



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 10:03 AM EST

PDB ID : 7FTK  
Title : Crystal Structure of apo human cyclic GMP-AMP synthase  
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Deposited on : 2023-02-08  
Resolution : 2.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

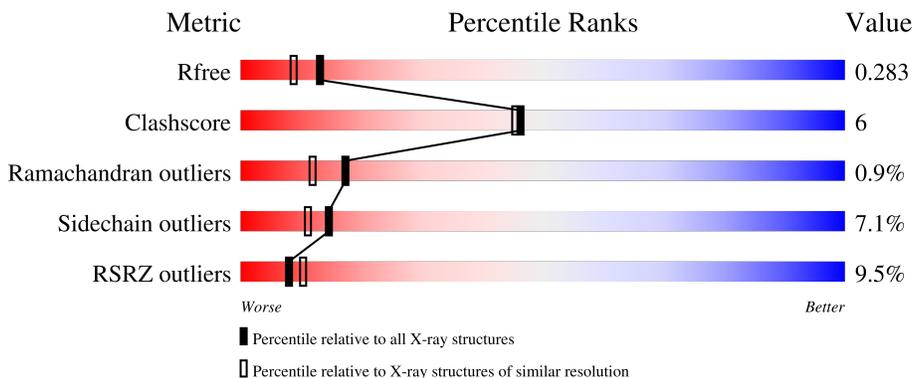
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	362	 10% 74% 19% • 6%
1	B	362	 8% 75% 18% • •

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5801 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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2847	1830	484	517	16	0	4	0
1	B	352	2932	1881	500	535	16	0	4	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

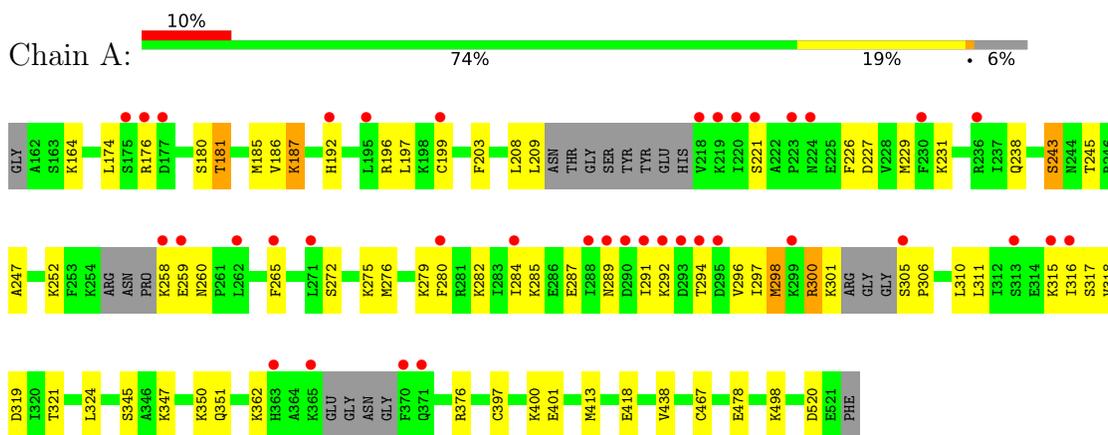
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	9	Total	O	0	0
			9	9		

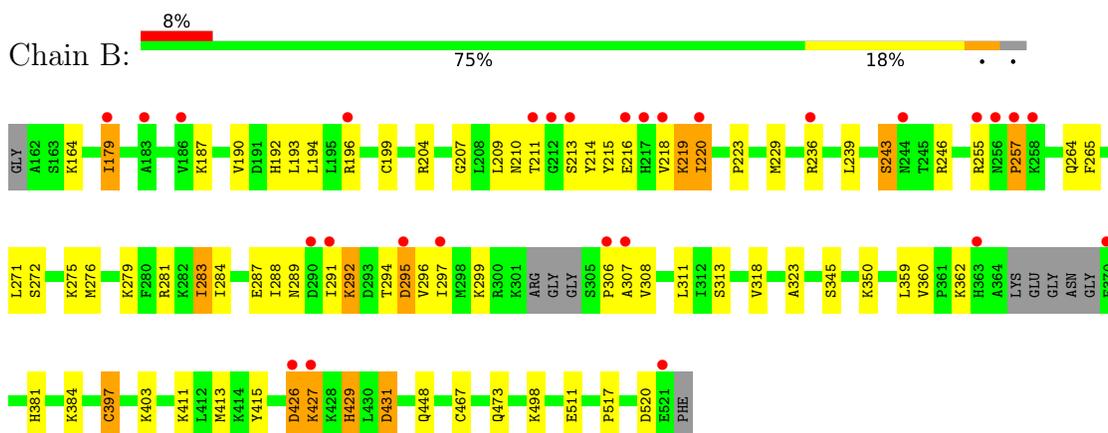
### 3 Residue-property plots [i](#)

