



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 02:48 AM EDT

PDB ID : 2P2Q  
Title : Acetyl-CoA Synthetase, R584E mutation  
Authors : Reger, A.S.; Gulick, A.M.  
Deposited on : unknown  
Resolution : 2.42 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

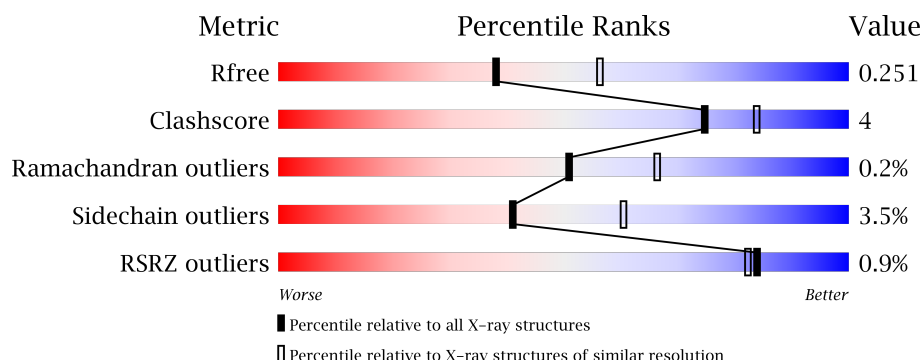
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	652	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	652	<div> <div>86%</div> <div>11%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10131 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.

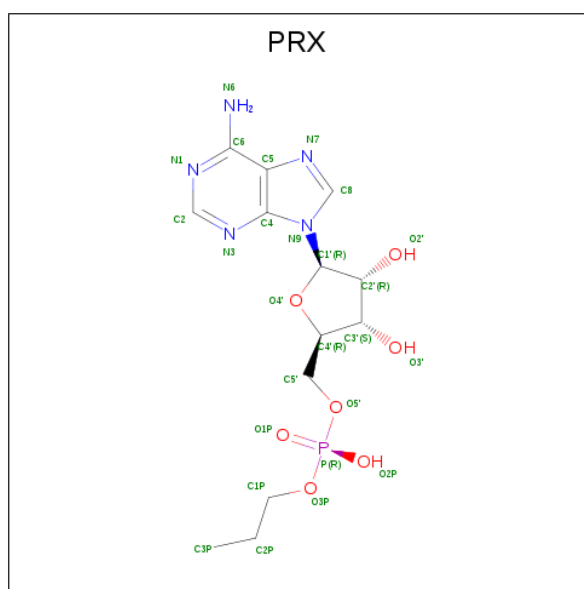
- Molecule 1 is a protein called Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			4905	3122	836	929	18			
1	B	636	Total	C	N	O	S	0	0	0
			4933	3141	843	931	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	584	GLU	ARG	ENGINEERED	UNP Q8ZKF6
B	584	GLU	ARG	ENGINEERED	UNP Q8ZKF6

- 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		

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

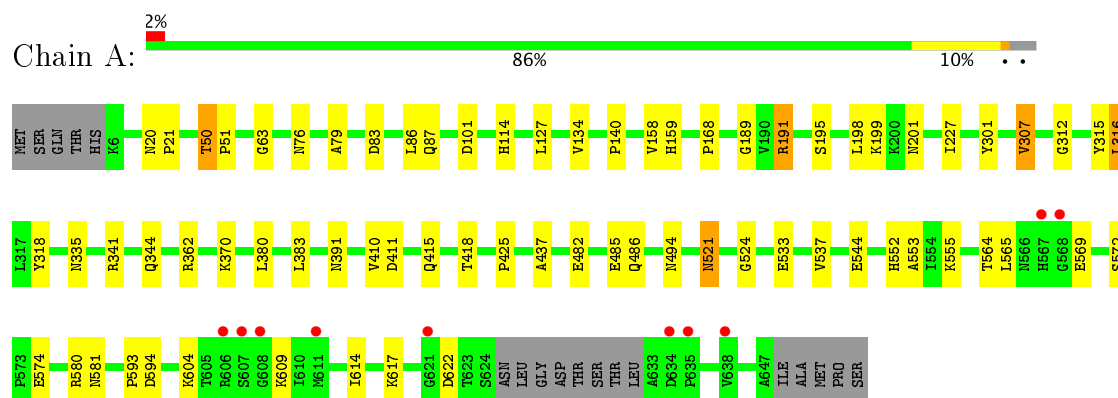
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	123	Total	O	0	0
			123	123		

