



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2016 – 08:29 PM EDT

PDB ID : 5K85  
Title : Crystal Structure of Acetyl-CoA Synthetase in Complex with Adenosine-5'-p  
ropylphosphate and Coenzyme A from *Cryptococcus neoformans* H99  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID); Fox III,  
D.; Delker, S.L.; Potts, K.T.; Lorimer, D.D.; Edwards, T.E.; Mutz, M.W.;  
SSGCID  
Deposited on : 2016-05-27  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939



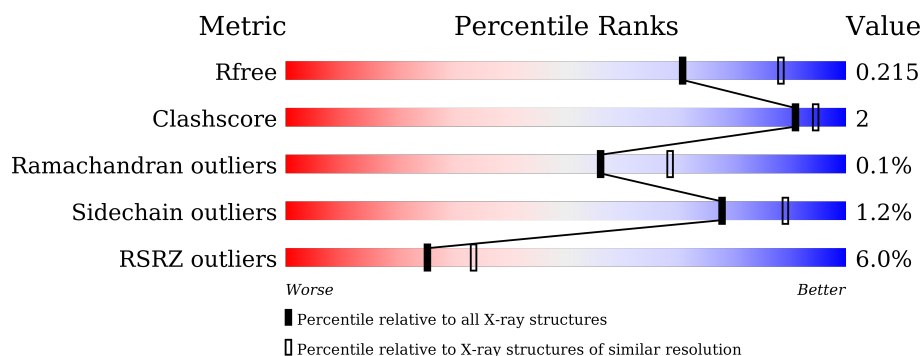
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	B	694	<div> <div>2%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
1	C	694	<div> <div>11%</div> <div>79%</div> <div>5%</div> <div>16%</div> </div>

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
3	EDO	A	702	-	-	-	X
3	EDO	A	703	-	-	-	X
3	EDO	A	704	-	-	-	X
3	EDO	A	705	-	-	-	X
3	EDO	A	706	-	-	-	X
3	EDO	B	703	-	-	-	X



## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15536 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetyl-coenzyme A synthetase.

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

There are 45 discrepancies between the modelled and reference sequences:

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

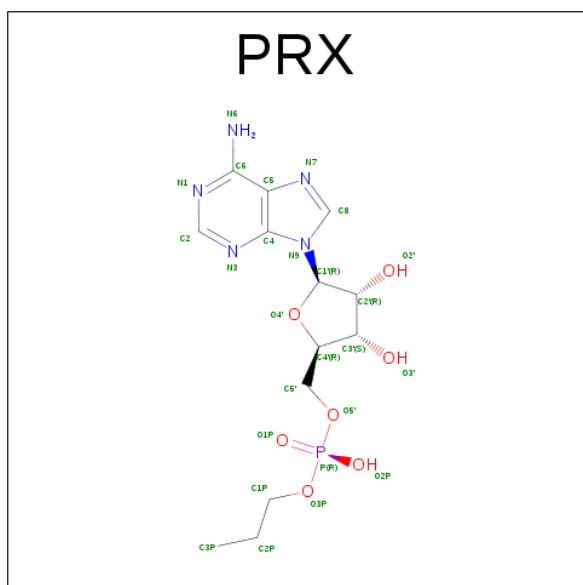
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression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

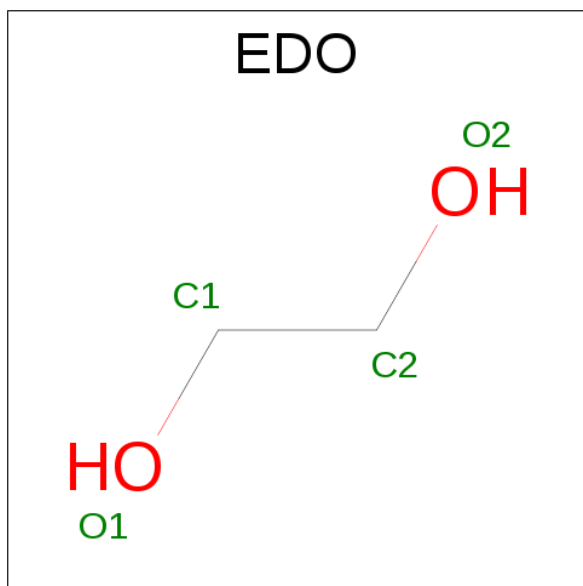
- Molecule 2 is ADENOSINE-5'-MONOPHOSPHATE-PROPYL ESTER (three-letter code: PRX) (formula:  $C_{13}H_{20}N_5O_7P$ ).