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: Cyclic GMP-AMP synthase



- Molecule 1: Cyclic GMP-AMP synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.13Å 120.41Å 127.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.21 – 2.12 60.21 – 2.13	Depositor EDS
% Data completeness (in resolution range)	90.0 (60.21-2.12) 87.3 (60.21-2.13)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.12rc1_2801	Depositor
R, $R_{free}$	0.212 , 0.278 0.215 , 0.283	Depositor DCC
$R_{free}$ test set	1880 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3947e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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:  
ZN

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	0.42	0/2911	0.58	0/3896
1	B	0.42	1/3002 (0.0%)	0.55	0/4025
All	All	0.42	1/5913 (0.0%)	0.56	0/7921

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	397	CYS	CB-SG	9.28	1.98	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	219	LYS	Peptide
1	B	307	ALA	Peptide

### 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	2847	0	2915	35	0
1	B	2932	0	2981	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	0	0	0
3	B	9	0	0	0	0
All	All	5801	0	5896	73	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 6.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HD21	1:B:207:GLY:HA2	1.67	0.76
1:B:289:ASN:HA	1:B:292:LYS:HB2	1.74	0.69
1:B:196:ARG:O	1:B:196:ARG:NH1	2.22	0.68
1:A:209:LEU:HD23	1:A:229:MET:HE2	1.75	0.67
1:B:397:CYS:HA	1:B:403:LYS:HD3	1.77	0.66
1:B:431:ASP:OD1	1:B:431:ASP:N	2.17	0.65
1:B:295:ASP:HB2	1:B:313:SER:HA	1.82	0.62
1:B:243:SER:O	1:B:243:SER:OG	2.19	0.58
1:A:310:LEU:O	1:A:317:SER:HA	2.06	0.56
1:A:229:MET:HG2	1:A:321:THR:HB	1.87	0.55
1:A:196:ARG:HG2	1:A:287:GLU:CD	2.26	0.55
1:A:221:SER:OG	1:A:418:GLU:OE1	2.18	0.55
1:A:243:SER:O	1:A:243:SER:OG	2.24	0.54
1:B:413[B]:MET:SD	1:B:467:CYS:HB3	2.47	0.54
1:B:265:PHE:CD2	1:B:276:MET:HE2	2.43	0.53
1:A:238:GLN:HB3	1:A:252:LYS:HB2	1.90	0.53
1:A:186:VAL:HG21	1:A:226:PHE:CD2	2.44	0.53
1:B:255:ARG:C	1:B:257:PRO:HD2	2.29	0.52
1:A:258:LYS:HG2	1:A:259:GLU:H	1.75	0.52
1:A:298:MET:O	1:A:298:MET:HG3	2.10	0.52
1:B:216:GLU:HG2	1:B:384:LYS:HA	1.92	0.52
1:B:283:ILE:O	1:B:287:GLU:HG2	2.11	0.51
1:B:281:ARG:HG2	1:B:308:VAL:HG22	1.94	0.50
1:A:208:LEU:O	1:A:231:LYS:NZ	2.45	0.50
