WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2022 – 01:09 pm BST

|		
PDB ID	:	6ZSV
Title	:	Structure of crocagin biosynthetic protein CgnB
Authors	:	Koehnke, J.; Adam, S.
Deposited on	:	2020-07-16
Resolution	:	2.30 Å(reported)

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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	Percentile Ranks	Value
Rfree		0.305
Clashscore		9
Ramachandran outliers		0.2%
Sidechain outliers		0
RSRZ outliers		47.9%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
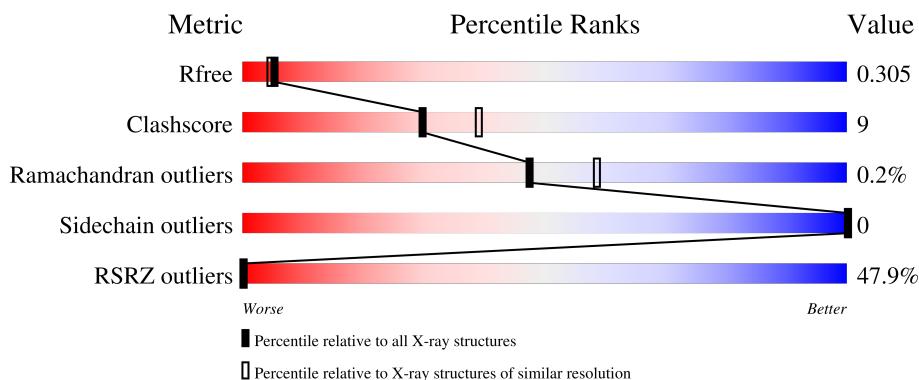
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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 <=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	317	44% / 78% 17% •
1	B	317	49% / 81% 17% •
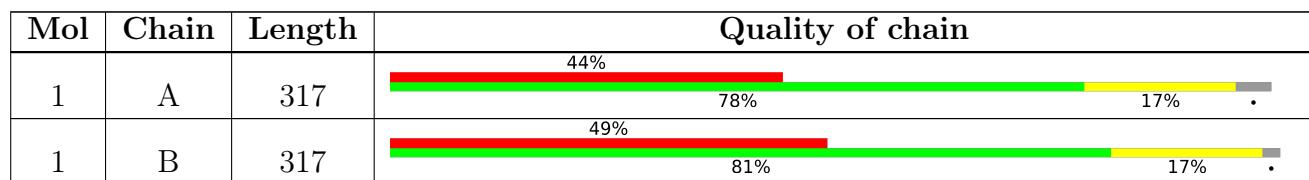
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9608 atoms, of which 4709 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total	C	H	N	O	S	0	0	0
			4734	1505	2336	405	469	19			
1	B	310	Total	C	H	N	O	S	0	0	0
			4809	1528	2373	411	477	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A0K1EBZ5
A	-6	ALA	-	expression tag	UNP A0A0K1EBZ5
A	-5	MET	-	expression tag	UNP A0A0K1EBZ5
A	-4	ALA	-	expression tag	UNP A0A0K1EBZ5
A	-3	ASP	-	expression tag	UNP A0A0K1EBZ5
A	-2	ILE	-	expression tag	UNP A0A0K1EBZ5
A	-1	GLY	-	expression tag	UNP A0A0K1EBZ5
A	0	SER	-	expression tag	UNP A0A0K1EBZ5
B	-7	GLY	-	expression tag	UNP A0A0K1EBZ5
B	-6	ALA	-	expression tag	UNP A0A0K1EBZ5
B	-5	MET	-	expression tag	UNP A0A0K1EBZ5
B	-4	ALA	-	expression tag	UNP A0A0K1EBZ5
B	-3	ASP	-	expression tag	UNP A0A0K1EBZ5
B	-2	ILE	-	expression tag	UNP A0A0K1EBZ5
B	-1	GLY	-	expression tag	UNP A0A0K1EBZ5
B	0	SER	-	expression tag	UNP A0A0K1EBZ5

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

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

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- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total 26	O 26	0	0
3	B	35	Total 35	O 35	0	0