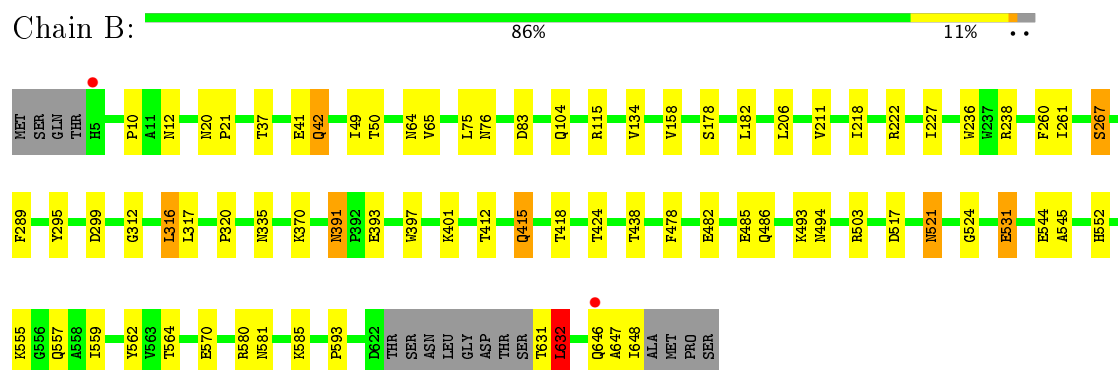
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.05Å 95.53Å 164.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.42 47.77 – 2.42	Depositor EDS
% Data completeness (in resolution range)	94.2 (35.00-2.42) 93.4 (47.77-2.42)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.42Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.184 , 0.245 0.190 , 0.251	Depositor DCC
$R_{free}$ test set	2655 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: 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	0.66	0/5036	0.71	2/6871 (0.0%)
1	B	0.65	1/5065 (0.0%)	0.69	3/6910 (0.0%)
All	All	0.65	1/10101 (0.0%)	0.70	5/13781 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	482	GLU	CG-CD	5.58	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	LEU	CA-CB-CG	6.65	130.59	115.30
1	B	580	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	632	LEU	CA-CB-CG	6.11	129.36	115.30
1	A	411	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	101	ASP	CB-CG-OD1	-5.13	113.69	118.30

