Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 12:15 PM EDT

PDB ID	:	5IFI
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 (i) 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 (i)) were used in the production of this report:

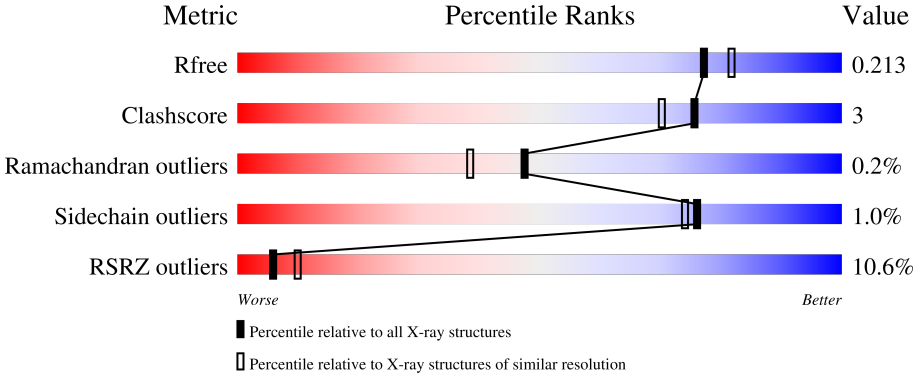
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 <=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	3% 86% 6% 7%
1	C	694	20% 74% 8% 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 (i)

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
			Total	C	N	O	S			
1	A	650	5045	3221	858	939	27	0	7	0
1	B	642	5010	3190	858	936	26	0	11	0
1	C	567	4187	2668	712	784	23	0	1	0

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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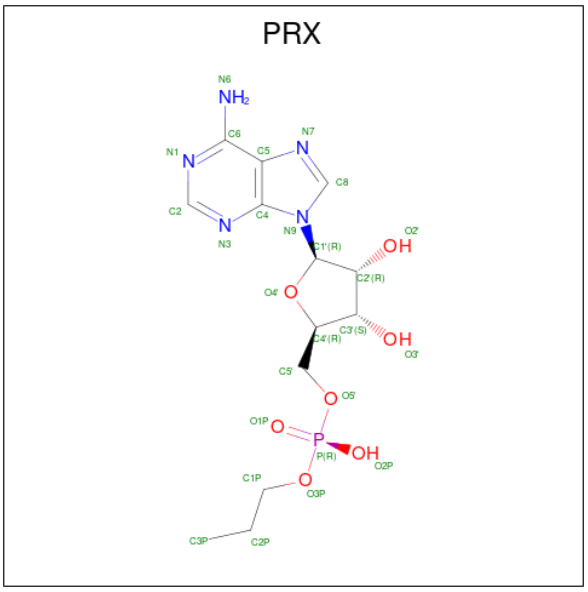
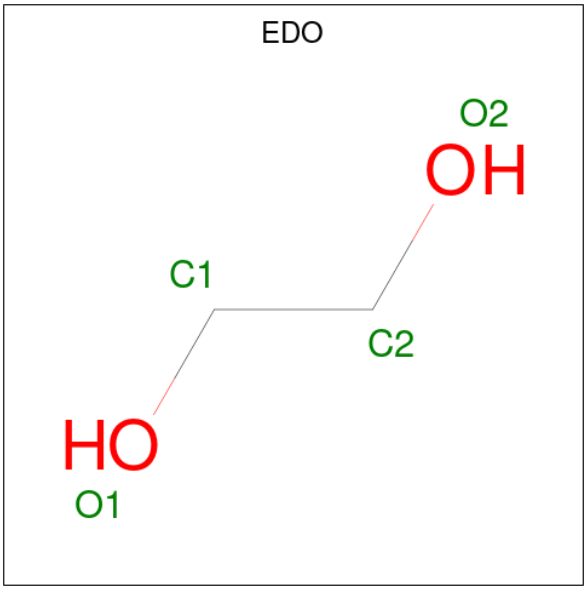
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
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 (three-letter code: 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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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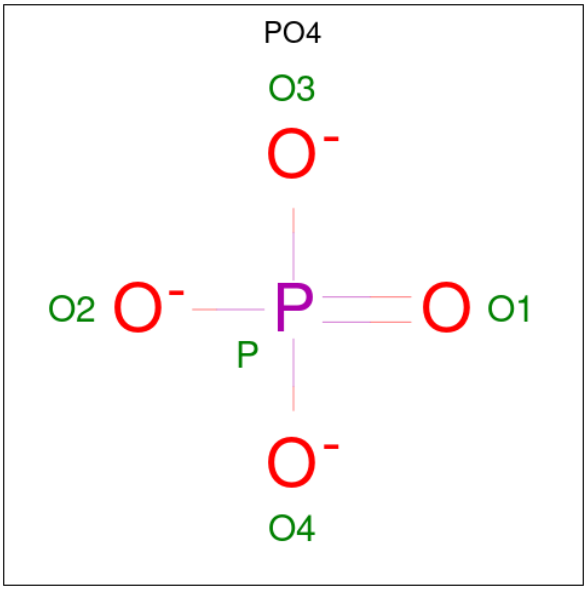
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	C	1	4	2	2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

- Molecule 5 is water.

