	PRX	N1-C2-N3	-6.39	118.91	128.58
2	A	701	PRX	C5-N7-C8	6.06	112.98	103.45
2	C	701	PRX	C5-N7-C8	6.01	112.90	103.45
2	A	701	PRX	C5-C4-N9	-5.95	99.33	105.81
2	C	701	PRX	C6-C5-C4	5.90	125.23	117.18
2	A	701	PRX	N1-C2-N3	-5.87	119.69	128.58
2	B	701	PRX	C5-N7-C8	5.86	112.65	103.45
2	A	701	PRX	O4'-C1'-N9	5.76	119.15	108.09
2	B	701	PRX	O4'-C1'-N9	5.58	118.81	108.09
2	C	701	PRX	N1-C2-N3	-5.54	120.20	128.58
2	A	701	PRX	C6-C5-C4	5.24	124.34	117.18
2	B	701	PRX	C2-N1-C6	5.00	126.94	118.73
2	C	701	PRX	C2'-C1'-N9	4.80	125.24	113.30
2	A	701	PRX	C2-N1-C6	4.73	126.50	118.73
2	B	701	PRX	C6-C5-C4	4.68	123.57	117.18
2	C	701	PRX	C2-N1-C6	4.37	125.90	118.73
2	C	701	PRX	C1'-N9-C8	-3.75	118.78	127.09
2	A	701	PRX	C4-N9-C1'	-3.24	119.06	126.63
2	A	701	PRX	C2'-C1'-N9	3.12	121.07	113.30
2	B	701	PRX	C2'-C1'-N9	3.05	120.88	113.30
2	B	701	PRX	C4-N9-C1'	-2.92	119.80	126.63
2	A	701	PRX	N9-C8-N7	-2.88	109.85	113.94
2	B	701	PRX	N9-C8-N7	-2.59	110.26	113.94
2	B	701	PRX	C2-N3-C4	2.50	117.94	111.83
2	A	701	PRX	C2-N3-C4	2.47	117.86	111.83
2	C	701	PRX	C2-N3-C4	2.38	117.64	111.83