1:A:196:ARG:O	1:A:199:CYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:HG13	1:B:411:LYS:HG2	1.94	0.49
1:A:245:THR:O	1:A:245:THR:OG1	2.26	0.49
1:A:300:ARG:HG2	1:A:301:LYS:N	2.28	0.48
1:B:296:VAL:HA	1:B:311:LEU:O	2.13	0.48
1:A:362:LYS:HZ2	1:A:376:ARG:NH1	2.11	0.48
1:B:271:LEU:HD11	1:B:276:MET:HE3	1.96	0.48
1:A:245:THR:O	1:A:247:ALA:N	2.48	0.47
1:A:164:LYS:NZ	1:A:520:ASP:OD1	2.40	0.47
1:B:220:ILE:HD11	1:B:415:TYR:HB2	1.96	0.47
1:A:478:GLU:OE1	1:A:498:LYS:NZ	2.43	0.47
1:B:272:SER:HB3	1:B:275:LYS:HB2	1.97	0.46
1:B:196:ARG:NH1	1:B:199:CYS:HB2	2.31	0.46
1:B:193:LEU:HD13	1:B:284:ILE:HD12	1.97	0.45
1:B:306:PRO:HD3	1:B:362:LYS:NZ	2.31	0.45
1:A:305:SER:N	1:A:306:PRO:HD2	2.31	0.45
1:B:427:LYS:HB3	1:B:427:LYS:HE2	1.35	0.45
1:B:517:PRO:O	1:B:520:ASP:HB2	2.17	0.45
1:A:280:PHE:O	1:A:284:ILE:HD12	2.17	0.45
1:A:272:SER:OG	1:A:275:LYS:HG2	2.16	0.45
1:B:211:THR:HG21	1:B:381:HIS:HA	1.99	0.44
1:B:323:ALA:HB2	1:B:360:VAL:HG12	1.99	0.44
1:B:192:HIS:NE2	1:B:291:ILE:HD13	2.33	0.44
1:B:288:ILE:HD13	1:B:288:ILE:HA	1.83	0.44
1:B:214:TYR:HA	1:B:219:LYS:HB2	1.99	0.44
1:A:315:LYS:HD3	1:A:315:LYS:HA	1.85	0.43
1:A:181:THR:O	1:A:185:MET:HG2	2.18	0.43
1:A:413[B]:MET:SD	1:A:467:CYS:HB3	2.58	0.43
1:A:400:LYS:HE2	1:A:401:GLU:OE1	2.19	0.43
1:B:215:TYR:HB3	1:B:384:LYS:HE3	2.01	0.43
1:B:218:VAL:O	1:B:218:VAL:HG12	2.19	0.42
1:A:285:LYS:O	1:A:289:ASN:HB2	2.20	0.42
1:B:179:ILE:HG22	1:B:223:PRO:HG3	2.02	0.42
1:B:511:GLU:OE1	1:B:517:PRO:HD2	2.20	0.42
1:A:187:LYS:HD3	1:A:187:LYS:HA	1.59	0.42
1:A:265:PHE:CE2	1:A:276:MET:HG3	2.55	0.41
1:A:347:LYS:O	1:A:351:GLN:HG3	2.21	0.41
1:B:209:LEU:HD23	1:B:229:MET:HE2	2.02	0.41
1:B:236:ARG:HH21	1:B:255:ARG:HG3	1.85	0.41
1:A:192:HIS:CE1	1:A:291:ILE:HD12	2.54	0.41
1:A:260:ASN:OD1	1:A:260:ASN:N	2.48	0.41
1:A:265:PHE:HZ	1:A:279:LYS:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.92	0.41
1:B:239:LEU:HD21	1:B:359:LEU:HD11	2.02	0.41
1:B:164:LYS:HE3	1:B:164:LYS:HB2	1.76	0.41
1:A:197:LEU:O	1:A:203:PHE:HB2	2.22	0.40
1:B:271:LEU:HD11	1:B:276:MET:CE	2.51	0.40
1:A:362:LYS:NZ	1:A:376:ARG:HD3	2.37	0.40
1:A:311:LEU:HD11	1:A:315:LYS:HA	2.01	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	336/362 (93%)	317 (94%)	17 (5%)	2 (1%)	25 20
1	B	350/362 (97%)	326 (93%)	20 (6%)	4 (1%)	14 9
All	All	686/724 (95%)	643 (94%)	37 (5%)	6 (1%)	17 12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	345	SER
1	B	345	SER
1	B	426	ASP
1	B	429	HIS
1	B	257	PRO