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<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

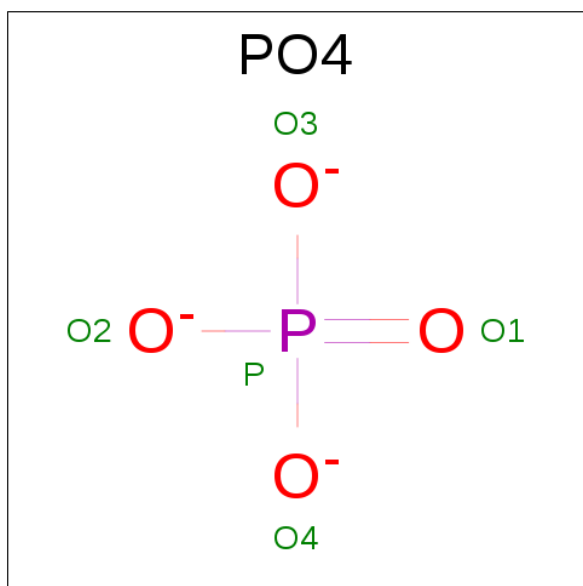
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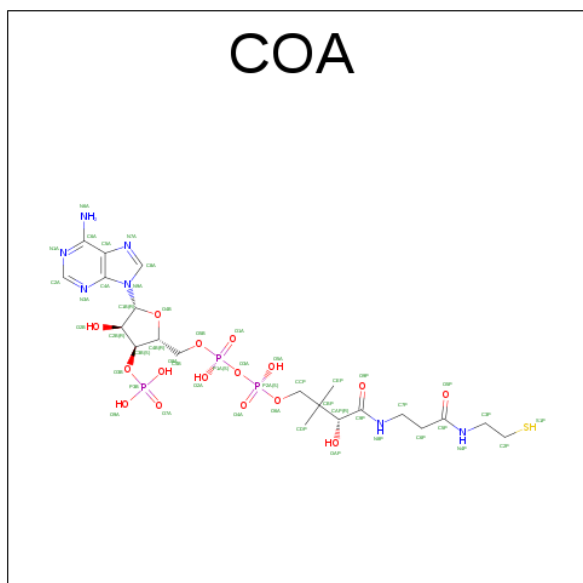
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).





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

- Molecule 6 is water.

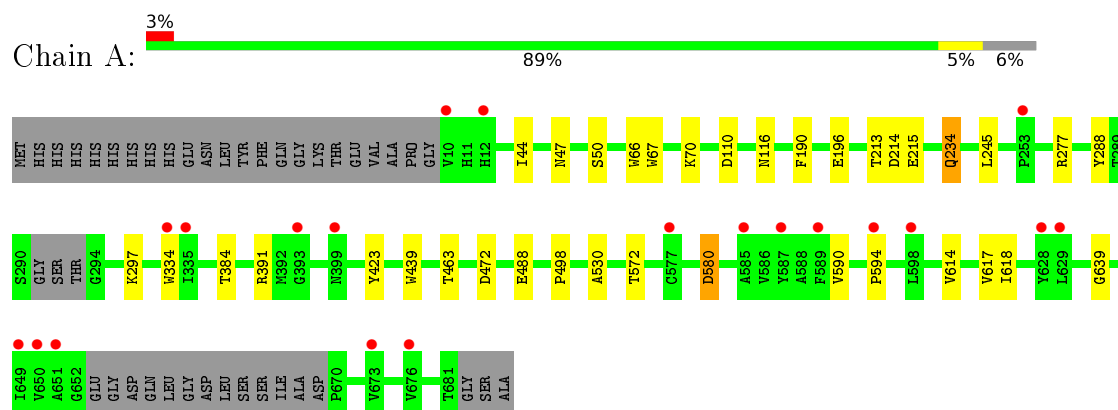
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	303	Total	O	0	0
			303	303		
6	B	280	Total	O	0	0
			280	280		
6	C	158	Total	O	0	0
			158	158		