3 Residue-property plots ⓘ

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: Uncharacterized protein
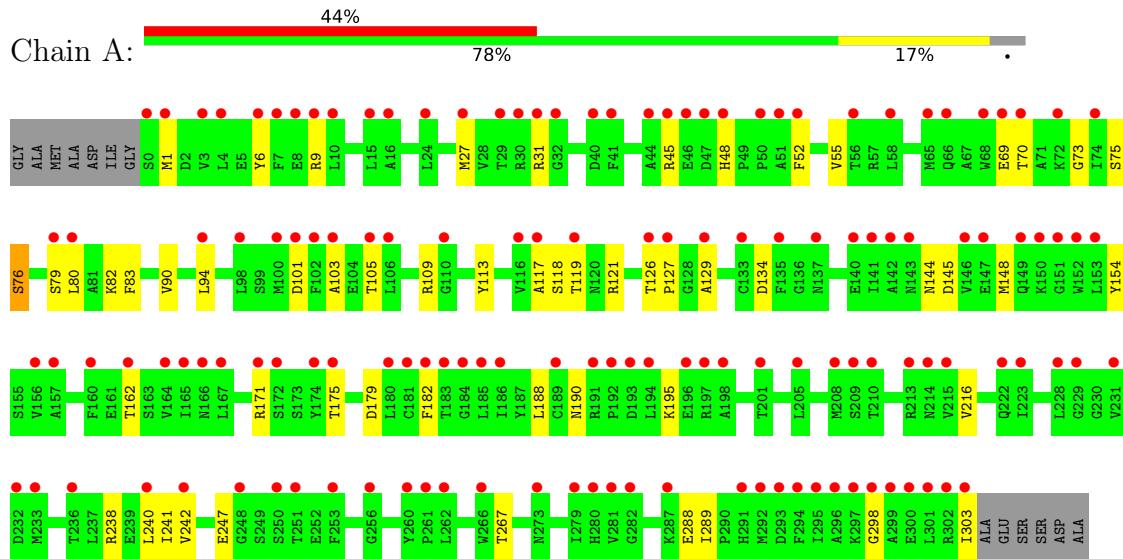
- Molecule 1: Uncharacterized protein
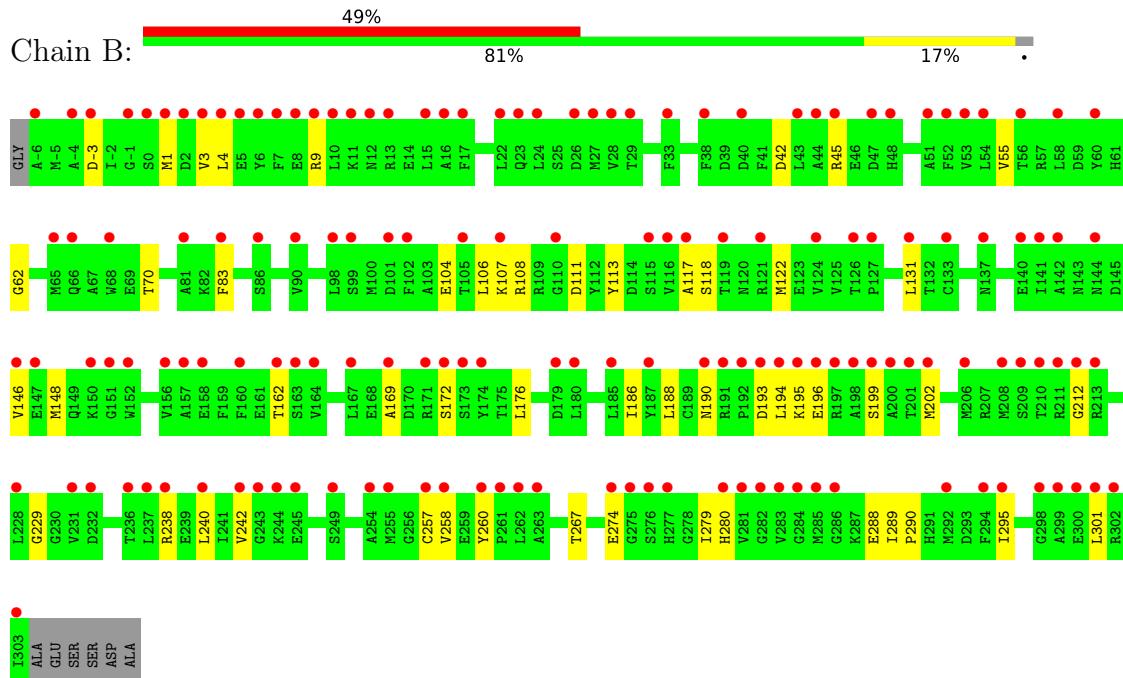
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.45Å 67.50Å 86.15Å 90.00° 95.99° 90.00°	Depositor
Resolution (Å)	36.17 – 2.30 36.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (36.17-2.30) 95.5 (36.17-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.283 , 0.305 0.284 , 0.305	Depositor DCC
R_{free} test set	1339 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.789	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9608	wwPDB-VP
Average B, all atoms (Å^2)	67.0	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 53.10 % 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 4.4252e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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	0.28	0/2441	0.46	0/3296
1	B	0.29	0/2479	0.46	0/3347
All	All	0.28	0/4920	0.46	0/6643