2	C	701	PRX	N9-C8-N7	-2.08	110.98	113.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	701	PRX	C1'

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	705	EDO	O1-C1-C2-O2
3	C	703	EDO	O1-C1-C2-O2
3	A	709	EDO	O1-C1-C2-O2
3	A	702	EDO	O1-C1-C2-O2

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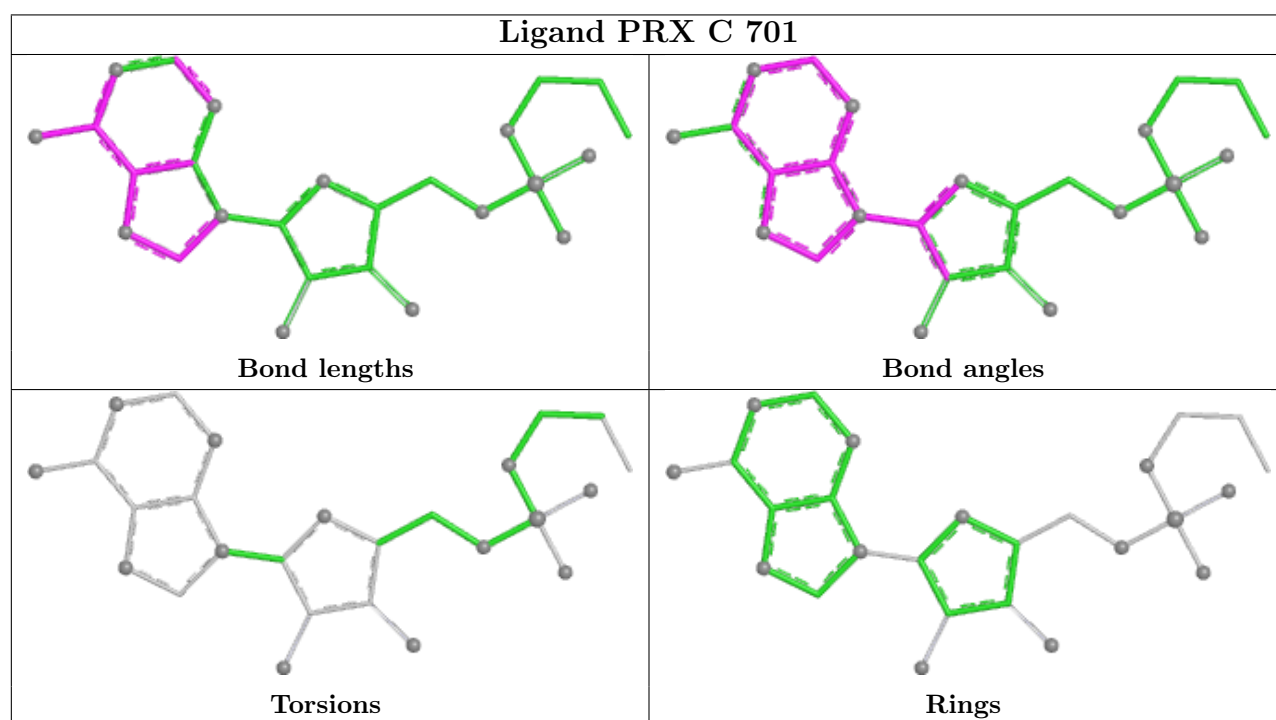
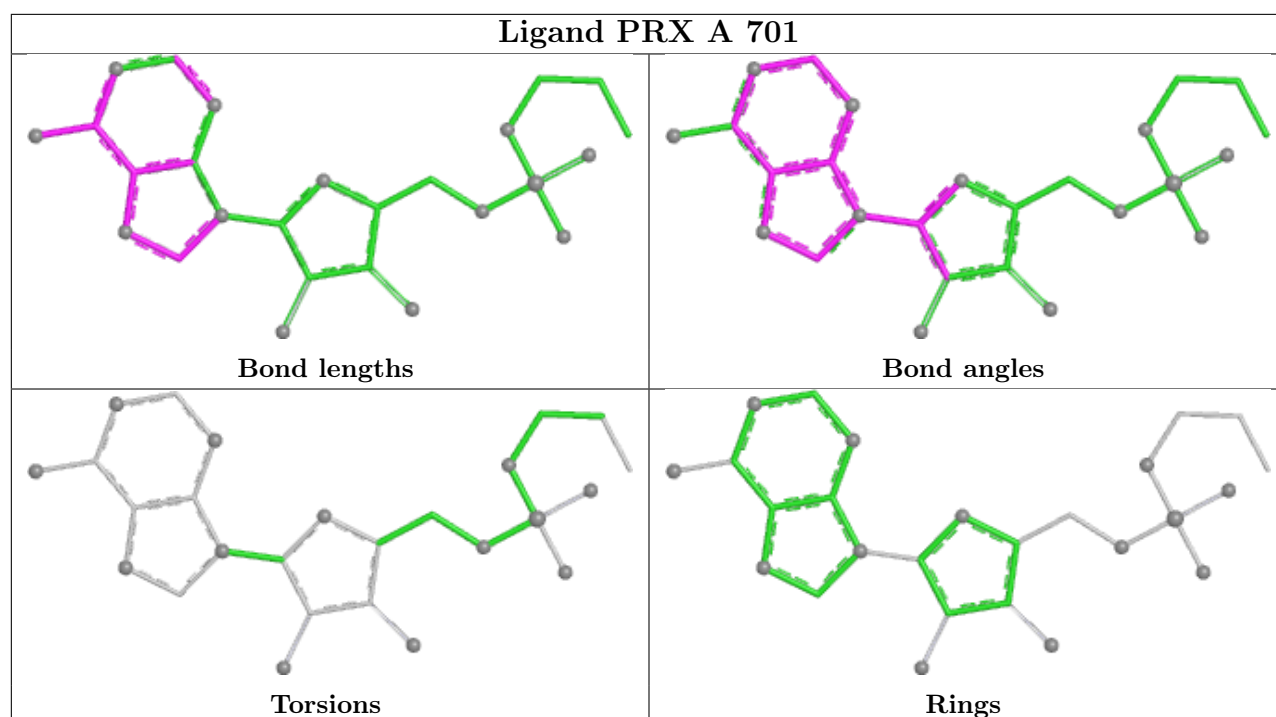
Mol	Chain	Res	Type	Atoms
3	A	707	EDO	O1-C1-C2-O2
3	A	711	EDO	O1-C1-C2-O2
3	B	707	EDO	O1-C1-C2-O2
3	B	709	EDO	O1-C1-C2-O2

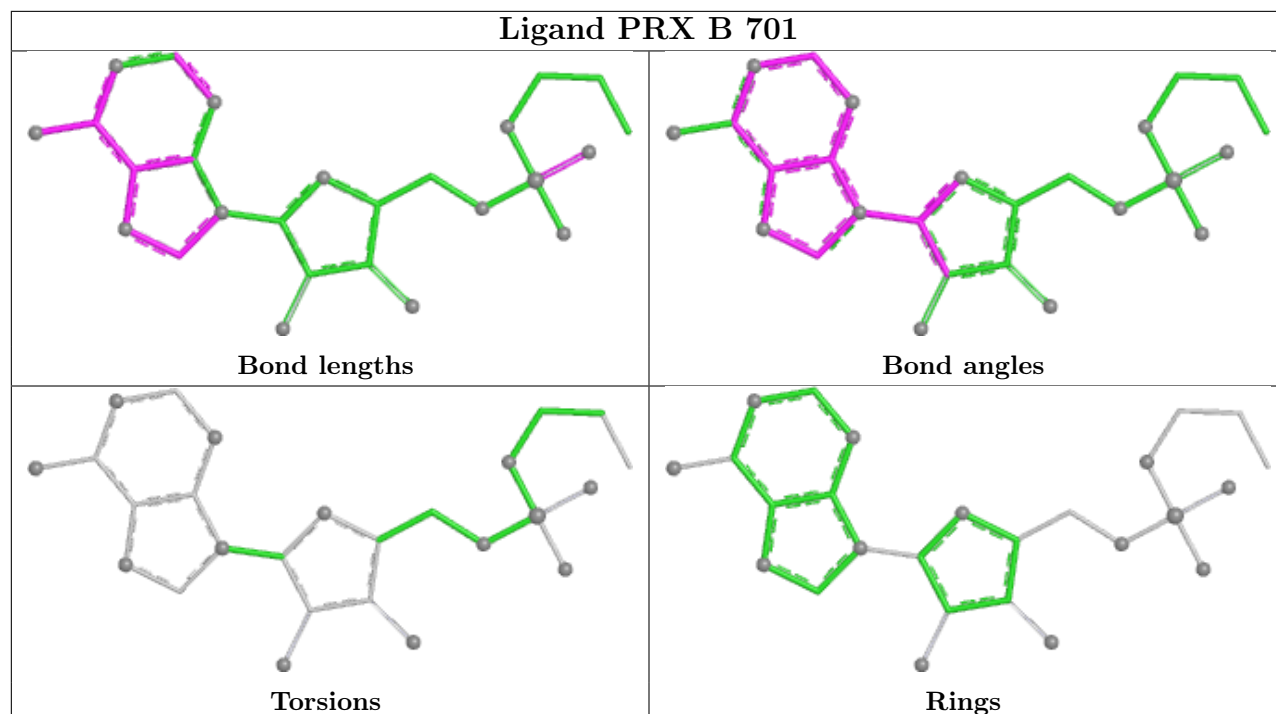
There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	PRX	1	0
3	A	707	EDO	1	0
2	C	701	PRX	2	0
3	C	702	EDO	1	0
3	B	706	EDO	1	0
2	B	701	PRX	1	0
3	C	703	EDO	2	0
3	A	702	EDO	1	0
3	A	710	EDO	1	0
3	B	708	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, 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	650/694 (93%)	0.27	34 (5%)	33 38	12, 36, 70, 94	7 (1%)
1	B	642/694 (92%)	0.30	39 (6%)	27 31	14, 35, 67, 102	11 (1%)
1	C	567/694 (81%)	1.14	133 (23%)	2 2	21, 55, 100, 128	1 (0%)
