



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 4K8V / pdb_00004k8v
Title : Structure of cyclic GMP-AMP Synthase (cGAS)
Authors : Gao, P.; Wu, Y.; Patel, D.J.
Deposited on : 2013-04-18
Resolution : 2.00 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

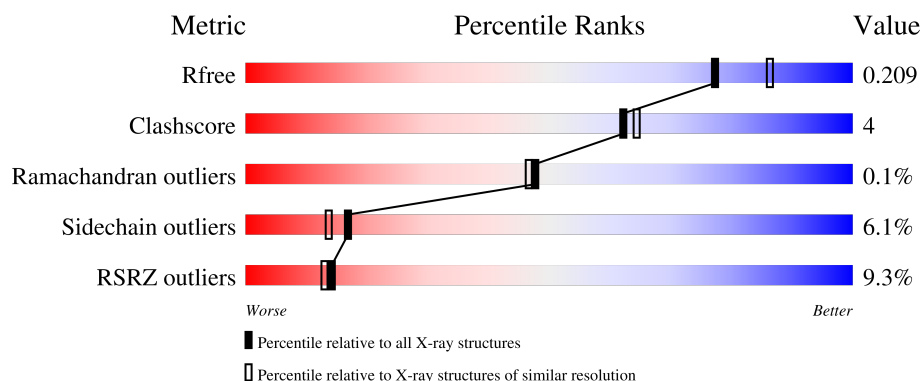
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	3% 90% 9% .
1	B	362	6% 85% 13% .
1	C	362	% 90% 8% .
1	D	362	27% 78% 19% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13318 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	C	362	Total	C	N	O	S	0	0	0
			2989	1922	509	545	13			
1	A	362	Total	C	N	O	S	0	0	0
			2990	1922	509	546	13			
1	B	362	Total	C	N	O	S	0	0	0
			2989	1922	509	545	13			
1	D	362	Total	C	N	O	S	0	0	0
			2989	1922	509	545	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	146	SER	-	expression tag	UNP Q8C6L5
A	146	SER	-	expression tag	UNP Q8C6L5
B	146	SER	-	expression tag	UNP Q8C6L5
D	146	SER	-	expression tag	UNP Q8C6L5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

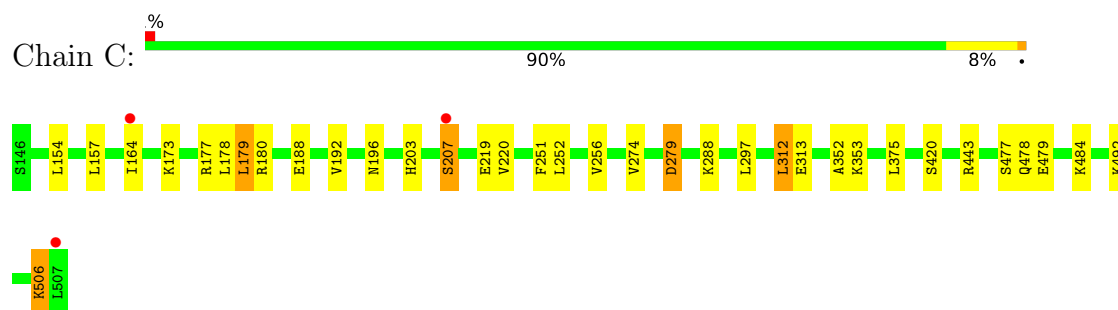
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	481	Total 481	O 481	0	0
3	A	406	Total 406	O 406	0	0
3	B	275	Total 275	O 275	0	0
3	D	195	Total 195	O 195	0	0

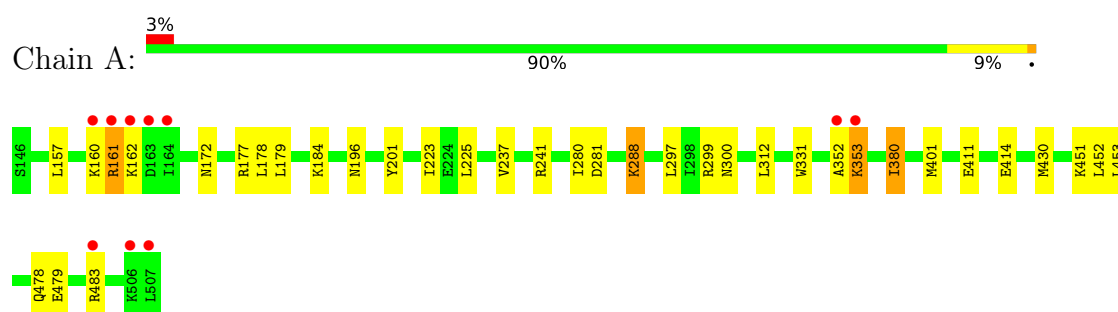
3 Residue-property plots [i](#)

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.