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	76	SER	Mainchain

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	2398	2336	2338	46	1
1	B	2436	2373	2375	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	26	0	0	14	0
3	B	35	0	0	9	1
All	All	4899	4709	4713	90	1

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 9.

All (90) 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:45:ARG:O	1:A:48:HIS:ND1	1.84	1.11
1:B:257:CYS:SG	3:B:504:HOH:O	2.25	0.94
1:A:101:ASP:OD1	3:A:501:HOH:O	1.88	0.91
1:B:122:MET:SD	3:B:533:HOH:O	2.29	0.91
1:A:121:ARG:NE	1:A:134:ASP:OD1	2.07	0.87
1:A:288:GLU:O	3:A:502:HOH:O	1.94	0.83
1:A:240:LEU:HD12	1:A:241:ILE:HG23	1.61	0.82
1:B:196:GLU:OE2	3:B:502:HOH:O	2.00	0.80
1:A:75:SER:OG	3:A:503:HOH:O	2.02	0.78
1:B:288:GLU:O	3:B:503:HOH:O	2.04	0.76
1:A:119:THR:HG21	1:A:303:ILE:HD12	1.68	0.74
1:A:27:MET:HE2	1:A:94:LEU:HD12	1.69	0.74
1:A:52:PHE:HA	3:A:507:HOH:O	1.87	0.74
1:A:105:THR:OG1	3:A:504:HOH:O	2.07	0.72
1:A:247:GLU:O	3:A:505:HOH:O	2.07	0.71
1:B:107:LYS:NZ	1:B:111:ASP:OD1	2.23	0.71
1:A:145:ASP:OD2	3:A:506:HOH:O	2.10	0.70
1:B:162:THR:N	3:B:504:HOH:O	2.24	0.69
1:A:6:TYR:OH	3:A:507:HOH:O	2.11	0.69
1:A:103:ALA:N	3:A:501:HOH:O	2.25	0.67
1:B:4:LEU:CD2	1:B:106:LEU:HD12	2.24	0.67
1:B:202:MET:HE1	1:B:240:LEU:HD13	1.78	0.65
1:B:202:MET:HE3	1:B:290:PRO:HG2	1.80	0.64
1:B:195:LYS:O	1:B:199:SER:OG	2.10	0.64
1:A:27:MET:CE	1:A:94:LEU:HD12	2.28	0.64
1:B:193:ASP:OD1	1:B:194:LEU:N	2.32	0.63
1:A:27:MET:HE1	1:A:90:VAL:HG12	1.81	0.62
1:B:62:GLY:HA2	3:B:526:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD23	1:B:106:LEU:HD12	1.82	0.61
1:A:190:ASN:ND2	3:A:509:HOH:O	2.34	0.60
1:A:48:HIS:CE1	1:A:73:GLY:HA3	2.37	0.59
1:B:117:ALA:N	3:B:505:HOH:O	2.34	0.59
1:A:75:SER:N	3:A:503:HOH:O	2.34	0.59
1:A:117:ALA:HB3	3:A:513:HOH:O	2.04	0.57
1:A:27:MET:O	1:A:31:ARG:NH1	2.38	0.57
1:B:42:ASP:OD2	1:B:45:ARG:HG3	2.05	0.56
1:A:182:PHE:CE1	1:A:216:VAL:HG23	2.41	0.56
1:B:186:ILE:HD11	1:B:274:GLU:HB2	1.86	0.56
1:A:240:LEU:HD12	1:A:241:ILE:CG2	2.33	0.56
1:B:131:LEU:HD21	1:B:176:LEU:HD22	1.87	0.56
1:B:3:VAL:HG23	1:B:146:VAL:O	2.06	0.56