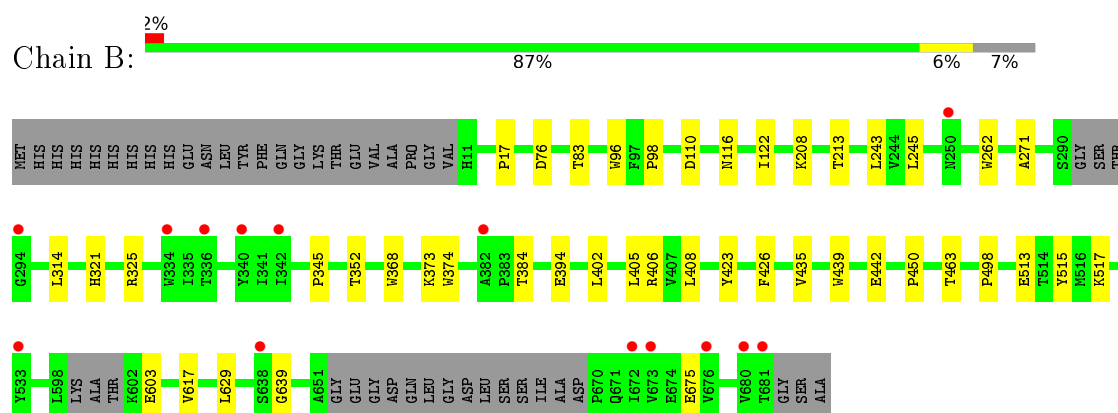
### 3 Residue-property plots [i](#)

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

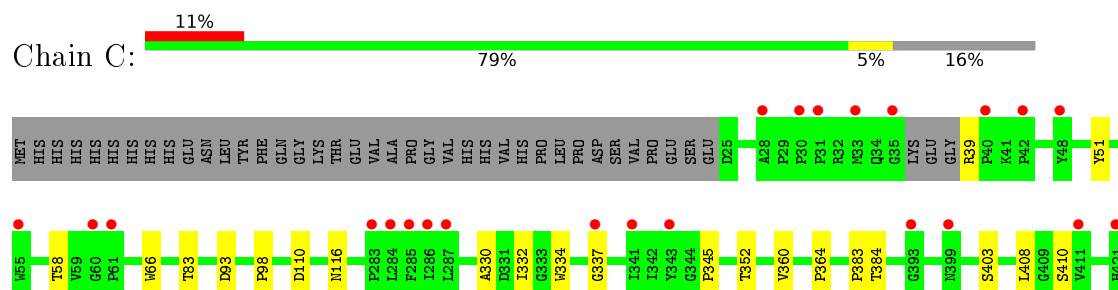
- Molecule 1: Acetyl-coenzyme A synthetase



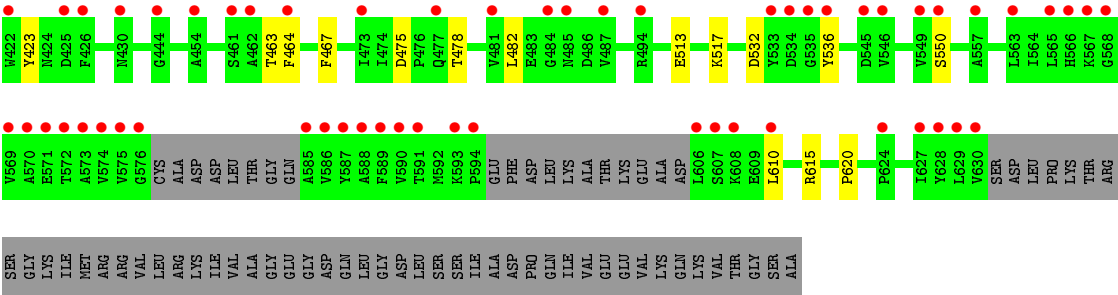
- Molecule 1: Acetyl-coenzyme A synthetase