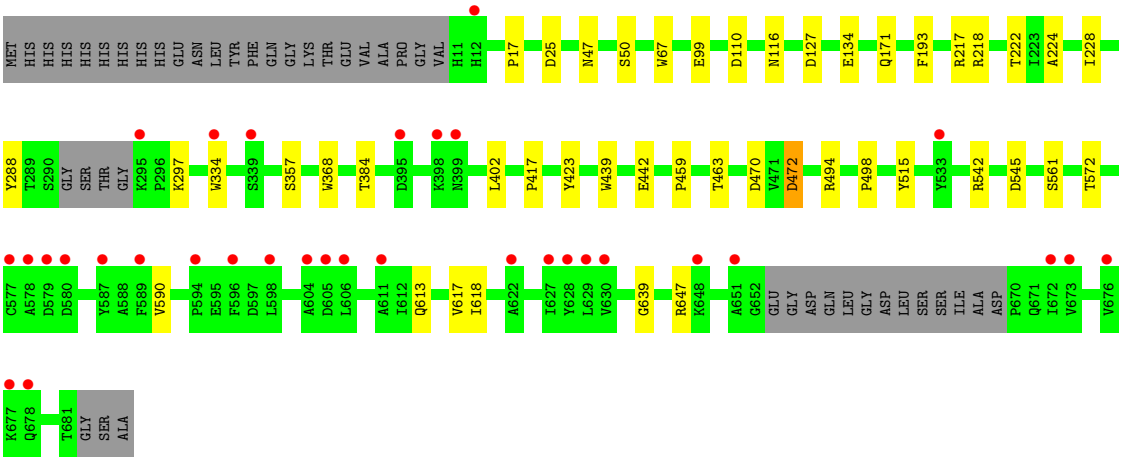
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	398	399	399	0	1
			Total	O		
5	B	385	386	386	0	2
			Total	O		
5	C	186	187	187	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

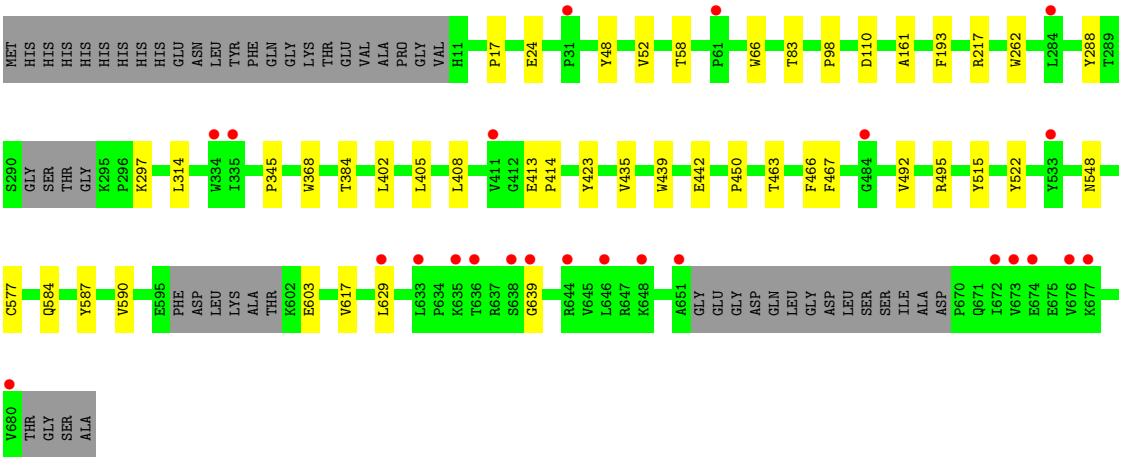
• Molecule 1: Acetyl-coenzyme A synthetase

Chain A:



• Molecule 1: Acetyl-coenzyme A synthetase

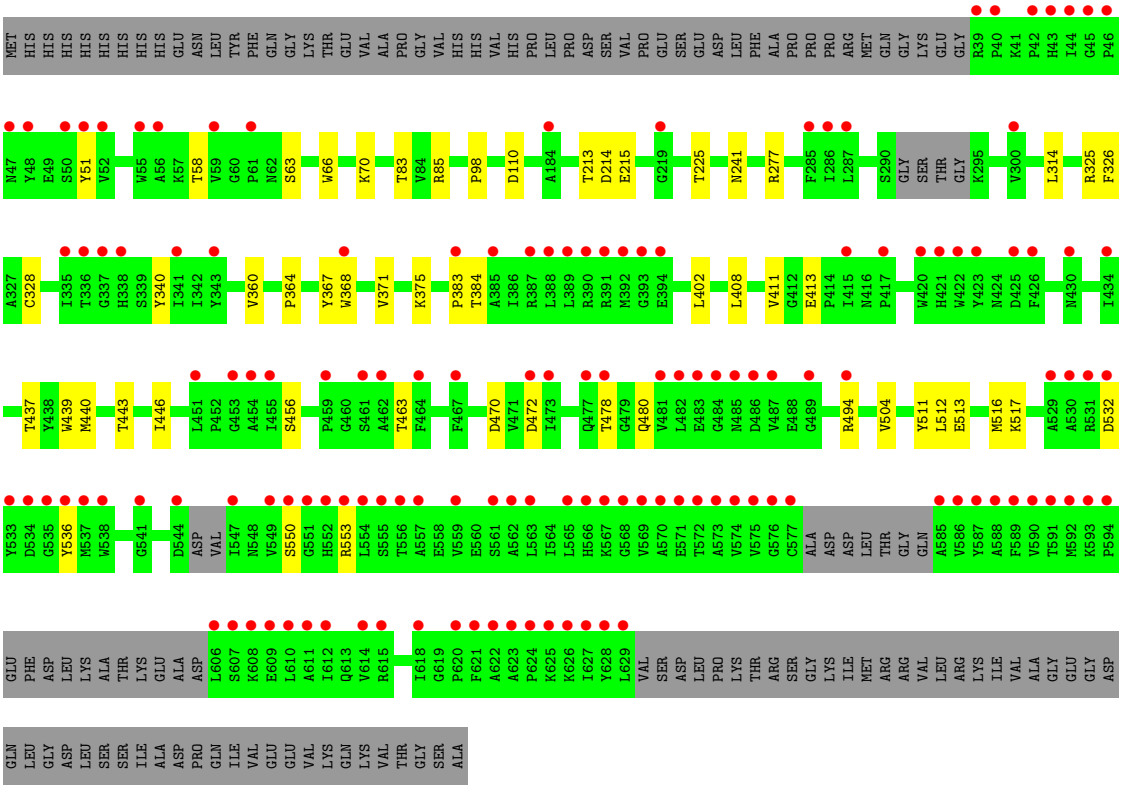
Chain B:



• Molecule 1: Acetyl-coenzyme A synthetase

Chain C:

20%
74%
8%
18%


MET HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY LYS THR GLU VAL ALA PRO GLY VAL HIS HIS VAL HIS PRO LEU PRO ASP SER VAL PRO GLU SER GLU ASP LEU PHE ALA PRO PRO PRO ARG MET GLN GLY LYS GLU GLY
R39 P40 K41 P42 H43 I44 G45 P46
N47 Y48 E49 S50 Y51 V52 W55 A56 K57 T58 V59 G60 P61 N62 S63 W66 K70 T83 V84 R85 P98 D110 A184 T213 D214 E215 G219 T225 N241 R277 F285 I286 L287 S290 GLY SER THR GLY K295 V300 L314 R325 F326
A327 G328 I335 T336 G337 H338 S339 Y340 I341 I342 Y343 V360 P364 Y367 W368 V371 K375 P383 T384 A385 I386 R387 L388 L389 R390 R391 M392 G393 E394 L402 L408 V411 G412 E413 P414 I415 N416 P417 W420 H421 W422 Y423 N424 D425 F426 M430 I434
T437 Y438 W439 M440 T443 I446 L451 P452 G453 A454 I455 S456 F459 G460 S461 A462 T463 F464 F467 D470 V471 D472 I473 Q477 T478 G479 Q480 V481 L482 E483 G484 N485 D486 V487 E488 G489 R494 V504 Y511 L512 E513 M516 K517 A529 A530 R531 D532
Y533 D534 G535 Y536 M537 W538 G541 D544 ASP VAL I547 N548 V549 S550 G551 H552 R553 L554 S555 T556 A557 E558 V559 E560 S561 A562 L563 I564 L565 H566 K567 G568 V569 A570 E571 T572 A573 V574 V575 G576 C577 ALA ASP ASP LEU THR GLY GLN A585 V586 Y587 A588 F589 V590 T591 M592 K593 P594
GLU PHE ASP LEU LYS ALA THR LYS GLU ALA ASP L606 S607 K608 E609 L610 A611 I612 Q613 V614 R615 I618 G619 P620 F621 A622 A623 P624 K625 K626 I627 Y628 L629 VAL SER ASP LEU PRO LYS THR ARG SER GLY LYS ILE MET ARG ARG VAL LEU ARG LYS ILE VAL ALA GLY GLU GLY ASP
GLN LEU GLY ASP LEU SER SER ILE ALA ASP PRO GLN ILE VAL GLU GLU VAL LYS GLN LYS VAL THR GLY SER ALA

4 Data and refinement statistics (i)

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 48.46 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (41.84-1.95) 98.7 (48.46-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.95Å)	Xtriage
Refinement program	PHENIX (DEV_2328: ???)	Depositor
R, R_{free}	0.185 , 0.213 0.185 , 0.213	Depositor DCC
R_{free} test set	8031 reflections (5.02%)	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)	0.32 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.37	0/5198	0.53	0/7094
1	B	0.34	0/5156	0.51	0/7032
1	C	0.31	0/4301	0.49	0/5888
All	All	0.34	0/14655	0.51	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	27	0
1	B	5010	0	4725	22	0
1	C	4187	0	3785	36	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	1	0
5	C	187	0	0	2	0
All	All	15384	0	13465	85	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 (85) 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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	47	38
1	B	645/694 (93%)	625 (97%)	19 (3%)	1 (0%)	47	38
1	C	558/694 (80%)	537 (96%)	20 (4%)	1 (0%)	47	38
All	All	1854/2082 (89%)	1790 (96%)	61 (3%)	3 (0%)	47	38