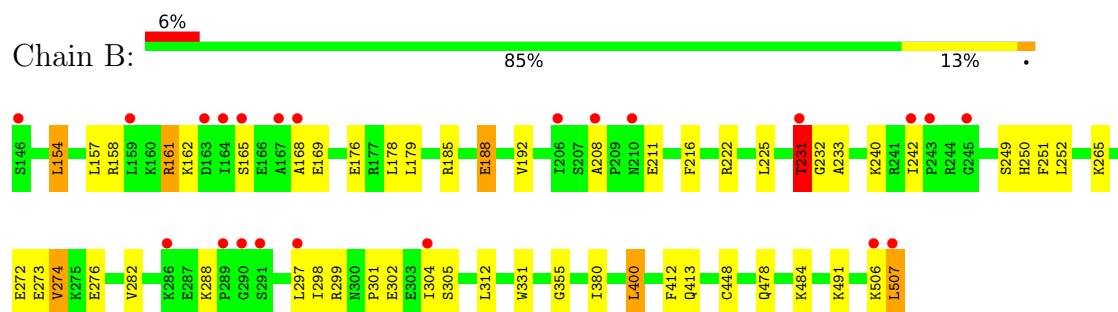
- Molecule 1: Cyclic GMP-AMP synthase



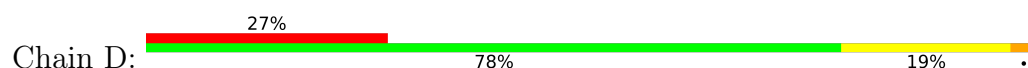
- Molecule 1: Cyclic GMP-AMP synthase

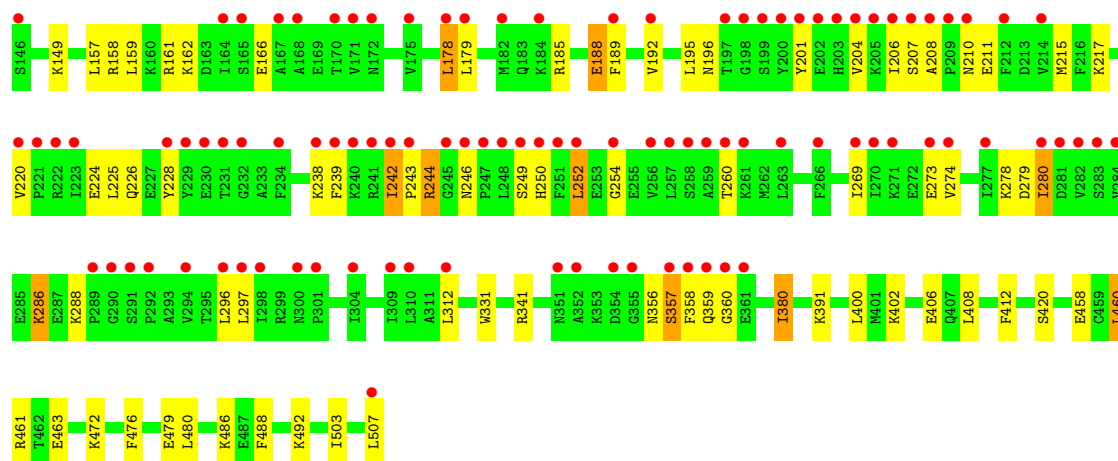


- Molecule 1: Cyclic GMP-AMP synthase



- Molecule 1: Cyclic GMP-AMP synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.56Å 84.15Å 124.72Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	44.07 – 2.00 44.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (44.07-2.00) 98.1 (44.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.175 , 0.208 0.176 , 0.209	Depositor DCC
R_{free} test set	5939 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l 0.007 for -k,-h,-l 0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13318	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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	0.57	0/3055	0.80	2/4102 (0.0%)
1	B	0.53	0/3054	0.79	2/4100 (0.0%)
1	C	0.63	0/3054	0.81	3/4100 (0.1%)
1	D	0.49	0/3054	0.85	4/4100 (0.1%)
All	All	0.56	0/12217	0.81	11/16402 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	220	VAL	CA-C-N	8.42	128.43	119.76
1	D	220	VAL	C-N-CA	8.42	128.43	119.76
1	D	357	SER	N-CA-C	8.21	121.39	108.67
1	C	352	ALA	CA-C-N	-6.31	114.33	122.79
1	C	352	ALA	C-N-CA	-6.31	114.33	122.79
1	D	239	PHE	N-CA-C	5.66	118.71	108.69
1	C	352	ALA	N-CA-C	-5.17	102.87	110.52
1	B	231	THR	N-CA-C	5.14	115.96	108.14
1	A	288	LYS	CA-C-N	5.04	125.33	119.93
1	A	288	LYS	C-N-CA	5.04	125.33	119.93
1	B	412	PHE	N-CA-C	5.03	116.60	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2990	0	3038	17	0
1	B	2989	0	3038	28	0
1	C	2989	0	3038	17	0
1	D	2989	0	3038	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	406	0	0	5	0
3	B	275	0	0	4	0
3	C	481	0	0	6	0
3	D	195	0	0	0	0
All	All	13318	0	12152	99	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 (99) 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:448:CYS:SG	3:B:865:HOH:O	2.34	0.85
1:B:231:THR:HG23	3:B:721:HOH:O	1.85	0.75
1:D:185:ARG:NH1	1:D:273:GLU:OE2	2.22	0.72
1:C:506:LYS:HZ2	1:C:506:LYS:HB2	1.54	0.70
1:D:201:TYR:O	1:D:402:LYS:NZ	2.26	0.67
1:D:206:ILE:HG23	1:D:406:GLU:HG3	1.79	0.65
