



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:08 PM UTC

PDB ID : 7FTK / pdb_00007ftk
Title : Crystal Structure of apo human cyclic GMP-AMP synthase
Authors : Leibrock, L.; Benz, J.; Groebke-Zbinden, K.; Rudolph, M.G.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

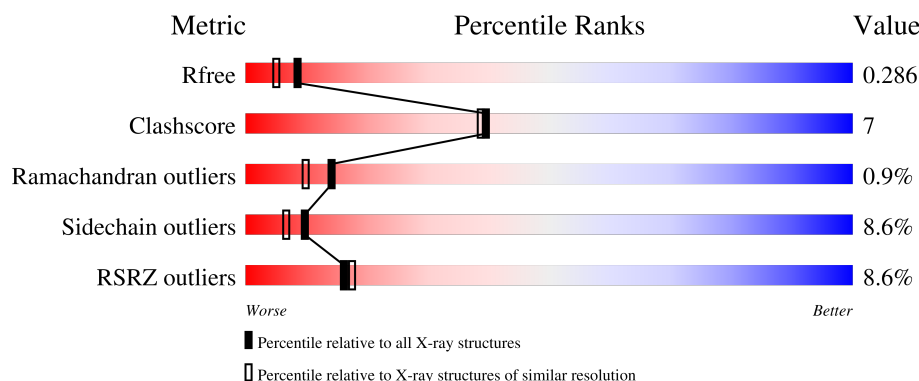
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 ≥ 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	7% 73% 19% 6%
1	B	362	9% 74% 19% .

2 Entry composition

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
1	A	342	Total	C	N	O	S	0	4	0
			2847	1830	484	517	16			
1	B	352	Total	C	N	O	S	0	4	0
			2932	1881	500	535	16			

- Molecule 2 is ZINC ION (CCD ID: 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		

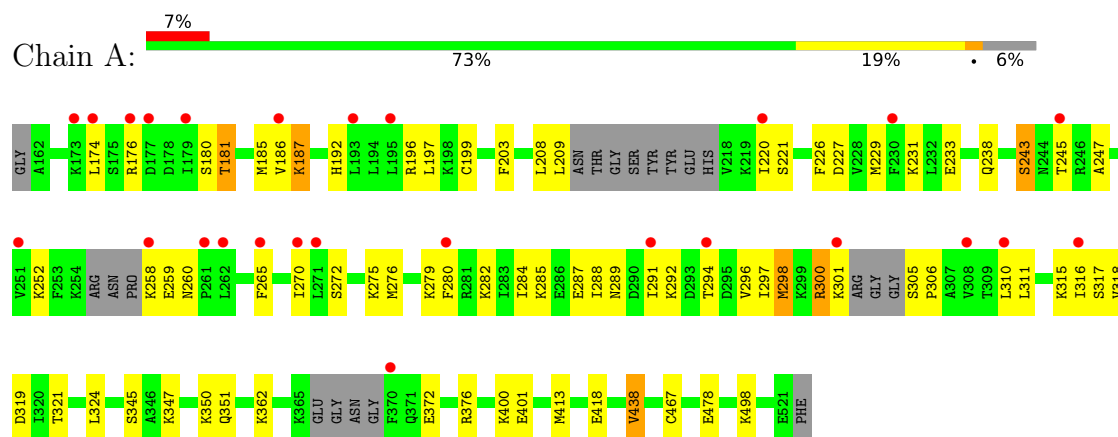
- Molecule 3 is water.

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

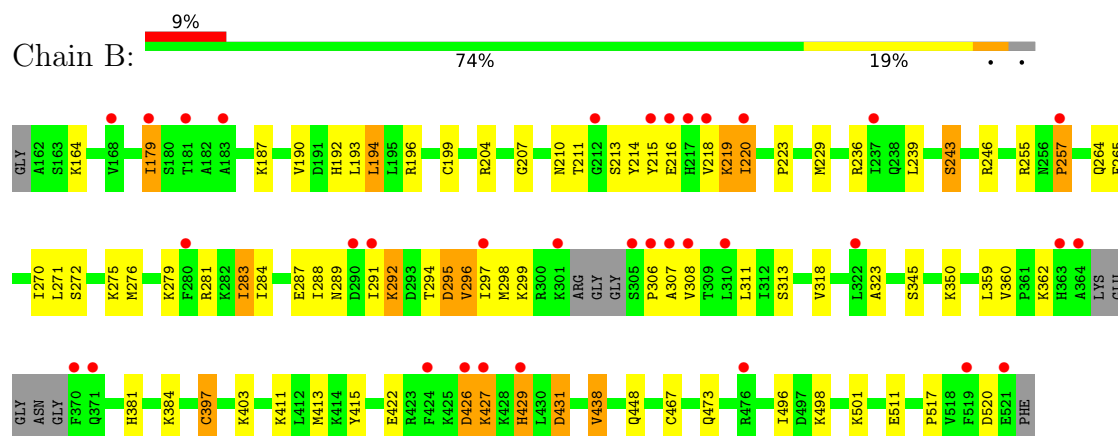
3 Residue-property plots [i](#)

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, α , β , γ	50.13Å 120.41Å 127.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.21 – 2.12 60.21 – 2.12	Depositor EDS
% Data completeness (in resolution range)	90.0 (60.21-2.12) 87.3 (60.21-2.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.12rc1_2801	Depositor
R, R_{free}	0.212 , 0.278 0.220 , 0.286	Depositor DCC
R_{free} test set	1880 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5801	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.38	0/2911	0.58	0/3896
1	B	0.34	1/3002 (0.0%)	0.53	0/4025
All	All	0.36	1/5913 (0.0%)	0.55	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	5.08	1.98	1.81

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	37	0
1	B	2932	0	2981	41	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	78	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 7.