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 (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	513/576 (89%)	508 (99%)	5 (1%)	76	74
1	B	505/576 (88%)	499 (99%)	6 (1%)	71	68
1	C	390/576 (68%)	386 (99%)	4 (1%)	76	74
All	All	1408/1728 (82%)	1393 (99%)	15 (1%)	76	71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	110	ASP
1	A	116	ASN
1	A	423	TYR
1	A	472	ASP
1	B	110	ASP
1	B	193	PHE
1	B	217[A]	ARG
1	B	217[B]	ARG
1	B	262	TRP
1	B	423	TYR
1	C	51	TYR
1	C	110	ASP
1	C	314	LEU
1	C	408	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	B	116	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	EDO	C	703	-	3,3,3	0.24	0	2,2,2	0.19	0
2	PRX	A	701	-	25,28,28	2.49	7 (28%)	27,41,41	2.33	4 (14%)
3	EDO	A	709	-	3,3,3	0.49	0	2,2,2	0.19	0
3	EDO	B	710	-	3,3,3	0.48	0	2,2,2	0.25	0
3	EDO	A	708	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	A	704	-	3,3,3	0.44	0	2,2,2	0.46	0
4	PO4	B	702	-	4,4,4	0.97	0	6,6,6	0.40	0
3	EDO	B	711	-	3,3,3	0.49	0	2,2,2	0.37	0
3	EDO	B	708	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	B	707	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	B	706	-	3,3,3	0.51	0	2,2,2	0.24	0
3	EDO	A	711	-	3,3,3	0.46	0	2,2,2	0.34	0
2	PRX	B	701	-	25,28,28	2.61	9 (36%)	27,41,41	2.30	4 (14%)
3	EDO	A	710	-	3,3,3	0.49	0	2,2,2	0.26	0
3	EDO	A	705	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	B	709	-	3,3,3	0.42	0	2,2,2	0.48	0
3	EDO	C	702	-	3,3,3	0.39	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	B	704	-	4,4,4	0.87	0	6,6,6	0.43	0
2	PRX	C	701	-	25,28,28	2.69	8 (32%)	27,41,41	2.10	4 (14%)
4	PO4	B	703	-	4,4,4	0.91	0	6,6,6	0.37	0
3	EDO	A	706	-	3,3,3	0.40	0	2,2,2	0.54	0
3	EDO	A	703	-	3,3,3	0.38	0	2,2,2	0.60	0
3	EDO	A	702	-	3,3,3	0.61	0	2,2,2	0.07	0
4	PO4	B	705	-	4,4,4	0.90	0	6,6,6	0.42	0
3	EDO	A	707	-	3,3,3	0.41	0	2,2,2	0.37	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	703	-	-	1/1/1/1	-
2	PRX	A	701	-	-	0/11/31/31	0/3/3/3
3	EDO	A	709	-	-	1/1/1/1	-
3	EDO	B	710	-	-	0/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	B	711	-	-	0/1/1/1	-
3	EDO	B	708	-	-	0/1/1/1	-
3	EDO	B	707	-	-	1/1/1/1	-
3	EDO	B	706	-	-	0/1/1/1	-
3	EDO	A	711	-	-	1/1/1/1	-
2	PRX	B	701	-	-	0/11/31/31	0/3/3/3
3	EDO	A	710	-	-	0/1/1/1	-
3	EDO	A	705	-	-	1/1/1/1	-
3	EDO	B	709	-	-	1/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
2	PRX	C	701	-	1/1/5/5	0/11/31/31	0/3/3/3
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	A	702	-	-	1/1/1/1	-
3	EDO	A	707	-	-	1/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	PRX	C8-N7	-7.89	1.20	1.34
2	B	701	PRX	C8-N7	-7.70	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PRX	C8-N7	-6.98	1.22	1.34
2	C	701	PRX	C2-N3	6.40	1.42	1.32
2	B	701	PRX	C2-N3	6.23	1.42	1.32
2	A	701	PRX	C2-N3	6.18	1.42	1.32
2	C	701	PRX	C5-C4	4.57	1.53	1.40
2	A	701	PRX	C5-C4	4.30	1.52	1.40
2	B	701	PRX	C5-C4	4.16	1.51	1.40
2	C	701	PRX	C6-C5	-3.89	1.28	1.43
2	B	701	PRX	C6-C5	-3.70	1.29	1.43
2	A	701	PRX	C6-C5	-3.62	1.29	1.43
2	C	701	PRX	C6-N6	3.21	1.45	1.34
2	A	701	PRX	C6-N6	3.03	1.45	1.34
2	B	701	PRX	C6-N6	2.99	1.44	1.34
2	A	701	PRX	C2'-C1'	-2.56	1.49	1.53
2	B	701	PRX	C2'-C1'	-2.55	1.49	1.53
2	C	701	PRX	C2'-C1'	-2.38	1.50	1.53
2	B	701	PRX	O4'-C1'	-2.27	1.37	1.41
2	A	701	PRX	C6-N1	-2.26	1.27	1.37
2	B	701	PRX	C6-N1	-2.21	1.27	1.37
2	B	701	PRX	P-O2P	-2.10	1.45	1.55
2	C	701	PRX	C6-N1	-2.07	1.28	1.37
2	C	701	PRX	O4'-C1'	-2.01	1.38	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	PRX	C4-C5-N7	-7.60	101.48	109.40
2	C	701	PRX	C4-C5-N7	-7.19	101.91	109.40
2	B	701	PRX	C4-C5-N7	-7.04	102.06	109.40
2	B	701	PRX	N3-C2-N1	-6.25	118.91	128.68
2	A	701	PRX	N3-C2-N1	-5.75	119.69	128.68
2	C	701	PRX	N3-C2-N1	-5.43	120.20	128.68
2	B	701	PRX	C2-N1-C6	4.79	126.94	118.75
2	A	701	PRX	C2-N1-C6	4.53	126.50	118.75
2	A	701	PRX	C1'-N9-C4	-4.32	119.06	126.64
2	C	701	PRX	C2-N1-C6	4.18	125.90	118.75
2	B	701	PRX	C1'-N9-C4	-3.90	119.80	126.64
2	C	701	PRX	O4'-C1'-C2'	2.10	110.00	106.93

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	701	PRX	C1'

All (8) torsion outliers are listed below:

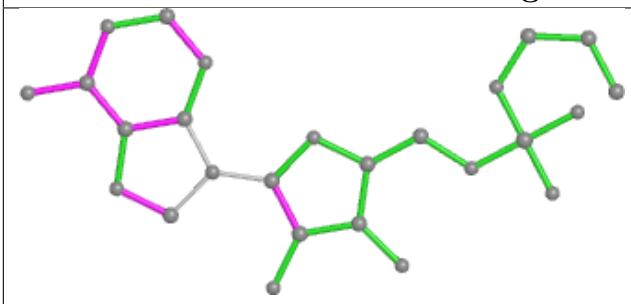
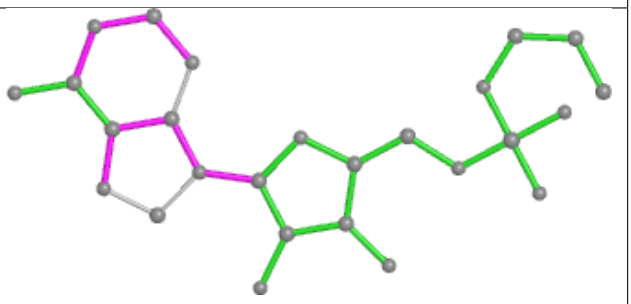
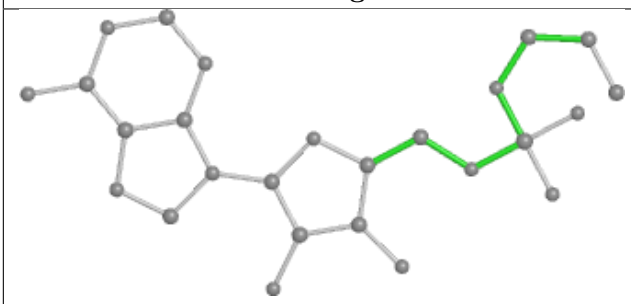
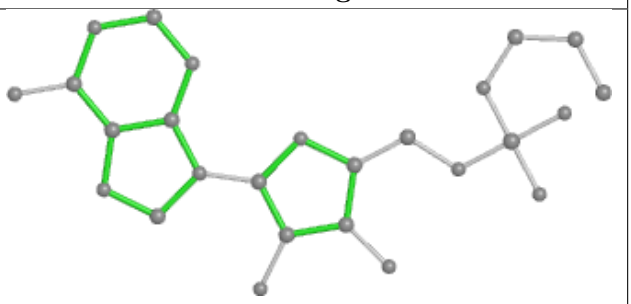
Mol	Chain	Res	Type	Atoms
3	A	705	EDO	O1-C1-C2-O2
3	C	703	EDO	O1-C1-C2-O2
3	A	709	EDO	O1-C1-C2-O2
3	A	702	EDO	O1-C1-C2-O2
3	A	711	EDO	O1-C1-C2-O2
3	A	707	EDO	O1-C1-C2-O2
3	B	707	EDO	O1-C1-C2-O2
3	B	709	EDO	O1-C1-C2-O2

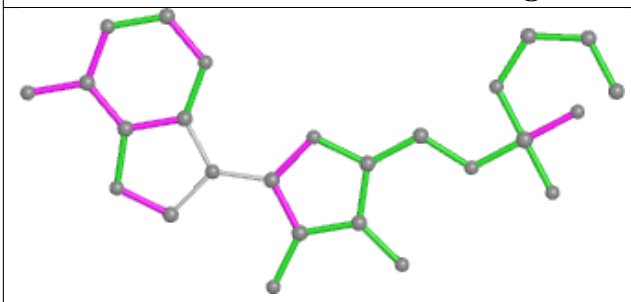
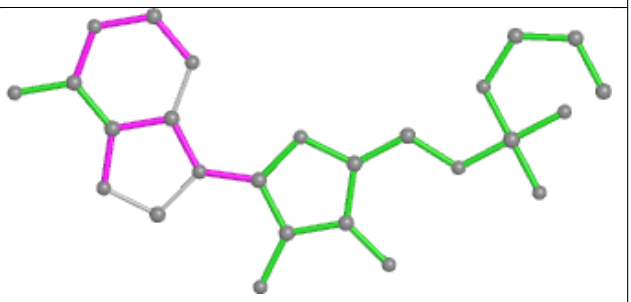
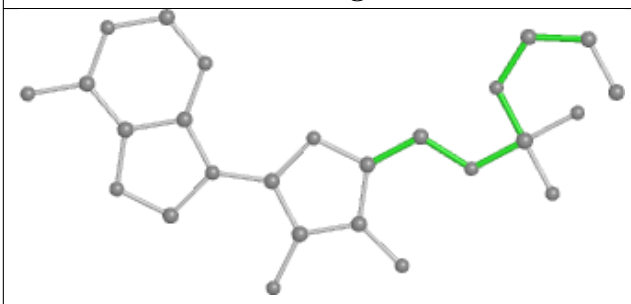
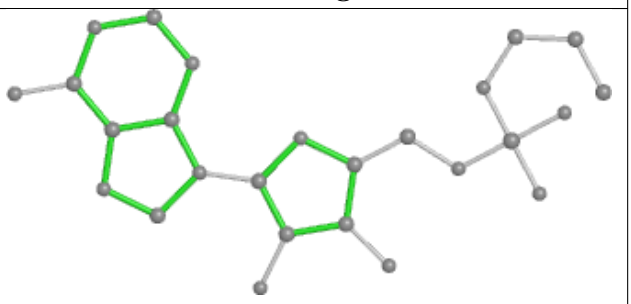
There are no ring outliers.

10 monomers are involved in 12 short contacts:

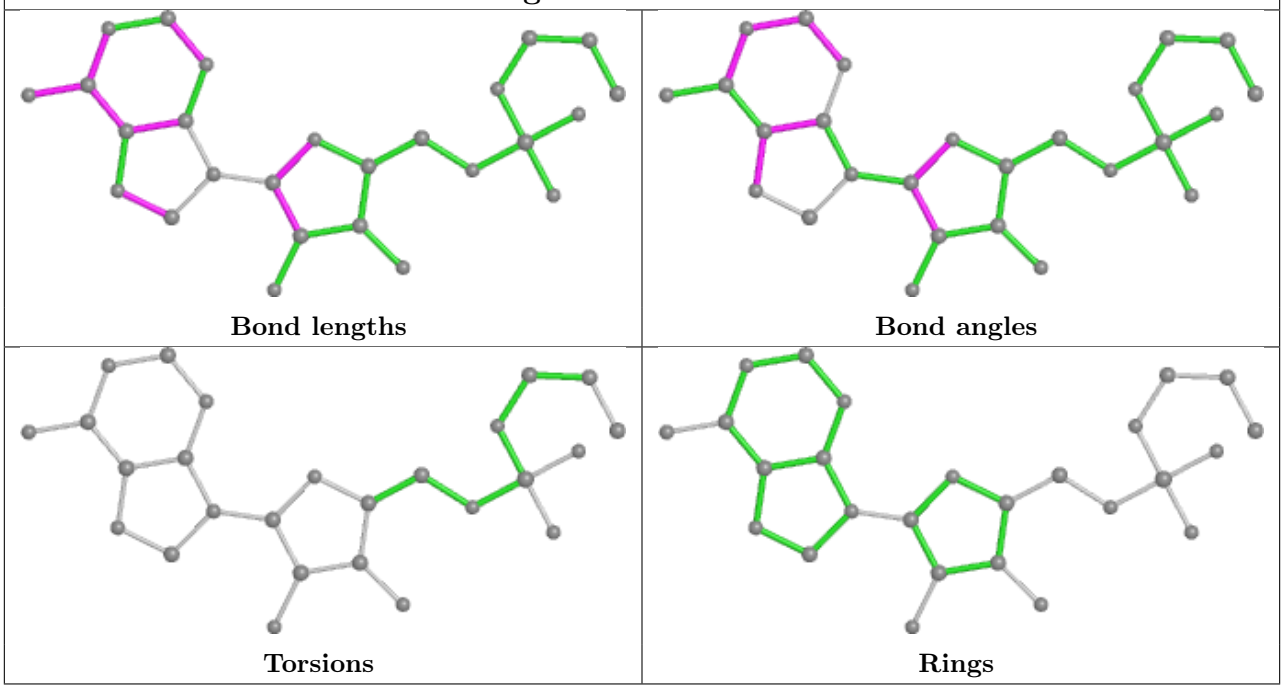
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	EDO	2	0
2	A	701	PRX	1	0
3	B	708	EDO	1	0
3	B	706	EDO	1	0
2	B	701	PRX	1	0
3	A	710	EDO	1	0
3	C	702	EDO	1	0
2	C	701	PRX	2	0
3	A	702	EDO	1	0
3	A	707	EDO	1	0

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 then 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.

Ligand PRX A 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PRX B 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PRX C 701