1:D:188:GLU:H	1:D:188:GLU:CD	2.09	0.60
1:D:356:ASN:C	1:D:359:GLN:HG2	2.26	0.60
1:A:331:TRP:O	1:A:380:ILE:HD13	2.02	0.59
1:B:231:THR:OG1	1:B:233:ALA:N	2.35	0.58
1:A:479:GLU:HG3	3:A:886:HOH:O	2.03	0.57
1:D:463:GLU:HG2	1:D:486:LYS:HE3	1.84	0.57
1:D:458:GLU:OE2	1:D:461:ARG:NH2	2.35	0.57
1:D:158:ARG:O	1:D:161:ARG:HG2	2.04	0.57
1:B:506:LYS:HG2	1:B:507:LEU:N	2.20	0.57
1:C:188:GLU:H	1:C:188:GLU:CD	2.13	0.56
1:D:488:PHE:CZ	1:D:492:LYS:HE2	2.40	0.56
1:A:161:ARG:HG3	1:A:162:LYS:N	2.20	0.56
1:A:281:ASP:HB3	1:A:299:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ALA:HB3	1:D:211:GLU:HG3	1.88	0.55
1:C:279:ASP:OD1	1:C:279:ASP:N	2.32	0.54
1:B:188:GLU:H	1:B:188:GLU:CD	2.16	0.53
1:B:165:SER:HA	1:B:168:ALA:HB3	1.91	0.53
1:C:203:HIS:ND1	1:C:375:LEU:HD12	2.23	0.52
1:B:185:ARG:NH1	1:B:272:GLU:OE1	2.41	0.52
1:D:260:THR:OG1	1:D:360:GLY:HA3	2.09	0.52
1:D:207:SER:HB3	1:D:211:GLU:HB2	1.91	0.52
1:D:178:LEU:HD12	1:D:296:LEU:HD11	1.91	0.52
1:D:204:VAL:O	1:D:402:LYS:NZ	2.38	0.52
1:D:412:PHE:CZ	1:D:492:LYS:HE3	2.45	0.52
1:D:286:LYS:HE3	1:D:288:LYS:HG2	1.93	0.51
1:C:188:GLU:HG3	1:C:251:PHE:CE2	2.46	0.50
1:C:196:ASN:HB3	3:C:1101:HOH:O	2.10	0.50
1:D:250:HIS:HD1	1:D:250:HIS:H	1.60	0.50
1:B:273:GLU:CD	3:B:943:HOH:O	2.54	0.50
1:B:154:LEU:HD13	1:B:400:LEU:HD13	1.93	0.50
1:C:220:VAL:HG21	1:C:312:LEU:HG	1.93	0.49
1:B:222:ARG:HE	1:B:242:ILE:HG12	1.78	0.49
1:A:196:ASN:HB3	3:A:1002:HOH:O	2.11	0.48
1:C:256:VAL:HG13	3:C:701:HOH:O	2.13	0.48
1:B:273:GLU:OE1	3:B:943:HOH:O	2.20	0.48
1:D:228:TYR:HE1	1:D:358:PHE:CD2	2.32	0.48
1:D:246:ASN:O	1:D:249:SER:OG	2.20	0.48
1:C:420:SER:HB2	3:C:1031:HOH:O	2.13	0.48
1:B:222:ARG:HH21	1:B:242:ILE:HD13	1.79	0.48
1:D:252:LEU:C	1:D:254:GLY:H	2.22	0.48
1:D:278:LYS:O	1:D:280:ILE:N	2.47	0.48
1:C:492:LYS:NZ	3:C:1000:HOH:O	2.44	0.47
1:C:207:SER:HB2	3:C:1142:HOH:O	2.13	0.47
1:B:231:THR:OG1	1:B:232:GLY:N	2.47	0.47
1:A:411:GLU:O	1:B:355:GLY:HA2	2.15	0.47
1:D:195:LEU:HD23	1:D:215:MET:HE2	1.97	0.46
1:B:491:LYS:HB3	1:B:491:LYS:HE2	1.71	0.46
1:D:460:LEU:HD13	1:D:476:PHE:CE2	2.50	0.46
1:D:341:ARG:HH11	1:D:341:ARG:HB3	1.80	0.46
1:B:188:GLU:CD	1:B:250:HIS:HE2	2.24	0.46
1:D:206:ILE:HG13	1:D:420:SER:HB3	1.97	0.46