- Molecule 1: Acetyl-coenzyme A synthetase









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.80 Å 186.09 Å 85.32 Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	27.57 – 2.30 48.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (27.57-2.30) 97.5 (48.70-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (DEV_2443: ???)	Depositor
R, $R_{free}$	0.179 , 0.217 0.177 , 0.215	Depositor DCC
$R_{free}$ test set	1992 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: COA, PO4, 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	0/5250	0.52	0/7164
1	B	0.35	0/5282	0.52	0/7196
1	C	0.33	0/4541	0.49	0/6209
All	All	0.35	0/15073	0.51	0/20569

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5090	0	4836	20	0
1	B	5121	0	4902	20	0
1	C	4413	0	4084	22	0
2	A	26	0	19	1	0
2	B	26	0	19	1	0
2	C	26	0	19	0	0
3	A	28	0	42	3	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	48	0	32	5	0
6	A	303	0	0	1	0
6	B	280	0	0	1	0
6	C	158	0	0	0	0
All	All	15536	0	13971	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ALA:HB1	5:C:801:COA:H32	1.97	0.47
1:C:463:THR:OG1	1:C:464:PHE:N	2.47	0.47
1:B:373:LYS:HE3	1:B:374:TRP:NE1	2.29	0.47
1:A:190[A]:PHE:CZ	1:A:334[A]:TRP:HB2	2.50	0.47
1:C:58:THR:HG21	1:C:467:PHE:HB3	1.95	0.47
1:C:83:THR:O	1:C:98:PRO:HD2	2.15	0.47
1:A:288:TYR:HA	1:A:297:LYS:O	2.16	0.46
1:A:67:TRP:CZ3	1:A:498:PRO:HG2	2.52	0.45
1:A:66:TRP:CZ2	1:A:70:LYS:HE3	2.52	0.45
1:A:580:ASP:N	1:A:580:ASP:OD1	2.42	0.44
1:B:213:THR:HG22	1:B:245:LEU:HB3	1.99	0.44
1:A:614:VAL:HG13	1:A:618:ILE:HD12	2.00	0.44
1:C:532:ASP:OD2	1:C:536:TYR:HB2	2.18	0.44
1:C:345:PRO:HB2	1:C:352:THR:HB	1.99	0.43
1:C:513:GLU:HA	1:C:517:LYS:HG3	2.00	0.43
1:B:243:LEU:HD11	1:B:262:TRP:HA	2.01	0.43
1:C:384:THR:OG1	1:C:550:SER:HA	2.18	0.43
1:B:83:THR:O	1:B:98:PRO:HD2	2.20	0.42
1:C:58:THR:HG22	1:C:66:TRP:CD2	2.54	0.42
1:B:321:HIS:HD2	1:B:406[B]:ARG:HH22	1.68	0.42
1:B:435:VAL:HG12	1:B:450:PRO:HG2	2.02	0.42
1:B:271:ALA:HB3	1:C:93:ASP:HB3	2.01	0.42
1:B:122:ILE:HA	1:B:352:THR:O	2.20	0.42
1:A:488[A]:GLU:HG3	1:A:530:ALA:HB2	2.01	0.42
1:B:208:LYS:NZ	6:B:825:HOH:O	2.53	0.41
1:A:214:ASP:OD1	1:A:215:GLU:N	2.52	0.41
1:B:96:TRP:CD1	1:B:498:PRO:HA	2.54	0.41
1:A:213:THR:HG22	1:A:245:LEU:HB3	2.02	0.41
1:C:383:PRO:HG3	1:C:410:SER:OG	2.21	0.40
1:C:475:ASP:HB2	1:C:482:LEU:HD21	2.02	0.40
1:B:394:GLU:HG2	1:B:426:PHE:CZ	2.57	0.40
1:C:408:LEU:HB3	1:C:423:TYR:CE2	2.56	0.40
1:A:572:THR:HG22	1:A:590:VAL:HA	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	656/694 (94%)	637 (97%)	18 (3%)	1 (0%)	52	64
1	B	654/694 (94%)	634 (97%)	19 (3%)	1 (0%)	52	64
1	C	576/694 (83%)	555 (96%)	21 (4%)	0	100	100
All	All	1886/2082 (91%)	1826 (97%)	58 (3%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	518/576 (90%)	511 (99%)	7 (1%)	74	86
1	B	528/576 (92%)	521 (99%)	7 (1%)	76	87
1	C	427/576 (74%)	423 (99%)	4 (1%)	84	93
All	All	1473/1728 (85%)	1455 (99%)	18 (1%)	78	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP

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Mol	Chain	Res	Type
1	A	116	ASN
1	A	234	GLN
1	A	277	ARG
1	A	423	TYR
1	A	472	ASP
1	A	580	ASP
1	B	76	ASP
1	B	110	ASP
1	B	116	ASN
1	B	325[A]	ARG
1	B	325[B]	ARG
1	B	423	TYR
1	B	675	GLU
1	C	51	TYR
1	C	110	ASP
1	C	116	ASN
1	C	610	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PRX	A	701	-	25,28,28	2.31	7 (28%)	24,41,41	2.80	3 (12%)
3	EDO	A	702	-	3,3,3	0.57	0	2,2,2	0.08	0
3	EDO	A	703	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	A	704	-	3,3,3	0.51	0	2,2,2	0.36	0
3	EDO	A	705	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	A	706	-	3,3,3	0.41	0	2,2,2	0.42	0
3	EDO	A	707	-	3,3,3	0.40	0	2,2,2	0.52	0
3	EDO	A	708	-	3,3,3	0.45	0	2,2,2	0.51	0
4	PO4	B	701	-	4,4,4	0.67	0	6,6,6	0.23	0
2	PRX	B	702	-	25,28,28	2.34	6 (24%)	24,41,41	2.85	3 (12%)
3	EDO	B	703	-	3,3,3	0.46	0	2,2,2	0.67	0
3	EDO	B	704	-	3,3,3	0.43	0	2,2,2	0.44	0
5	COA	C	801	-	41,50,50	3.48	13 (31%)	49,75,75	1.55	6 (12%)
2	PRX	C	802	-	25,28,28	2.40	6 (24%)	24,41,41	2.67	3 (12%)
3	EDO	C	803	-	3,3,3	0.42	0	2,2,2	0.54	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
2	PRX	A	701	-	-	0/11/31/31	0/3/3/3
3	EDO	A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	A	704	-	-	0/1/1/1	0/0/0/0
3	EDO	A	705	-	-	0/1/1/1	0/0/0/0
3	EDO	A	706	-	-	0/1/1/1	0/0/0/0
3	EDO	A	707	-	-	0/1/1/1	0/0/0/0
3	EDO	A	708	-	-	0/1/1/1	0/0/0/0
4	PO4	B	701	-	-	0/0/0/0	0/0/0/0
2	PRX	B	702	-	-	0/11/31/31	0/3/3/3
3	EDO	B	703	-	-	0/1/1/1	0/0/0/0
3	EDO	B	704	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	COA	C	801	-	-	0/44/64/64	0/3/3/3
2	PRX	C	802	-	-	0/11/31/31	0/3/3/3
3	EDO	C	803	-	-	0/1/1/1	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	801	COA	C2B-C3B	-11.64	1.26	1.53
5	C	801	COA	O4B-C1B	-8.94	1.28	1.41
2	C	802	PRX	C8-N7	-6.61	1.22	1.34
2	B	702	PRX	C8-N7	-6.48	1.22	1.34
2	A	701	PRX	C8-N7	-6.03	1.23	1.34
5	C	801	COA	C5B-C4B	-4.04	1.38	1.51
2	C	802	PRX	C6-C5	-2.51	1.29	1.42
2	B	702	PRX	C6-C5	-2.50	1.29	1.42
5	C	801	COA	OAP-CAP	-2.40	1.37	1.42
5	C	801	COA	O9P-C9P	-2.34	1.18	1.23
2	A	701	PRX	C6-C5	-2.29	1.31	1.42
2	A	701	PRX	C6-N1	-2.19	1.27	1.37
2	B	702	PRX	C6-N1	-2.15	1.27	1.37
2	C	802	PRX	C6-N1	-2.11	1.27	1.37
2	A	701	PRX	C5-N7	2.07	1.46	1.39
5	C	801	COA	P1A-O5B	2.10	1.68	1.59
5	C	801	COA	C6P-C5P	2.21	1.55	1.51
5	C	801	COA	C6A-N6A	2.50	1.44	1.34
5	C	801	COA	O3B-C3B	2.58	1.52	1.44
2	C	802	PRX	C6-N6	2.74	1.45	1.34
2	B	702	PRX	C6-N6	2.81	1.45	1.34
2	A	701	PRX	C6-N6	2.83	1.45	1.34
5	C	801	COA	O4B-C4B	4.35	1.55	1.45
2	B	702	PRX	C5-C4	5.42	1.52	1.40
2	B	702	PRX	C2-N3	5.49	1.41	1.32
2	A	701	PRX	C5-C4	5.52	1.52	1.40
2	C	802	PRX	C5-C4	5.66	1.53	1.40
2	A	701	PRX	C2-N3	5.73	1.42	1.32
2	C	802	PRX	C2-N3	5.74	1.42	1.32
5	C	801	COA	C5P-N4P	6.82	1.49	1.33
5	C	801	COA	C9P-N8P	8.01	1.50	1.33
5	C	801	COA	C2B-C1B	8.76	1.67	1.53