### 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	324/334 (97%)	304 (94%)	20 (6%)	18	15
1	B	333/334 (100%)	307 (92%)	26 (8%)	12	9
All	All	657/668 (98%)	611 (93%)	46 (7%)	14	11

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LEU
1	A	180	SER
1	A	181	THR
1	A	187	LYS
1	A	227	ASP
1	A	243	SER
1	A	282	LYS
1	A	292	LYS
1	A	294	THR
1	A	296	VAL
1	A	297	ILE
1	A	298	MET
1	A	300	ARG
1	A	316	ILE
1	A	318	VAL
1	A	319	ASP
1	A	324	LEU
1	A	350	LYS
1	A	397	CYS
1	A	438	VAL
1	B	179	ILE
1	B	187	LYS
1	B	190	VAL
1	B	204	ARG
1	B	210	ASN
1	B	213	SER
1	B	220	ILE

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Mol	Chain	Res	Type
1	B	243	SER
1	B	246	ARG
1	B	264	GLN
1	B	279	LYS
1	B	283	ILE
1	B	292	LYS
1	B	294	THR
1	B	295	ASP
1	B	297	ILE
1	B	299	LYS
1	B	318	VAL
1	B	350	LYS
1	B	426	ASP
1	B	427	LYS
1	B	429	HIS
1	B	431	ASP
1	B	448	GLN
1	B	473	GLN
1	B	498	LYS

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

Mol	Chain	Res	Type
1	B	224	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	342/362 (94%)	0.43	38 (11%) <b>5</b> <b>6</b>	36, 70, 137, 168	0
1	B	352/362 (97%)	0.31	28 (7%) <b>12</b> <b>15</b>	41, 77, 132, 181	0
All	All	694/724 (95%)	0.37	66 (9%) <b>8</b> <b>10</b>	36, 75, 136, 181	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	THR	8.0
1	B	370	PHE	6.5
1	A	195	LEU	6.5
1	B	290	ASP	6.5
1	B	212	GLY	6.4
1	A	280	PHE	5.5
1	A	315	LYS	5.5
1	A	220	ILE	4.8
1	A	293	ASP	4.7
1	A	289	ASN	4.5
1	B	183	ALA	4.3
1	B	217	HIS	4.3
1	B	426	ASP	4.3
1	A	219	LYS	4.1
1	A	291	ILE	4.1
1	B	521	GLU	3.8
1	A	223	PRO	3.7
1	B	295	ASP	3.6
1	A	177	ASP	3.5
1	B	307	ALA	3.5
1	A	258	LYS	3.3
1	B	256	ASN	3.3
1	B	306	PRO	3.2
1	A	284	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	LYS	3.2
1	A	305	SER	3.1
1	B	213	SER	3.1
1	B	220	ILE	3.1
1	B	427	LYS	3.1
1	A	218	VAL	3.1
1	A	176	ARG	3.0
1	A	370	PHE	3.0
1	A	199	CYS	3.0
1	A	299	LYS	3.0
1	B	218	VAL	3.0
1	B	297	ILE	2.9
1	A	259	GLU	2.9
1	A	316	ILE	2.9
1	B	244	ASN	2.7
1	A	295	ASP	2.6
1	B	196	ARG	2.6
1	A	363	HIS	2.6
1	B	211	THR	2.6
1	B	255	ARG	2.5
1	B	179	ILE	2.5
1	A	175	SER	2.5
1	A	192	HIS	2.5
1	B	186	VAL	2.5
1	B	291	ILE	2.4
1	A	290	ASP	2.4
1	B	236	ARG	2.4
1	A	221	SER	2.4
1	A	230[A]	PHE	2.3
1	A	271	LEU	2.3
1	B	363	HIS	2.3
1	A	236	ARG	2.3
1	A	371	GLN	2.3
1	A	288	ILE	2.2
1	B	216	GLU	2.2
1	B	257	PRO	2.2
1	A	313	SER	2.2
1	B	258	LYS	2.2
1	A	224	ASN	2.2
1	A	262	LEU	2.1
1	A	365	LYS	2.1
1	A	265	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	600	1/1	0.99	0.13	53,53,53,53	0
2	ZN	B	600	1/1	1.00	0.10	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.