1:A:134:ASP:HB2	1:A:175:THR:HG22	1.89	0.54
1:A:83:PHE:O	1:A:195:LYS:NZ	2.31	0.54
1:B:83:PHE:O	1:B:195:LYS:NZ	2.31	0.54
1:B:238:ARG:O	1:B:242:VAL:HG23	2.08	0.54
1:B:289:ILE:HA	3:B:503:HOH:O	2.07	0.54
1:B:113:TYR:CE1	1:B:162:THR:HG23	2.43	0.53
1:B:83:PHE:CE2	1:B:186:ILE:HD12	2.43	0.53
1:B:3:VAL:HG12	1:B:106:LEU:HD11	1.91	0.53
1:B:83:PHE:HE2	1:B:186:ILE:HD12	1.74	0.52
1:A:69:GLU:N	3:A:510:HOH:O	2.43	0.51
1:A:45:ARG:O	1:A:48:HIS:CE1	2.61	0.50
1:B:3:VAL:HG22	1:B:148:MET:HG3	1.92	0.50
1:A:83:PHE:CZ	1:A:188:LEU:HD12	2.49	0.48
1:A:126:THR:HB	1:A:127:PRO:HD2	1.96	0.48
1:A:76:SER:HA	1:A:154:TYR:O	2.14	0.47
1:B:258:VAL:HG11	1:B:260:TYR:CE1	2.49	0.47
1:A:1:MET:O	1:A:148:MET:N	2.43	0.47
1:B:188:LEU:HD21	1:B:190:ASN:OD1	2.13	0.47
1:A:267:THR:O	1:A:267:THR:HG22	2.15	0.47
1:B:70:THR:HG22	1:B:70:THR:O	2.14	0.47
1:B:4:LEU:HD21	1:B:106:LEU:HD12	1.98	0.46
1:A:113:TYR:CE1	1:A:162:THR:HG23	2.51	0.45
1:B:212:GLY:H	1:B:229:GLY:HA2	1.81	0.45
1:B:267:THR:HG22	1:B:267:THR:O	2.16	0.45
1:A:171:ARG:HD3	1:A:175:THR:OG1	2.17	0.45
1:B:3:VAL:CG1	1:B:106:LEU:HD11	2.47	0.44
1:A:55:VAL:CG2	1:A:79:SER:HA	2.48	0.44
1:A:80:LEU:HD23	1:A:90:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HB1	1:A:179:ASP:HB2	2.01	0.43
1:A:241:ILE:HG22	1:A:289:ILE:HG21	2.00	0.43
1:A:188:LEU:HD21	1:A:190:ASN:OD1	2.18	0.43
1:A:238:ARG:O	1:A:242:VAL:HG23	2.18	0.43
1:B:118:SER:N	3:B:505:HOH:O	2.28	0.43
1:A:126:THR:HB	1:A:127:PRO:CD	2.50	0.42
1:A:82:LYS:HD2	1:A:190:ASN:OD1	2.19	0.42
1:A:70:THR:O	1:A:70:THR:HG22	2.20	0.42
1:B:202:MET:CE	1:B:290:PRO:HG2	2.50	0.42
1:B:113:TYR:CZ	1:B:162:THR:HG23	2.55	0.42
1:A:109:ARG:NH1	1:A:144:ASN:HA	2.34	0.41
1:B:169:ALA:N	1:B:172:SER:OG	2.53	0.41
1:B:258:VAL:HG11	1:B:260:TYR:CZ	2.55	0.41
1:B:279:ILE:HD11	1:B:301:LEU:HG	2.03	0.41
1:B:1:MET:HE2	1:B:9:ARG:HD2	2.03	0.41
1:A:1:MET:HE3	1:A:9:ARG:CD	2.51	0.41
1:A:118:SER:N	3:A:513:HOH:O	2.52	0.41
1:B:42:ASP:HB3	1:B:45:ARG:HD3	2.02	0.41
1:B:280:HIS:HB3	1:B:295:ILE:HA	2.02	0.41
1:B:55:VAL:HG23	1:B:55:VAL:O	2.21	0.40
1:B:104:GLU:OE2	1:B:108:ARG:NH2	2.48	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLY:O	3:B:502:HOH:O[1_565]	2.15	0.05