All (15) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	PRX	N3-C2-N1	-11.56	119.79	128.87
2	A	701	PRX	N3-C2-N1	-11.27	120.02	128.87
2	C	802	PRX	N3-C2-N1	-11.12	120.13	128.87
5	C	801	COA	N3A-C2A-N1A	-8.18	122.45	128.87
2	B	702	PRX	C1'-N9-C4	-5.84	120.28	126.81
2	A	701	PRX	C1'-N9-C4	-5.81	120.32	126.81
2	C	802	PRX	C1'-N9-C4	-4.91	121.33	126.81
5	C	801	COA	C4B-O4B-C1B	-2.20	107.31	109.64
5	C	801	COA	C2P-C3P-N4P	-2.04	108.39	112.44
5	C	801	COA	CAP-C9P-N8P	2.02	121.06	116.31
5	C	801	COA	C7P-C6P-C5P	2.04	115.72	112.22
5	C	801	COA	C3B-C2B-C1B	2.60	105.72	100.06
2	C	802	PRX	C2-N1-C6	3.98	125.87	118.77
2	A	701	PRX	C2-N1-C6	4.07	126.03	118.77
2	B	702	PRX	C2-N1-C6	4.11	126.10	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	PRX	1	0
3	A	702	EDO	2	0
3	A	706	EDO	1	0
2	B	702	PRX	1	0
5	C	801	COA	5	0