All (78) 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: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:A:221:SER:OG	1:A:418:GLU:OE1	2.18	0.61
1:B:243:SER:O	1:B:243:SER:OG	2.19	0.60
1:A:196:ARG:HG2	1:A:287:GLU:CD	2.26	0.60
1:B:255:ARG:C	1:B:257:PRO:HD2	2.29	0.57
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:209:LEU:HD23	1:A:229:MET:HE2	1.89	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: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:A:258:LYS:HG2	1:A:259:GLU:H	1.75	0.52
1:A:285:LYS:HB2	1:A:298:MET:HE2	1.90	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:B:413[B]:MET:HE2	1:B:438:VAL:HG22	1.94	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:B:496:ILE:O	1:B:501:LYS:NZ	2.45	0.48
1:A:413[A]:MET:HE3	1:A:438:VAL:HG22	1.97	0.47
1:A:245:THR:O	1:A:247:ALA:N	2.48	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:362:LYS:HZ2	1:A:376:ARG:NH1	2.15	0.45
1:A:362:LYS:HZ1	1:A:376:ARG:HD3	1.81	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:229:MET:HE2	1:B:229:MET:HB3	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:276:MET:HE3	1:B:276:MET:HB2	1.90	0.41
1:B:413[A]:MET:HE3	1:B:438:VAL:HG22	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:B:265:PHE:CD2	1:B:276:MET:HE2	2.56	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 ⓘ

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	336/362 (93%)	317 (94%)	17 (5%)	2 (1%)	21	18
1	B	350/362 (97%)	326 (93%)	20 (6%)	4 (1%)	11	7
All	All	686/724 (95%)	643 (94%)	37 (5%)	6 (1%)	14	10

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 ⓘ

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%)	300 (93%)	24 (7%)	13	10
1	B	333/334 (100%)	301 (90%)	32 (10%)	8	5
All	All	657/668 (98%)	601 (92%)	56 (8%)	10	7

All (56) 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	220	ILE
1	A	227	ASP
1	A	233	GLU
1	A	243	SER
1	A	270	ILE
1	A	282	LYS
1	A	288	ILE
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	372	GLU
1	A	438	VAL
1	B	179	ILE
1	B	187	LYS
1	B	190	VAL

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Mol	Chain	Res	Type
1	B	194	LEU
1	B	204	ARG
1	B	210	ASN
1	B	213	SER
1	B	220	ILE
1	B	243	SER
1	B	246	ARG
1	B	264	GLN
1	B	270	ILE
1	B	279	LYS
1	B	283	ILE
1	B	292	LYS
1	B	294	THR
1	B	295	ASP
1	B	296	VAL
1	B	297	ILE
1	B	298	MET
1	B	299	LYS
1	B	318	VAL
1	B	350	LYS
1	B	422	GLU
1	B	426	ASP
1	B	427	LYS
1	B	429	HIS
1	B	431	ASP
1	B	438	VAL
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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	514	ASN
1	B	224	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	342/362 (94%)	0.54	26 (7%)	20 21	26, 69, 137, 168	4 (1%)
1	B	352/362 (97%)	0.66	34 (9%)	13 14	33, 77, 132, 181	4 (1%)
All	All	694/724 (95%)	0.60	60 (8%)	16 17	26, 75, 136, 181	8 (1%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	ALA	4.1
1	A	174	LEU	3.9
1	A	370	PHE	3.9
1	B	217	HIS	3.7
1	A	294	THR	3.7
1	A	179	ILE	3.6
1	B	364	ALA	3.6
1	B	212	GLY	3.5
1	B	218	VAL	3.5
1	B	363	HIS	3.4
1	B	306	PRO	3.3
1	A	280	PHE	3.3
1	B	301	LYS	3.2
1	A	220	ILE	3.1
1	A	271	LEU	3.1
1	A	270	ILE	3.0
1	B	519	PHE	3.0
1	A	291	ILE	2.9
1	B	220	ILE	2.8
1	A	301	LYS	2.8
1	A	316	ILE	2.8
1	B	183	ALA	2.8
1	A	258	LYS	2.7
1	B	215	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	177	ASP	2.6
1	B	290	ASP	2.6
1	A	265	PHE	2.6
1	B	179	ILE	2.6
1	B	297	ILE	2.6
1	B	291	ILE	2.5
1	A	173	LYS	2.5
1	B	322	LEU	2.5
1	B	429	HIS	2.5
1	B	216	GLU	2.4
1	A	195	LEU	2.4
1	A	193	LEU	2.4
1	B	426	ASP	2.4
1	A	176	ARG	2.3
1	A	251	VAL	2.3
1	B	257	PRO	2.3
1	A	308	VAL	2.2
1	A	262	LEU	2.2
1	B	310	LEU	2.2
1	B	521	GLU	2.2
1	A	245	THR	2.2
1	A	261	PRO	2.2
1	B	476	ARG	2.2
1	A	230[A]	PHE	2.2
1	B	424	PHE	2.1
1	B	168	VAL	2.1
1	B	305	SER	2.1
1	B	181	THR	2.1
1	B	237	ILE	2.1
1	A	310	LEU	2.1
1	B	308	VAL	2.1
1	B	371	GLN	2.0
1	B	427	LYS	2.0
1	A	186	VAL	2.0
1	B	280	PHE	2.0
1	B	370	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	600	1/1	0.99	0.05	53,53,53,53	0
2	ZN	B	600	1/1	0.99	0.02	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.