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.36	33 (5%)	28	37	15, 36, 70, 94	0
1	B	642/694 (92%)	0.31	24 (3%)	41	51	19, 36, 67, 102	0
1	C	567/694 (81%)	1.31	140 (24%)	0	0	21, 55, 100, 128	0
All	All	1859/2082 (89%)	0.63	197 (10%)	6	10	15, 39, 88, 128	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	628	TYR	8.2
1	C	585	ALA	8.0
1	C	484	GLY	7.8
1	C	587	TYR	7.6
1	B	676	VAL	7.3
1	B	334[A]	TRP	7.1
1	C	627	ILE	7.1
1	C	575	VAL	6.9
1	C	554	LEU	6.7
1	C	610	LEU	6.6
1	C	577	CYS	6.4
1	C	44	ILE	6.3
1	C	589	PHE	6.2
1	C	629	LEU	6.1
1	C	570	ALA	6.0
1	C	606	LEU	5.7
1	C	586	VAL	5.7
1	C	624	PRO	5.5
1	C	453	GLY	5.4
1	C	535	GLY	5.4
1	C	536	TYR	5.3
1	C	568	GLY	5.3
1	C	590	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	611	ALA	5.3
1	C	454	ALA	5.3
1	C	473	ILE	5.2
1	C	534	ASP	5.2
1	C	591	THR	5.1
1	B	638	SER	5.1
1	C	576	GLY	5.1
1	C	459	PRO	5.1
1	A	673	VAL	5.0
1	A	334[A]	TRP	5.0
1	C	549	VAL	5.0
1	A	577	CYS	5.0
1	C	612	ILE	5.0
1	A	629	LEU	4.9
1	C	541	GLY	4.8
1	C	573	ALA	4.7
1	C	588	ALA	4.7
1	C	572	THR	4.7
1	C	574	VAL	4.6
1	C	461	SER	4.6
1	C	608	LYS	4.5
1	C	455	ILE	4.4
1	C	550	SER	4.4
1	C	533	TYR	4.4
1	C	607	SER	4.3
1	A	678	GLN	4.3
1	C	614	VAL	4.3
1	C	48	TYR	4.2
1	A	676	VAL	4.2
1	B	636	THR	4.2
1	B	680	VAL	4.2
1	C	485	ASN	4.2
1	B	651	ALA	4.2
1	B	533	TYR	4.1
1	C	45	GLY	4.1
1	C	569	VAL	4.0
1	C	417	PRO	4.0
1	C	571	GLU	4.0
1	B	672	ILE	3.9
1	C	420	TRP	3.9
1	C	532	ASP	3.8
1	C	42	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	40	PRO	3.8
1	C	615	ARG	3.8
1	C	563	LEU	3.8
1	C	481	VAL	3.8
1	A	604	ALA	3.7
1	C	556	THR	3.7
1	B	673	VAL	3.7
1	C	46	PRO	3.7
1	C	566	HIS	3.6
1	C	56	ALA	3.6
1	C	626	LYS	3.6
1	C	555	SER	3.6
1	C	622	ALA	3.5
1	C	425	ASP	3.5
1	C	422	TRP	3.4
1	C	537	MET	3.4
1	C	594	PRO	3.4
1	A	580	ASP	3.4
1	C	529	ALA	3.4
1	C	391	ARG	3.4
1	C	390	ARG	3.4
1	A	598	LEU	3.4
1	C	478	THR	3.3
1	C	477	GLN	3.3
1	C	625	LYS	3.3
1	C	61	PRO	3.3
1	C	55	TRP	3.2
1	C	530	ALA	3.2
1	C	423	TYR	3.2
1	C	368	TRP	3.2
1	A	399	ASN	3.2
1	C	52	VAL	3.1
1	A	579	ASP	3.1
1	C	426	PHE	3.1
1	C	559	VAL	3.1
1	A	606	LEU	3.1
1	B	61	PRO	3.1
1	C	592	MET	3.1
1	C	621	PHE	3.1
1	C	39	ARG	3.1
1	C	531	ARG	3.1
1	A	628	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	47	ASN	3.0
1	C	483	GLU	3.0
1	A	672	ILE	2.9
1	A	622	ALA	2.8
1	B	639	GLY	2.8
1	A	651	ALA	2.8
1	A	395	ASP	2.8
1	C	219	GLY	2.8
1	C	392	MET	2.8
1	B	677	LYS	2.8
1	C	557	ALA	2.8
1	C	487	VAL	2.8
1	C	623	ALA	2.8
1	C	538	TRP	2.8
1	A	627	ILE	2.8
1	C	286	ILE	2.7
1	C	50	SER	2.7
1	C	415	ILE	2.7
1	A	533	TYR	2.7
1	C	343	TYR	2.7
1	B	629	LEU	2.7
1	C	430	ASN	2.7
1	C	593	LYS	2.7
1	C	467	PHE	2.6
1	C	552	HIS	2.6
1	C	486	ASP	2.6
1	C	285	PHE	2.5
1	C	393	GLY	2.5
1	C	287	LEU	2.5
1	C	553	ARG	2.5
1	C	300	VAL	2.5
1	A	596	PHE	2.5
1	C	336[A]	THR	2.5
1	C	335	ILE	2.5
1	A	587	TYR	2.5
1	C	184	ALA	2.5
1	B	648	LYS	2.5
1	C	421	HIS	2.4
1	C	434	ILE	2.4
1	C	561	SER	2.4
1	C	565	LEU	2.4
1	A	594	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	484	GLY	2.4
1	C	494	ARG	2.4
1	C	464	PHE	2.4
1	B	635	LYS	2.4
1	A	605	ASP	2.4
1	C	389	LEU	2.4
1	A	630	VAL	2.3
1	C	394	GLU	2.3
1	C	482	LEU	2.3
1	C	551	GLY	2.3
1	C	544	ASP	2.3
1	B	674	GLU	2.3
1	C	341	ILE	2.3
1	A	611	ALA	2.3
1	B	646	LEU	2.3
1	A	648	LYS	2.3
1	B	411	VAL	2.3
1	C	51	TYR	2.3
1	C	462	ALA	2.3
1	C	472	ASP	2.2
1	C	43	HIS	2.2
1	C	620	PRO	2.2
1	A	578	ALA	2.2
1	C	562	ALA	2.2
1	C	338	HIS	2.2
1	C	567	LYS	2.2
1	B	284	LEU	2.2
1	C	609	GLU	2.2
1	C	385	ALA	2.2
1	C	387	ARG	2.2
1	A	295	LYS	2.2
1	A	12	HIS	2.2
1	A	398	LYS	2.2
1	B	633	LEU	2.1
1	C	388	LEU	2.1
1	A	677	LYS	2.1
1	C	59	VAL	2.1
1	B	335	ILE	2.1
1	C	451	LEU	2.1
1	B	644	ARG	2.1
1	C	547	ILE	2.1
1	C	618	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	383	PRO	2.1
1	C	337	GLY	2.1
1	A	589	PHE	2.1
1	A	339	SER	2.0
1	B	31	PRO	2.0
1	C	489	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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, 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	0.57	0.24	66,69,71,72	0
3	EDO	A	702	4/4	0.65	0.23	38,39,39,43	0
3	EDO	A	711	4/4	0.73	0.24	72,74,75,76	0
3	EDO	A	709	4/4	0.78	0.15	59,60,60,61	0
3	EDO	B	710	4/4	0.78	0.40	66,67,67,69	0
4	PO4	B	705	5/5	0.81	0.24	112,112,112,113	0
4	PO4	B	704	5/5	0.84	0.21	88,89,90,91	0
3	EDO	A	703	4/4	0.86	0.20	51,51,53,53	0
3	EDO	A	710	4/4	0.86	0.25	62,64,66,66	0
3	EDO	B	708	4/4	0.86	0.16	50,51,52,53	0
3	EDO	B	709	4/4	0.87	0.22	43,44,46,49	0
3	EDO	A	708	4/4	0.87	0.14	43,43,44,45	0
3	EDO	A	706	4/4	0.88	0.14	55,56,56,57	0
4	PO4	B	703	5/5	0.88	0.15	102,102,102,103	0
2	PRX	C	701	26/26	0.89	0.17	46,60,68,68	0
3	EDO	A	704	4/4	0.90	0.28	52,53,53,53	0
4	PO4	B	702	5/5	0.91	0.17	107,107,107,107	0