1:A:414:GLU:OE1	3:A:938:HOH:O	2.21	0.46
1:B:299:ARG:HA	1:B:302:GLU:O	2.15	0.46
1:D:408:LEU:HD23	1:D:503:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:HD2	1:C:180:ARG:HH21	1.81	0.45
1:A:483:ARG:NE	3:A:1011:HOH:O	2.49	0.45
1:D:149:LYS:HE3	1:D:149:LYS:HB2	1.75	0.45
1:D:244:ARG:H	1:D:244:ARG:HG2	1.43	0.45
1:B:192:VAL:CG2	1:B:216:PHE:HB3	2.46	0.45
1:D:331:TRP:O	1:D:380:ILE:HD13	2.17	0.45
1:A:430:MET:HE2	1:A:452:LEU:HA	1.99	0.45
1:B:299:ARG:HB2	1:B:301:PRO:O	2.17	0.45
1:A:380:ILE:HD12	1:A:380:ILE:O	2.17	0.45
1:D:242:ILE:O	1:D:242:ILE:HG13	2.18	0.44
1:C:443:ARG:HG3	1:A:451:LYS:HE2	1.99	0.44
1:A:157:LEU:HD12	1:A:160:LYS:HD3	2.00	0.44
1:B:158:ARG:O	1:B:161:ARG:HG2	2.17	0.44
1:D:226:GLN:OE1	1:D:238:LYS:NZ	2.41	0.44
1:C:477:SER:OG	1:C:479:GLU:HG2	2.17	0.44
1:A:401:MET:SD	1:A:453:LEU:HD23	2.58	0.44
1:B:507:LEU:H	1:B:507:LEU:HD22	1.82	0.44
1:C:506:LYS:NZ	3:C:968:HOH:O	2.51	0.43
1:B:298:ILE:O	1:B:304:ILE:N	2.51	0.43
1:D:189:PHE:HD2	1:D:269:ILE:HD12	1.83	0.43
1:B:331:TRP:O	1:B:380:ILE:HD13	2.18	0.43
1:D:279:ASP:N	1:D:279:ASP:OD1	2.51	0.43
1:A:352:ALA:O	1:A:353:LYS:C	2.61	0.42
1:D:286:LYS:O	1:D:286:LYS:HG2	2.16	0.42
1:B:222:ARG:HB3	1:B:240:LYS:HB2	2.02	0.42
1:D:162:LYS:O	1:D:166:GLU:HG3	2.19	0.42
1:D:278:LYS:C	1:D:280:ILE:N	2.77	0.42
1:C:179:LEU:HD12	1:C:192:VAL:HG13	2.01	0.42
1:B:274:VAL:HG13	1:B:282:VAL:HB	2.00	0.42
1:B:188:GLU:OE1	1:B:265:LYS:NZ	2.53	0.42
1:C:219:GLU:HA	1:C:313:GLU:HB3	2.01	0.42
1:B:188:GLU:HG3	1:B:251:PHE:CE2	2.55	0.41
1:D:278:LYS:C	1:D:280:ILE:H	2.29	0.41
1:A:483:ARG:CD	3:A:1011:HOH:O	2.69	0.40
1:A:157:LEU:HD21	1:A:201:TYR:CE2	2.56	0.40
1:D:480:LEU:HA	1:D:480:LEU:HD23	1.79	0.40
1:A:223:ILE:HG23	1:A:237:VAL:HG13	2.04	0.40
1:B:208:ALA:HB3	1:B:211:GLU:HG3	2.02	0.40
1:D:242:ILE:HA	1:D:243:PRO:HD3	1.89	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	360/362 (99%)	352 (98%)	6 (2%)	2 (1%)	21	17
1	B	360/362 (99%)	347 (96%)	13 (4%)	0	100	100
1	C	360/362 (99%)	354 (98%)	6 (2%)	0	100	100
1	D	360/362 (99%)	338 (94%)	22 (6%)	0	100	100
All	All	1440/1448 (99%)	1391 (97%)	47 (3%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	ARG
1	A	300	ASN