All	All	1859/2082 (89%)	0.54	206 (11%)	10 12	12, 39, 88, 128	19 (1%)

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	676	VAL	5.6
1	C	533	TYR	5.3
1	C	425	ASP	5.2
1	C	577	CYS	5.1
1	B	680	VAL	5.1
1	A	670	PRO	4.9
1	B	633	LEU	4.9
1	C	554	LEU	4.9
1	C	426	PHE	4.8
1	C	421	HIS	4.7
1	C	594	PRO	4.7
1	B	638	SER	4.7
1	C	550	SER	4.6
1	B	670	PRO	4.5
1	A	652	GLY	4.5
1	B	634	PRO	4.5
1	C	552	HIS	4.4
1	B	632	ASP	4.4
1	C	408	LEU	4.4
1	B	646	LEU	4.4
1	C	416	ASN	4.3
1	C	453	GLY	4.3
1	B	636	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	549	VAL	4.2
1	C	547	ILE	4.2
1	B	533	TYR	4.1
1	C	587	TYR	4.1
1	C	415	ILE	4.1
1	B	651	ALA	4.0
1	B	673	VAL	4.0
1	B	671	GLN	4.0
1	C	555	SER	4.0
1	C	618	ILE	4.0
1	C	422	TRP	3.9
1	C	585	ALA	3.9
1	B	650	VAL	3.9
1	A	399	ASN	3.9
1	B	334[A]	TRP	3.9
1	C	586	VAL	3.9
1	C	621	PHE	3.9
1	A	681	THR	3.8
1	C	419	ALA	3.8
1	C	543	VAL	3.8
1	C	607	SER	3.8
1	C	295	LYS	3.8
1	C	386	ILE	3.8
1	B	637	ARG	3.7
1	B	649	ILE	3.7
1	C	627	ILE	3.7
1	A	673	VAL	3.6
1	C	570	ALA	3.6
1	C	395	ASP	3.6
1	B	639	GLY	3.6
1	C	574	VAL	3.6
1	C	368	TRP	3.5
1	C	575	VAL	3.5
1	C	530	ALA	3.5
1	C	551	GLY	3.5