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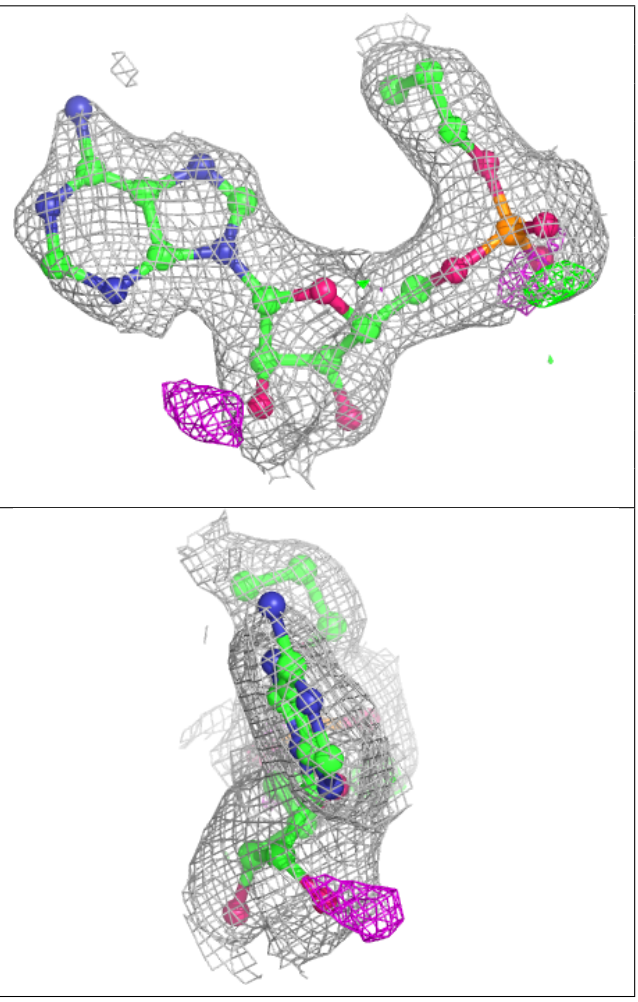
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	711	4/4	0.92	0.25	53,54,54,54	0
3	EDO	C	703	4/4	0.92	0.29	26,26,27,32	4
3	EDO	B	707	4/4	0.93	0.40	44,46,47,50	0
3	EDO	A	705	4/4	0.94	0.14	35,41,45,47	0
3	EDO	C	702	4/4	0.96	0.11	40,41,45,48	0
3	EDO	A	707	4/4	0.96	0.19	41,42,43,44	0
2	PRX	A	701	26/26	0.97	0.14	18,25,32,33	0
2	PRX	B	701	26/26	0.98	0.16	22,27,31,35	0

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

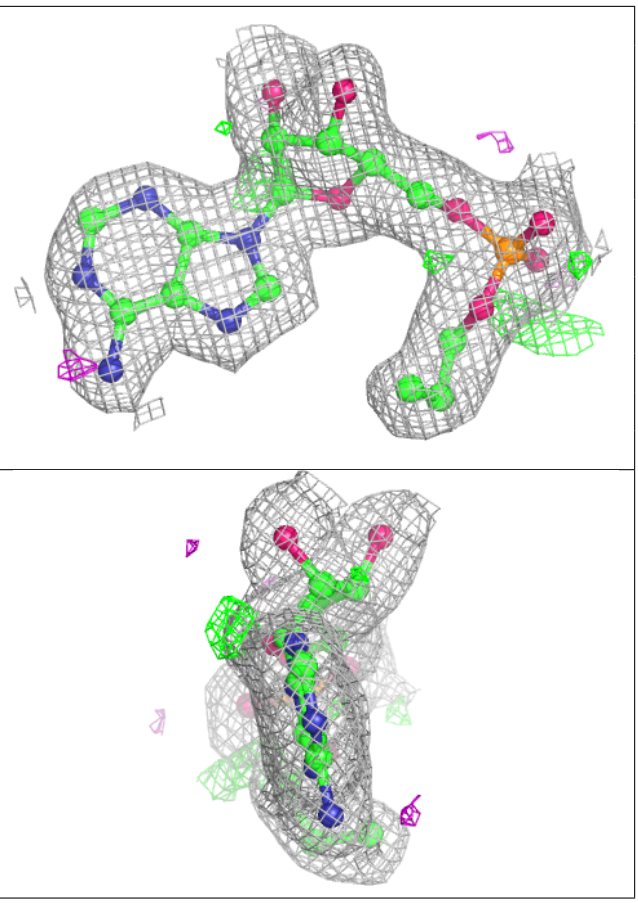
Electron density around PRX C 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



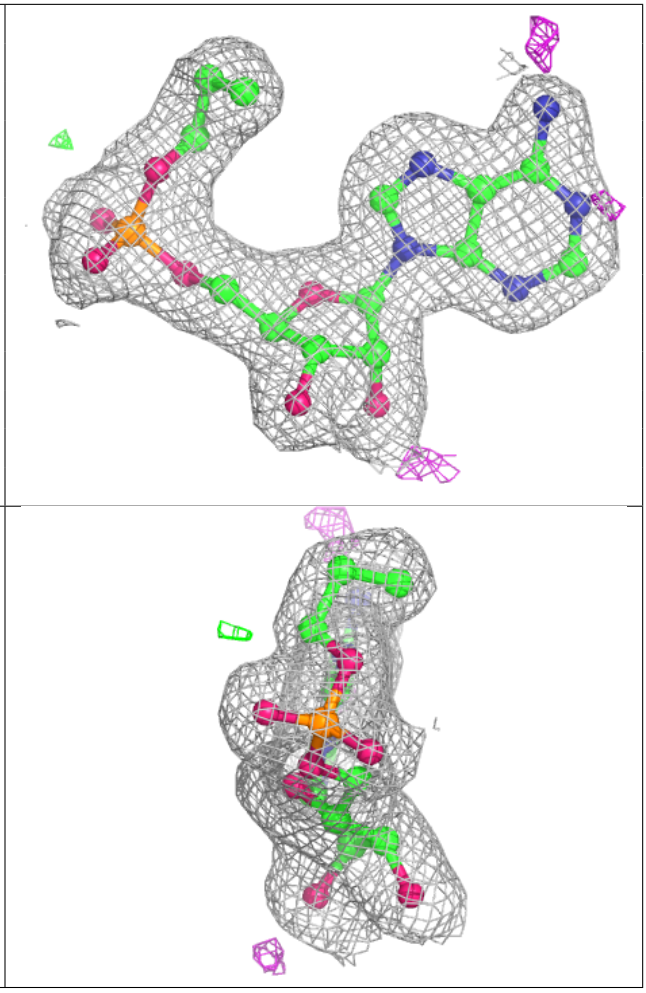
Electron density around PRX A 701:

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



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.