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	335/335 (100%)	321 (96%)	14 (4%)	26	25
1	B	335/335 (100%)	311 (93%)	24 (7%)	13	10
1	C	335/335 (100%)	318 (95%)	17 (5%)	21	19
1	D	335/335 (100%)	308 (92%)	27 (8%)	11	7
All	All	1340/1340 (100%)	1258 (94%)	82 (6%)	17	14

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	154	LEU
1	C	157	LEU
1	C	164	ILE
1	C	173	LYS
1	C	178	LEU
1	C	179	LEU
1	C	207	SER
1	C	252	LEU
1	C	274	VAL
1	C	279	ASP
1	C	288	LYS
1	C	297	LEU
1	C	312	LEU
1	C	353	LYS
1	C	478	GLN
1	C	484	LYS
1	C	506	LYS
1	A	172	ASN
1	A	177	ARG
1	A	178	LEU
1	A	179	LEU
1	A	184	LYS
1	A	225	LEU
1	A	241	ARG
1	A	280	ILE
1	A	288	LYS
1	A	297	LEU
1	A	312	LEU
1	A	353	LYS
1	A	380	ILE
1	A	478	GLN
1	B	154	LEU
1	B	157	LEU
1	B	161	ARG
1	B	162	LYS
1	B	169	GLU
1	B	176	GLU
1	B	178	LEU
1	B	179	LEU
1	B	188	GLU
1	B	225	LEU
1	B	231	THR
1	B	249	SER