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	302/317 (95%)	291 (96%)	11 (4%)	0	100	100
1	B	308/317 (97%)	298 (97%)	9 (3%)	1 (0%)	41	50
All	All	610/634 (96%)	589 (97%)	20 (3%)	1 (0%)	47	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-3	ASP

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	264/271 (97%)	264 (100%)	0	100	100
1	B	267/271 (98%)	267 (100%)	0	100	100
All	All	531/542 (98%)	531 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	149	GLN

5.3.3   RNA   ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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 ⓘ

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	304/317 (95%)	2.23	140 (46%)	0	0	32, 58, 86, 129	0
1	B	310/317 (97%)	2.15	154 (49%)	0	0	30, 57, 91, 128	0
All	All	614/634 (96%)	2.19	294 (47%)	0	0	30, 58, 90, 129	0

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	LYS	10.1
1	A	68	TRP	8.3
1	B	141	ILE	7.8
1	B	275	GLY	7.5
1	B	299	ALA	7.4
1	A	143	ASN	7.0
1	B	137	ASN	6.9
1	B	243	GLY	6.9
1	A	48	HIS	6.7
1	A	292	MET	6.3
1	A	116	VAL	6.2
1	A	157	ALA	6.1
1	B	38	PHE	6.0
1	A	47	ASP	5.9
1	A	105	THR	5.8
1	B	198	ALA	5.6
1	B	58	LEU	5.5
1	B	298	GLY	5.5
1	B	262	LEU	5.4
1	A	279	ILE	5.4
1	B	171	ARG	5.4
1	A	58	LEU	5.3
1	B	300	GLU	5.3
1	B	303	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	0	SER	5.2
1	A	10	LEU	5.1
1	A	233	MET	5.1
1	A	193	ASP	5.0
1	A	152	TRP	4.9
1	A	166	ASN	4.9
1	A	191	ARG	4.9
1	A	119	THR	4.8
1	B	162	THR	4.8
1	B	33	PHE	4.7
1	A	210	THR	4.7
1	B	163	SER	4.7
1	A	127	PRO	4.6
1	A	29	THR	4.6
1	B	167	LEU	4.6
1	A	103	ALA	4.5
1	A	15	LEU	4.5
1	B	11	LYS	4.5
1	A	151	GLY	4.5
1	A	9	ARG	4.5
1	A	147	GLU	4.4
1	A	298	GLY	4.3
1	A	1	MET	4.3
1	B	194	LEU	4.2
1	A	213	ARG	4.2
1	A	8	GLU	4.2
1	A	110	GLY	4.1
1	A	242	VAL	4.1
1	A	172	SER	4.1
1	A	303	ILE	4.1
1	A	299	ALA	4.0
1	B	51	ALA	4.0
1	A	208	MET	4.0
1	A	142	ALA	4.0
1	A	46	GLU	4.0
1	A	280	HIS	4.0
1	B	24	LEU	4.0
1	A	291	HIS	4.0
1	B	242	VAL	3.9
1	A	117	ALA	3.9
1	B	146	VAL	3.8
1	B	210	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	179	ASP	3.8
1	B	209	SER	3.8
1	A	44	ALA	3.8