1	A	602	LYS	3.5
1	C	423	TYR	3.4
1	C	420	TRP	3.4
1	C	629	LEU	3.4
1	C	430	ASN	3.4
1	C	417	PRO	3.4
1	A	649	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	44	ILE	3.4
1	A	639	GLY	3.3
1	C	559	VAL	3.3
1	A	598	LEU	3.3
1	A	672	ILE	3.3
1	C	611	ALA	3.3
1	C	553	ARG	3.3
1	C	576	GLY	3.3
1	A	533	TYR	3.2
1	C	418	GLU	3.2
1	C	481	VAL	3.2
1	B	629	LEU	3.2
1	B	635	LYS	3.2
1	C	606	LEU	3.2
1	B	641	ILE	3.1
1	C	624	PRO	3.1
1	C	610	LEU	3.1
1	C	427	ALA	3.1
1	C	48	TYR	3.1
1	C	531	ARG	3.1
1	C	564	ILE	3.0
1	C	397	VAL	3.0
1	B	642	MET	3.0
1	C	622	ALA	3.0
1	C	612	ILE	3.0
1	C	541	GLY	3.0
1	C	52	VAL	3.0
1	C	389	LEU	2.9
1	B	645	VAL	2.9
1	C	628	TYR	2.9
1	C	589	PHE	2.9
1	C	623	ALA	2.9
1	C	568	GLY	2.9
1	B	296	PRO	2.9
1	C	454	ALA	2.9
1	A	334[A]	TRP	2.9
1	C	486	ASP	2.9
1	C	42	PRO	2.8
1	C	615	ARG	2.8
1	B	672	ILE	2.8
1	C	399	ASN	2.8
1	C	451	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	619	GLY	2.8
1	C	534	ASP	2.8
1	A	193	PHE	2.8
1	C	446	ILE	2.7
1	A	680	VAL	2.7
1	B	61	PRO	2.7
1	C	432	CYS	2.7
1	C	296	PRO	2.7
1	C	536	TYR	2.6
1	A	621	PHE	2.6
1	C	558	GLU	2.6
1	C	473	ILE	2.6