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Mol	Chain	Res	Type
1	B	252	LEU
1	B	274	VAL
1	B	276	GLU
1	B	288	LYS
1	B	297	LEU
1	B	305	SER
1	B	312	LEU
1	B	400	LEU
1	B	413	GLN
1	B	478	GLN
1	B	484	LYS
1	B	507	LEU
1	D	157	LEU
1	D	159	LEU
1	D	178	LEU
1	D	179	LEU
1	D	188	GLU
1	D	192	VAL
1	D	196	ASN
1	D	210	ASN
1	D	217	LYS
1	D	224	GLU
1	D	225	LEU
1	D	242	ILE
1	D	244	ARG
1	D	252	LEU
1	D	274	VAL
1	D	280	ILE
1	D	286	LYS
1	D	297	LEU
1	D	312	LEU
1	D	357	SER
1	D	380	ILE
1	D	391	LYS
1	D	400	LEU
1	D	460	LEU
1	D	472	LYS
1	D	479	GLU
1	D	507	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	407	GLN
1	B	210	ASN
1	B	226	GLN
1	B	300	ASN
1	D	210	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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	362/362 (100%)	-0.42	10 (2%) 55 54	8, 21, 46, 83	0
1	B	362/362 (100%)	0.01	22 (6%) 27 26	12, 28, 73, 106	0
1	C	362/362 (100%)	-0.51	3 (0%) 82 82	10, 20, 42, 70	0
1	D	362/362 (100%)	0.99	99 (27%) 1 1	13, 45, 115, 159	0
All	All	1448/1448 (100%)	0.02	134 (9%) 14 13	8, 24, 92, 159	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	358	PHE	6.2
1	D	282	VAL	6.1
1	A	507	LEU	6.0
1	D	206	ILE	6.0
1	D	284	VAL	5.9
1	D	204	VAL	5.5
1	C	507	LEU	5.2
1	D	239	PHE	5.0
1	D	229	TYR	4.9
1	B	289	PRO	4.9
1	D	242	ILE	4.7
1	D	209	PRO	4.7
1	B	507	LEU	4.6
1	D	248	LEU	4.4
1	D	201	TYR	4.3
1	A	164	ILE	4.3
1	D	357	SER	4.3
1	D	247	PRO	4.2
1	D	240	LYS	4.2
1	D	280	ILE	4.2
1	D	257	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	203	HIS	4.0
1	D	243	PRO	4.0
1	D	360	GLY	3.9
1	D	270	ILE	3.9
1	D	208	ALA	3.9
1	D	241	ARG	3.9
1	D	274	VAL	3.8
1	D	198	GLY	3.8
1	D	228	TYR	3.8
1	B	242	ILE	3.7
1	D	231	THR	3.7
1	D	297	LEU	3.6
1	B	164	ILE	3.6
1	D	200	TYR	3.6
1	D	301	PRO	3.6
1	D	146	SER	3.6
1	D	250	HIS	3.5
1	D	251	PHE	3.5
1	D	298	ILE	3.4
1	D	304	ILE	3.4
1	D	296	LEU	3.4
1	D	164	ILE	3.3
1	D	352	ALA	3.3
1	D	256	VAL	3.2
1	D	269	ILE	3.2
1	D	310	LEU	3.2
1	B	146	SER	3.2
1	D	273	GLU	3.2
1	D	290	GLY	3.2
1	D	182	MET	3.2
1	D	202	GLU	3.1
1	D	234	PHE	3.1
1	D	254	GLY	3.1
1	D	292	PRO	3.0
1	D	355	GLY	3.0
1	D	266	PHE	3.0
1	D	260	THR	3.0
1	D	222	ARG	2.9
1	D	261	LYS	2.9
1	D	221	PRO	2.9
1	D	199	SER	2.9
1	B	208	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	167	ALA	2.9
1	D	507	LEU	2.9
1	B	167	ALA	2.9
1	D	351	ASN	2.8
1	B	243	PRO	2.8
1	D	175	VAL	2.8
1	D	283	SER	2.7
1	C	164	ILE	2.7
1	D	309	ILE	2.7
1	D	354	ASP	2.7
1	B	206	ILE	2.6
1	D	220	VAL	2.6
1	D	361	GLU	2.6
1	D	168	ALA	2.6
1	D	205	LYS	2.6
1	B	165	SER	2.6
1	D	277	ILE	2.6
1	D	300	ASN	2.6
1	B	506	LYS	2.5
1	D	291	SER	2.5
1	D	312	LEU	2.5
1	A	160	LYS	2.5
1	D	263	LEU	2.5
1	D	294	VAL	2.5
1	B	231	THR	2.5
1	D	178	LEU	2.5
1	B	163	ASP	2.4
1	A	161	ARG	2.4
1	D	189	PHE	2.4
1	B	210	ASN	2.4
1	D	246	ASN	2.4
1	D	289	PRO	2.4
1	B	159	LEU	2.4
1	D	281	ASP	2.4
1	D	171	VAL	2.4
1	B	297	LEU	2.4
1	D	252	LEU	2.4
1	D	172	ASN	2.4
1	D	223	ILE	2.4
1	D	207	SER	2.4
1	D	230	GLU	2.3
1	D	210	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	359	GLN	2.3
1	D	179	LEU	2.3
1	D	212	PHE	2.3
1	D	197	THR	2.3
1	A	162	LYS	2.3
1	D	271	LYS	2.3
1	A	352	ALA	2.2
1	B	304	ILE	2.2
1	D	238	LYS	2.2
1	D	259	ALA	2.2
1	C	207	SER	2.2
1	A	483	ARG	2.2
1	A	163	ASP	2.2
1	B	286	LYS	2.2
1	D	192	VAL	2.1
1	B	245	GLY	2.1
1	B	291	SER	2.1
1	D	165	SER	2.1
1	D	245	GLY	2.1
1	A	353	LYS	2.1
1	D	249	SER	2.1
1	D	258	SER	2.1
1	D	170	THR	2.1
1	D	184	LYS	2.1
1	D	214	VAL	2.1
1	B	168	ALA	2.1
1	D	232	GLY	2.0
1	A	506	LYS	2.0
1	B	290	GLY	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 ⓘ

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	B	601	1/1	0.99	0.01	15,15,15,15	0
2	ZN	A	601	1/1	1.00	0.01	11,11,11,11	0
2	ZN	C	601	1/1	1.00	0.01	13,13,13,13	0
2	ZN	D	601	1/1	1.00	0.01	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.