## 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	652/694 (93%)	-0.00	20 (3%)	52	62	23, 41, 79, 97	0
1	B	647/694 (93%)	-0.02	14 (2%)	65	73	27, 41, 71, 104	0
1	C	584/694 (84%)	0.64	79 (13%)	4	6	27, 57, 100, 114	0
All	All	1883/2082 (90%)	0.19	113 (6%)	25	33	23, 44, 88, 114	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	629	LEU	8.3
1	C	587	TYR	7.3
1	C	628	TYR	6.6
1	C	533	TYR	6.3
1	C	534	ASP	5.8
1	B	334[A]	TRP	5.6
1	C	606	LEU	5.6
1	B	676	VAL	5.3
1	C	31	PRO	5.3
1	C	570	ALA	5.1
1	C	42	PRO	5.0
1	C	627	ILE	4.9
1	A	577	CYS	4.8
1	C	48	TYR	4.7
1	C	589	PHE	4.6
1	C	575	VAL	4.5
1	C	607	SER	4.3
1	C	535	GLY	4.2
1	C	630	VAL	4.1
1	C	585	ALA	4.0
1	C	399	ASN	3.9
1	C	422	TRP	3.9
1	C	484	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	629	LEU	3.8
1	B	533	TYR	3.8
1	C	568	GLY	3.7
1	A	649	ILE	3.6
1	C	591	THR	3.6
1	C	485	ASN	3.5
1	C	30	PRO	3.5
1	C	588	ALA	3.4
1	C	565	LEU	3.4
1	C	566	HIS	3.3
1	C	569	VAL	3.3
1	A	587	TYR	3.3
1	C	610	LEU	3.3
1	C	35	GLY	3.3
1	C	590	VAL	3.3
1	C	536	TYR	3.2
1	C	426	PHE	3.2
1	A	10	VAL	3.2
1	C	586	VAL	3.2
1	C	33	MET	3.2
1	A	334[A]	TRP	3.2
1	C	567	LYS	3.2
1	B	673	VAL	3.1
1	B	680	VAL	3.0
1	A	650	VAL	3.0
1	C	571	GLU	3.0
1	C	572	THR	3.0
1	C	594	PRO	2.9
1	C	574	VAL	2.9
1	C	454	ALA	2.9
1	C	425	ASP	2.8
1	B	681	THR	2.8
1	C	473	ILE	2.8
1	C	608	LYS	2.8
1	C	61	PRO	2.8
1	A	399	ASN	2.8
1	C	550	SER	2.7
1	C	549	VAL	2.7
1	A	12	HIS	2.7
1	A	598	LEU	2.7
1	C	461	SER	2.6
1	C	593	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	285	PHE	2.6
1	A	253	PRO	2.6
1	A	651	ALA	2.6
1	C	343	TYR	2.6
1	C	487	VAL	2.6
1	C	462	ALA	2.6
1	C	286	ILE	2.5
1	C	545	ASP	2.5
1	C	284	LEU	2.4
1	A	594	PRO	2.4
1	C	481	VAL	2.4
1	C	287	LEU	2.4
1	C	393	GLY	2.4
1	C	576	GLY	2.4
1	C	464	PHE	2.4
1	A	673	VAL	2.3
1	C	624	PRO	2.3
1	A	628	TYR	2.3
1	C	444	GLY	2.3
1	C	494	ARG	2.3
1	B	382	ALA	2.2
1	C	60	GLY	2.2
1	B	340	TYR	2.2
1	C	421	HIS	2.2
1	C	430	ASN	2.2
1	A	589	PHE	2.2
1	C	573	ALA	2.2
1	C	563	LEU	2.2
1	C	40	PRO	2.2
1	A	676	VAL	2.2
1	C	55	TRP	2.2
1	C	477	GLN	2.2
1	B	250	ASN	2.1
1	C	546	VAL	2.1
1	C	341	ILE	2.1
1	C	283	PRO	2.1
1	B	336	THR	2.1
1	B	672	ILE	2.1
1	B	294	GLY	2.1
1	B	342	ILE	2.1
1	B	638	SER	2.1
1	A	393	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	2.1
1	A	585	ALA	2.0
1	C	28	ALA	2.0
1	C	411	VAL	2.0
1	C	337	GLY	2.0
1	C	557	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	A	703	4/4	0.91	0.28	19.63	58,58,58,58	0
3	EDO	A	706	4/4	0.95	0.20	7.73	58,58,59,59	0
3	EDO	A	704	4/4	0.85	0.19	7.33	58,58,59,59	0
3	EDO	A	705	4/4	0.90	0.20	7.10	63,63,63,63	0
3	EDO	A	702	4/4	0.72	0.24	5.56	55,56,56,57	0
3	EDO	B	703	4/4	0.92	0.14	2.08	42,43,43,43	0
5	COA	C	801	48/48	0.75	0.26	1.65	96,101,104,104	0
3	EDO	B	704	4/4	0.94	0.14	1.58	57,57,57,57	0
3	EDO	A	707	4/4	0.90	0.11	-0.16	46,46,46,46	0
2	PRX	A	701	26/26	0.97	0.16	-0.25	30,32,32,32	0
2	PRX	B	702	26/26	0.97	0.19	-0.34	29,31,35,35	0
2	PRX	C	802	26/26	0.91	0.15	-0.48	55,60,62,62	0
3	EDO	C	803	4/4	0.95	0.08	-1.99	45,45,45,46	0
4	PO4	B	701	5/5	0.89	0.22	-	93,94,94,94	0
3	EDO	A	708	4/4	0.74	0.24	-	75,75,76,76	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.