1	A	69	GLU	3.8
1	B	164	VAL	3.7
1	B	-3	ASP	3.7
1	A	126	THR	3.7
1	A	240	LEU	3.6
1	B	47	ASP	3.6
1	A	65	MET	3.6
1	B	286	GLY	3.6
1	B	193	ASP	3.6
1	B	4	LEU	3.5
1	B	98	LEU	3.5
1	B	68	TRP	3.5
1	B	22	LEU	3.5
1	A	4	LEU	3.4
1	B	245	GLU	3.4
1	A	70	THR	3.4
1	A	3	VAL	3.4
1	B	16	ALA	3.4
1	B	45	ARG	3.4
1	B	157	ALA	3.4
1	A	228	LEU	3.4
1	A	294	PHE	3.3
1	B	160	PHE	3.3
1	B	56	THR	3.3
1	B	102	PHE	3.3
1	B	236	THR	3.3
1	A	197	ARG	3.3
1	B	295	ILE	3.3
1	B	-1	GLY	3.3
1	A	50	PRO	3.2
1	A	52	PHE	3.2
1	A	32	GLY	3.2
1	B	127	PRO	3.2
1	B	86	SER	3.2
1	A	98	LEU	3.2
1	B	144	ASN	3.2
1	B	172	SER	3.2
1	B	10	LEU	3.2
1	A	223	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	231	VAL	3.2
1	B	121	ARG	3.2
1	A	262	LEU	3.2
1	A	175	THR	3.1
1	B	140	GLU	3.1
1	B	191	ARG	3.1
1	A	94	LEU	3.1
1	A	185	LEU	3.1
1	B	211	ARG	3.1
1	A	196	GLU	3.1
1	B	60	TYR	3.0
1	B	107	LYS	3.0
1	A	167	LEU	3.0
1	B	302	ARG	3.0
1	A	165	ILE	3.0
1	B	277	HIS	3.0
1	B	260	TYR	3.0
1	B	119	THR	3.0
1	A	149	GLN	3.0
1	A	194	LEU	3.0
1	B	124	VAL	3.0
1	B	301	LEU	3.0
1	A	282	GLY	3.0
1	A	180	LEU	2.9
1	A	101	ASP	2.9
1	B	281	VAL	2.9
1	B	238	ARG	2.9
1	B	15	LEU	2.9
1	B	27	MET	2.9
1	A	256	GLY	2.9
1	A	182	PHE	2.9
1	B	116	VAL	2.9
1	B	156	VAL	2.9
1	B	208	MET	2.9
1	B	29	THR	2.9
1	B	1	MET	2.9
1	B	0	SER	2.8
1	B	213	ARG	2.8
1	B	151	GLY	2.8
1	A	102	PHE	2.8
1	A	231	VAL	2.8
1	A	133	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	171	ARG	2.8
1	A	281	VAL	2.8
1	B	200	ALA	2.8
1	A	100	MET	2.8
1	A	174	TYR	2.8
1	A	192	PRO	2.7
1	A	146	VAL	2.7
1	B	115	SER	2.7
1	B	206	MET	2.7
1	A	186	ILE	2.7
1	A	181	CYS	2.7
1	B	258	VAL	2.7
1	B	294	PHE	2.7
1	B	180	LEU	2.7
1	A	24	LEU	2.7
1	A	45	ARG	2.7
1	B	169	ALA	2.7
1	A	160	PHE	2.7
1	B	8	GLU	2.6
1	B	81	ALA	2.6
1	B	285	MET	2.6
1	B	152	TRP	2.6
1	A	296	ALA	2.6
1	A	293	ASP	2.6
1	B	2	ASP	2.6
1	B	23	GLN	2.6
1	B	255	MET	2.6
1	A	302	ARG	2.6
1	B	197	ARG	2.6
1	A	156	VAL	2.6
1	B	173	SER	2.6
1	B	283	VAL	2.6
1	A	31	ARG	2.5
1	B	292	MET	2.5
1	B	101	ASP	2.5
1	B	117	ALA	2.5
1	B	126	THR	2.5
1	A	205	LEU	2.5
1	B	83	PHE	2.5
1	B	99	SER	2.5
1	B	5	GLU	2.5