1	C	556	THR	2.6
1	C	567	LYS	2.6
1	C	482	LEU	2.6
1	C	562	ALA	2.6
1	C	540	LYS	2.6
1	C	461	SER	2.6
1	A	581	LEU	2.6
1	C	435	VAL	2.6
1	C	563	LEU	2.5
1	C	462	ALA	2.5
1	C	390	ARG	2.5
1	C	406	ARG	2.5
1	C	477	GLN	2.5
1	B	640	LYS	2.5
1	C	548	ASN	2.5
1	A	395	ASP	2.5
1	C	402	LEU	2.5
1	C	474	ILE	2.5
1	A	671	GLN	2.4
1	B	674	GLU	2.4
1	C	434	ILE	2.4
1	A	578	ALA	2.4
1	C	457	THR	2.4
1	C	544	ASP	2.4
1	A	397	VAL	2.4
1	A	650	VAL	2.4
1	B	678	GLN	2.4
1	C	290	SER	2.4
1	C	527	ASP	2.4
1	A	296	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	424	ASN	2.4
1	C	396	HIS	2.4
1	B	630	VAL	2.4
1	C	478	THR	2.3
1	C	223	ILE	2.3
1	C	459	PRO	2.3
1	B	192[A]	GLY	2.3
1	C	428	GLY	2.3
1	C	460	GLY	2.3
1	B	290	SER	2.3
1	C	490	VAL	2.3
1	C	557	ALA	2.3
1	C	40	PRO	2.3
1	C	620	PRO	2.3
1	A	290	SER	2.3
1	C	429	LYS	2.3
1	C	590	VAL	2.3
1	C	617	VAL	2.3
1	C	455	ILE	2.2
1	A	676	VAL	2.2
1	C	572	THR	2.2
1	C	565	LEU	2.2
1	C	452	PRO	2.2
1	C	529	ALA	2.2
1	C	43	HIS	2.2
1	C	47	ASN	2.2
1	B	644	ARG	2.2
1	B	675	GLU	2.2
1	A	577	CYS	2.2
1	A	599	LYS	2.2
1	A	617	VAL	2.2
1	C	192	GLY	2.2
1	C	479	GLY	2.2
1	C	385	ALA	2.2