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	4905	0	4720	36	0
1	B	4933	0	4763	38	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
3	A	118	0	0	1	0
3	B	123	0	0	1	0
All	All	10131	0	9521	72	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 4.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:HG2	1:A:191:ARG:HH11	1.33	0.93
1:A:617:LYS:O	1:A:622:ASP:HB3	1.81	0.81
1:A:555:LYS:NZ	1:A:594:ASP:OD1	2.16	0.79
1:B:552:HIS:HD2	1:B:555:LYS:H	1.29	0.78
1:A:552:HIS:HD2	1:A:555:LYS:H	1.35	0.75
1:B:391:ASN:HD22	1:B:393:GLU:H	1.35	0.74
1:A:191:ARG:HG2	1:A:191:ARG:NH1	2.06	0.71
1:A:521:ASN:HD21	1:A:524:GLY:HA2	1.57	0.70
1:A:552:HIS:CD2	1:A:555:LYS:H	2.13	0.67
1:A:410:VAL:HA	1:A:425:PRO:HG2	1.80	0.64
1:B:391:ASN:ND2	1:B:393:GLU:H	1.97	0.62
1:B:552:HIS:CD2	1:B:555:LYS:H	2.14	0.62
1:B:415:GLN:HB3	2:B:998:PRX:H5'2	1.81	0.62
1:B:295:TYR:CE1	1:B:299:ASP:HB2	2.38	0.59
1:A:20:ASN:HB2	1:A:21:PRO:CD	2.34	0.58
1:A:604:LYS:HA	1:A:609:LYS:O	2.05	0.57
1:A:362:ARG:HD2	1:A:553:ALA:O	2.05	0.56
1:B:20:ASN:HB2	1:B:21:PRO:CD	2.36	0.56
1:B:415:GLN:HG3	1:B:418:THR:HG23	1.87	0.56
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.88	0.55
1:A:199:LYS:HG2	1:A:227:ILE:HD12	1.89	0.54
1:B:397:TRP:CE2	1:B:401:LYS:HG3	2.44	0.52
1:B:312:GLY:O	1:B:316:LEU:HB3	2.11	0.51
1:A:134:VAL:HA	1:A:158:VAL:O	2.11	0.51
1:B:493:LYS:O	1:B:494:ASN:HB2	2.11	0.50
1:B:544:GLU:HB2	1:B:564:THR:HB	1.93	0.50
1:B:134:VAL:HG11	1:B:178:SER:HB2	1.93	0.50
1:A:580:ARG:HD2	1:A:593:PRO:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:O	1:B:41:GLU:HG3	2.13	0.48
1:B:391:ASN:HD22	1:B:393:GLU:N	2.07	0.48
1:A:544:GLU:HB3	1:A:564:THR:HB	1.95	0.48
1:B:206:LEU:HD23	1:B:211:VAL:HG11	1.95	0.48
1:B:261:ILE:HD12	1:B:478:PHE:HB2	1.97	0.47
1:B:104:GLN:HE22	1:B:222:ARG:HH22	1.62	0.47
1:B:182:LEU:HD11	1:B:218:ILE:HG13	1.96	0.47
1:A:341:ARG:HA	1:A:344:GLN:NE2	2.30	0.46
1:B:10:PRO:HB2	1:B:12:ASN:OD1	2.16	0.46
1:B:521:ASN:O	1:B:557:GLN:HB2	2.15	0.46
1:A:189:GLY:O	1:A:195:SER:HA	2.15	0.46
1:A:482:GLU:HG3	3:A:1062:HOH:O	2.15	0.46
1:A:533:GLU:O	1:A:537:VAL:HG23	2.16	0.46
1:B:49:ILE:HG13	1:B:75:LEU:HA	1.98	0.46
1:B:20:ASN:HB2	1:B:21:PRO:HD2	2.00	0.44
1:B:412:THR:HG22	1:B:424:THR:OG1	2.18	0.44
1:B:65:VAL:HB	1:B:485:GLU:HG2	2.00	0.44
1:A:521:ASN:ND2	1:A:524:GLY:HA2	2.30	0.44
1:A:581:ASN:OD1	1:B:370:LYS:HE2	2.18	0.43
1:B:632:LEU:HD12	3:B:1121:HOH:O	2.18	0.43
1:B:531:GLU:HG3	1:B:531:GLU:H	1.59	0.43
1:A:159:HIS:HE1	1:A:318:TYR:OH	2.02	0.43
1:A:63:GLY:HA2	1:A:485:GLU:OE2	2.17	0.42
1:A:312:GLY:O	1:A:316:LEU:HB3	2.19	0.42
1:B:559:ILE:HB	1:B:593:PRO:HA	2.01	0.42
1:B:227:ILE:HD11	1:B:236:TRP:CH2	2.55	0.42
1:A:86:LEU:HD11	1:A:114:HIS:CG	2.55	0.42
1:A:168:PRO:HG3	1:A:201:ASN:HA	2.01	0.42
1:B:42:GLN:HA	1:B:42:GLN:NE2	2.34	0.42
1:B:289:PHE:CE1	1:B:320:PRO:HG3	2.55	0.41
1:A:140:PRO:HD3	1:A:198:LEU:CD1	2.50	0.41
1:A:370:LYS:HE2	1:B:581:ASN:OD1	2.20	0.41
1:A:380:LEU:HD13	1:A:383:LEU:HD21	2.02	0.41
1:A:76:ASN:HD22	1:A:79:ALA:H	1.67	0.41
1:B:158:VAL:HG13	1:B:260:PHE:HA	2.03	0.41
1:B:545:ALA:HA	1:B:562:TYR:O	2.21	0.41
1:A:50:THR:HA	1:A:51:PRO:HD2	1.79	0.41
1:A:565:LEU:HB3	1:A:569:GLU:HB2	2.03	0.41
1:B:267:SER:OG	1:B:517:ASP:HB2	2.21	0.41
1:B:647:ALA:O	1:B:648:ILE:HB	2.20	0.41
1:A:425:PRO:HD3	1:A:437:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLN:HB2	1:A:418:THR:HG23	2.02	0.41
1:A:301:TYR:HE1	1:A:315:TYR:O	2.04	0.41
1:B:521:ASN:HD21	1:B:524:GLY:HA2	1.86	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	630/652 (97%)	603 (96%)	26 (4%)	1 (0%)	51 66
1	B	632/652 (97%)	611 (97%)	20 (3%)	1 (0%)	51 66
All	All	1262/1304 (97%)	1214 (96%)	46 (4%)	2 (0%)	51 66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	438	THR
1	A	307	VAL