1	A	248	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	232	ASP	2.5
1	B	284	GLY	2.5
1	A	301	LEU	2.5
1	A	129	ALA	2.4
1	A	189	CYS	2.4
1	A	198	ALA	2.4
1	A	79	SER	2.4
1	A	135	PHE	2.4
1	A	164	VAL	2.4
1	B	280	HIS	2.4
1	A	201	THR	2.4
1	A	236	THR	2.4
1	B	7	PHE	2.4
1	B	90	VAL	2.4
1	B	244	LYS	2.4
1	A	162	THR	2.4
1	A	209	SER	2.4
1	A	30	ARG	2.4
1	A	184	GLY	2.4
1	A	140	GLU	2.4
1	A	215	VAL	2.4
1	A	273	ASN	2.4
1	B	150	LYS	2.3
1	B	276	SER	2.4
1	A	295	ILE	2.3
1	B	6	TYR	2.3
1	B	212	GLY	2.3
1	B	131	LEU	2.3
1	B	192	PRO	2.3
1	B	261	PRO	2.3
1	B	3	VAL	2.3
1	B	249	SER	2.3
1	B	133	CYS	2.3
1	B	282	GLY	2.3
1	A	106	LEU	2.3
1	A	141	ILE	2.3
1	A	261	PRO	2.3
1	A	297	LYS	2.3
1	B	28	VAL	2.3
1	B	44	ALA	2.3
1	A	266	TRP	2.3
1	B	9	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	41	PHE	2.3
1	B	17	PHE	2.3
1	B	254	ALA	2.3
1	B	263	ALA	2.3
1	A	56	THR	2.2
1	A	6	TYR	2.2
1	A	137	ASN	2.2
1	A	214	ASN	2.2
1	A	232	ASP	2.2
1	A	7	PHE	2.2
1	B	199	SER	2.2
1	B	110	GLY	2.2
1	B	48	HIS	2.2
1	B	174	TYR	2.2
1	B	26	ASP	2.2
1	B	66	GLN	2.2
1	A	229	GLY	2.2
1	A	253	PHE	2.2
1	B	12	ASN	2.2
1	B	190	ASN	2.2
1	B	196	GLU	2.2
1	B	147	GLU	2.2
1	A	51	ALA	2.2
1	A	250	SER	2.2
1	A	260	TYR	2.1
1	B	142	ALA	2.1
1	A	300	GLU	2.1
1	B	40	ASP	2.1
1	B	43	LEU	2.1
1	B	54	LEU	2.1
1	A	66	GLN	2.1
1	B	202	MET	2.1
1	B	274	GLU	2.1
1	B	65	MET	2.1
1	B	158	GLU	2.1
1	A	251	THR	2.1
1	B	187	TYR	2.1
1	A	40	ASP	2.1
1	B	195	LYS	2.1
1	A	287	LYS	2.1
1	B	53	VAL	2.1
1	A	74	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	2.1
1	B	237	LEU	2.1
1	A	27	MET	2.1
1	A	72	LYS	2.1
1	A	153	LEU	2.0
1	B	185	LEU	2.0
1	A	183	THR	2.0
1	B	105	THR	2.0
1	B	-4	ALA	2.0
1	B	240	LEU	2.0
1	A	16	ALA	2.0
1	A	222	GLN	2.0
1	B	201	THR	2.0
1	B	-6	ALA	2.0
1	B	52	PHE	2.0
1	B	257	CYS	2.0
1	B	228	LEU	2.0
1	B	13	ARG	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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($Å^2$)	Q<0.9
2	ZN	A	401	1/1	0.79	0.24	29,29,29,29	1
2	ZN	B	402	1/1	0.88	0.33	29,29,29,29	1
2	ZN	B	401	1/1	0.92	0.17	28,28,28,28	1
2	ZN	A	402	1/1	0.93	0.48	43,43,43,43	1

6.5 Other polymers ⓘ

There are no such residues in this entry.