1	C	566	HIS	2.1
1	C	485	ASN	2.1
1	C	448	ILE	2.1
1	B	631	SER	2.1
1	B	325[A]	ARG	2.1
1	C	388	LEU	2.1
1	C	510	ARG	2.1
1	A	604	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	538	TRP	2.1
1	A	12	HIS	2.1
1	C	322	PRO	2.1
1	A	612	ILE	2.1
1	C	608	LYS	2.1
1	C	405	LEU	2.1
1	A	622	ALA	2.1
1	B	591	THR	2.0
1	A	623	ALA	2.0
1	A	580	ASP	2.0
1	A	638	SER	2.0
1	C	456	SER	2.0
1	B	190	PHE	2.0
1	B	38	GLY	2.0
1	C	471	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(Å ²)	Q<0.9
3	EDO	B	706	4/4	0.74	0.21	66,69,71,72	0
4	PO4	B	705	5/5	0.74	0.13	112,112,112,113	0
3	EDO	A	711	4/4	0.78	0.23	72,74,75,76	0
3	EDO	A	702	4/4	0.80	0.18	38,39,39,43	0
3	EDO	B	710	4/4	0.81	0.18	66,67,67,69	0
4	PO4	B	703	5/5	0.82	0.12	102,102,102,103	0
3	EDO	A	704	4/4	0.82	0.21	52,53,53,53	0
3	EDO	A	703	4/4	0.83	0.21	51,51,53,53	0

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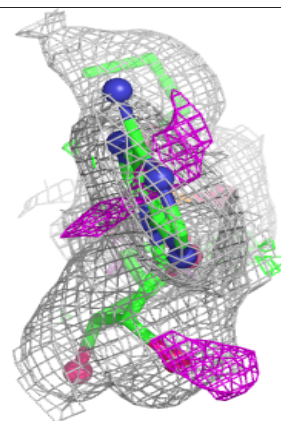
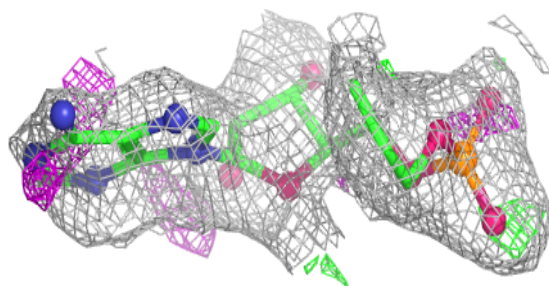
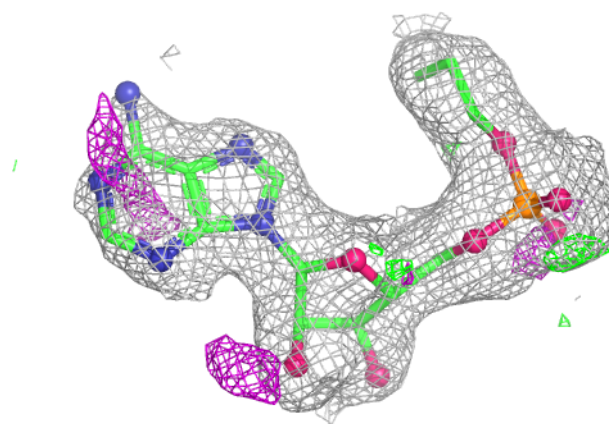
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	B	704	5/5	0.84	0.14	88,89,90,91	0