### 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	508/538 (94%)	493 (97%)	15 (3%)	46 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	513/538 (95%)	492 (96%)	21 (4%)	35	53
All	All	1021/1076 (95%)	985 (96%)	36 (4%)	41	60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	83	ASP
1	A	87	GLN
1	A	127	LEU
1	A	191	ARG
1	A	307	VAL
1	A	316	LEU
1	A	335	ASN
1	A	391	ASN
1	A	486	GLN
1	A	494	ASN
1	A	521	ASN
1	A	572	SER
1	A	574	GLU
1	A	614	ILE
1	B	42	GLN
1	B	50	THR
1	B	64	ASN
1	B	76	ASN
1	B	83	ASP
1	B	115	ARG
1	B	238	ARG
1	B	267	SER
1	B	317	LEU
1	B	335	ASN
1	B	391	ASN
1	B	415	GLN
1	B	486	GLN
1	B	503	ARG
1	B	521	ASN
1	B	531	GLU
1	B	570	GLU
1	B	585	LYS
1	B	631	THR
1	B	632	LEU
1	B	646	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	159	HIS
1	A	249	GLN
1	A	335	ASN
1	A	344	GLN
1	A	456	GLN
1	A	521	ASN
1	A	552	HIS
1	B	5	HIS
1	B	64	ASN
1	B	76	ASN
1	B	87	GLN
1	B	89	ASN
1	B	104	GLN
1	B	335	ASN
1	B	344	GLN
1	B	391	ASN
1	B	456	GLN
1	B	521	ASN
1	B	552	HIS
1	B	646	GLN

### 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](#)

2 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	999	-	25,28,28	0.68	0	25,41,41	1.80	2 (8%)
2	PRX	B	998	-	25,28,28	0.75	0	25,41,41	1.94	1 (4%)

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	999	-	-	0/11/31/31	0/3/3/3
2	PRX	B	998	-	-	0/11/31/31	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	PRX	N3-C2-N1	-8.87	121.13	128.86
2	A	999	PRX	N3-C2-N1	-7.86	122.02	128.86
2	A	999	PRX	C4-C5-N7	-2.29	107.20	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	998	PRX	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	634/652 (97%)	-0.35	10 (1%) 72 70	18, 25, 36, 47	0
1	B	636/652 (97%)	-0.39	2 (0%) 93 93	18, 26, 36, 58	0
All	All	1270/1304 (97%)	-0.37	12 (0%) 84 82	18, 25, 36, 58	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	646	GLN	5.0
1	B	5	HIS	3.0
1	A	567	HIS	2.8
1	A	638	VAL	2.8
1	A	607	SER	2.8
1	A	611	MET	2.7
1	A	606	ARG	2.5
1	A	608	GLY	2.5
1	A	568	GLY	2.4
1	A	634	ASP	2.2
1	A	621	GLY	2.0
1	A	635	PRO	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( $\text{\AA}^2$ )	Q<0.9
2	PRX	B	998	26/26	0.98	0.14	-0.77	15,20,21,21	0
2	PRX	A	999	26/26	0.98	0.12	-1.20	12,16,19,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.