3	EDO	A	708	4/4	0.85	0.19	43,43,44,45	0
4	PO4	B	702	5/5	0.86	0.21	107,107,107,107	0
3	EDO	B	707	4/4	0.86	0.25	44,46,47,50	0
3	EDO	B	709	4/4	0.86	0.18	43,44,46,49	0
3	EDO	A	706	4/4	0.86	0.16	55,56,56,57	0
3	EDO	A	710	4/4	0.87	0.15	62,64,66,66	0
3	EDO	B	708	4/4	0.87	0.17	50,51,52,53	0
2	PRX	C	701	26/26	0.87	0.14	46,60,68,68	0
3	EDO	A	709	4/4	0.87	0.16	59,60,60,61	0
3	EDO	B	711	4/4	0.89	0.14	53,54,54,54	0
3	EDO	A	707	4/4	0.90	0.21	41,42,43,44	0
3	EDO	A	705	4/4	0.92	0.13	35,41,45,47	0
3	EDO	C	702	4/4	0.92	0.12	40,41,45,48	0
3	EDO	C	703	4/4	0.93	0.15	26,26,27,32	4
2	PRX	B	701	26/26	0.97	0.06	22,27,31,35	0
2	PRX	A	701	26/26	0.97	0.07	18,25,32,33	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.

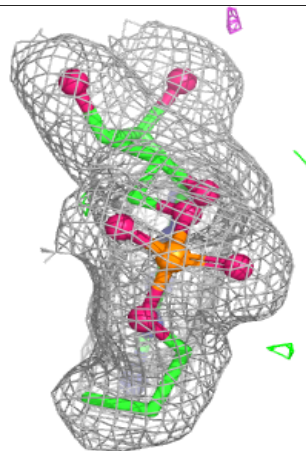
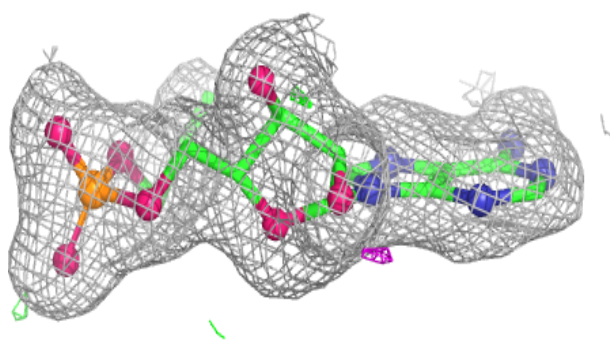
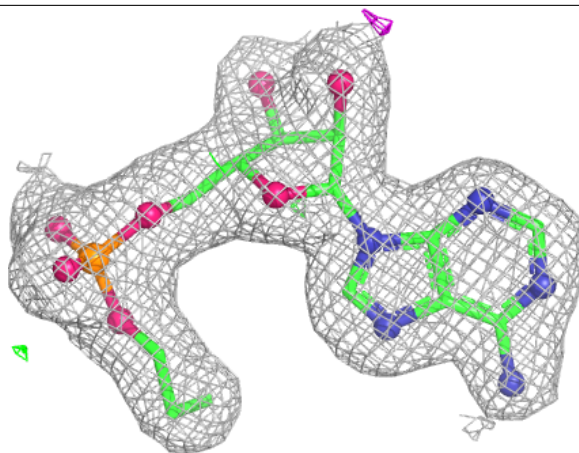
Electron density around PRX C 701:

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



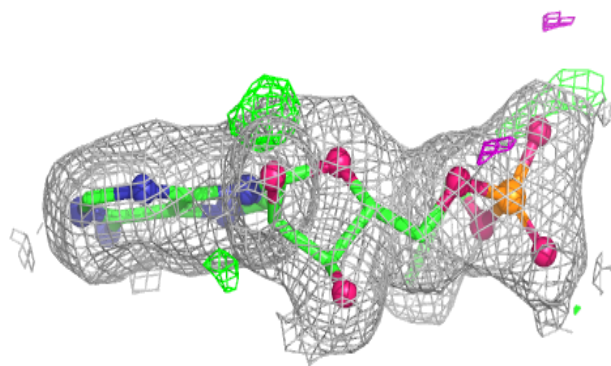
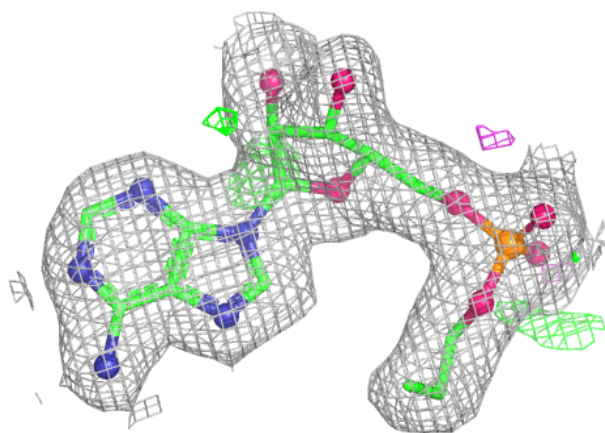
Electron density around PRX B 701:

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



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.