



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 09:57 PM UTC

PDB ID : 9M70 / pdb_00009m70
Title : Crystal Structure of the Carboxyltransferase Subunit of Acetyl-CoA carboxylase from *Chloroflexus aurantiacus*
Authors : Shen, J.J.; Wu, W.P.; Xu, X.L.
Deposited on : 2025-03-08
Resolution : 2.78 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

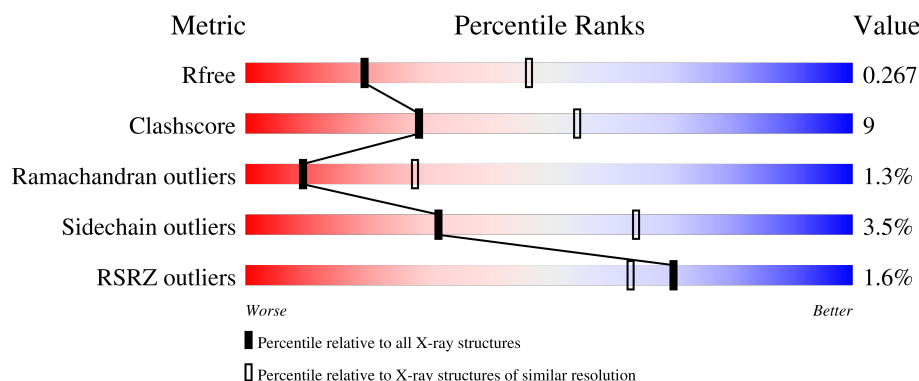
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	303	<div> <div>3%</div> <div>63% 21% 16%</div> </div>
1	C	303	<div> <div>%</div> <div>66% 18% 16%</div> </div>
2	B	273	<div> <div>%</div> <div>74% 20% ..</div> </div>
2	D	273	<div> <div>%</div> <div>68% 27% ..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7957 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 carboxylase carboxyl transferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1935	1213	344	357	21			
1	C	256	Total	C	N	O	S	0	0	0
			1935	1213	344	357	21			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	initiating methionine	UNP A9WBQ9
A	4	GLY	-	expression tag	UNP A9WBQ9
A	5	SER	-	expression tag	UNP A9WBQ9
A	6	SER	-	expression tag	UNP A9WBQ9
A	7	HIS	-	expression tag	UNP A9WBQ9
A	8	HIS	-	expression tag	UNP A9WBQ9
A	9	HIS	-	expression tag	UNP A9WBQ9
A	10	HIS	-	expression tag	UNP A9WBQ9
A	11	HIS	-	expression tag	UNP A9WBQ9
A	12	HIS	-	expression tag	UNP A9WBQ9
A	13	SER	-	expression tag	UNP A9WBQ9
A	14	SER	-	expression tag	UNP A9WBQ9
A	15	GLY	-	expression tag	UNP A9WBQ9
A	16	LEU	-	expression tag	UNP A9WBQ9
A	17	VAL	-	expression tag	UNP A9WBQ9
A	18	PRO	-	expression tag	UNP A9WBQ9
A	19	ARG	-	expression tag	UNP A9WBQ9
A	20	GLY	-	expression tag	UNP A9WBQ9
A	21	SER	-	expression tag	UNP A9WBQ9
A	22	HIS	-	expression tag	UNP A9WBQ9
A	23	MET	-	expression tag	UNP A9WBQ9
C	3	MET	-	initiating methionine	UNP A9WBQ9
C	4	GLY	-	expression tag	UNP A9WBQ9
C	5	SER	-	expression tag	UNP A9WBQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	SER	-	expression tag	UNP A9WBQ9
C	7	HIS	-	expression tag	UNP A9WBQ9
C	8	HIS	-	expression tag	UNP A9WBQ9
C	9	HIS	-	expression tag	UNP A9WBQ9
C	10	HIS	-	expression tag	UNP A9WBQ9
C	11	HIS	-	expression tag	UNP A9WBQ9
C	12	HIS	-	expression tag	UNP A9WBQ9
C	13	SER	-	expression tag	UNP A9WBQ9
C	14	SER	-	expression tag	UNP A9WBQ9
C	15	GLY	-	expression tag	UNP A9WBQ9
C	16	LEU	-	expression tag	UNP A9WBQ9
C	17	VAL	-	expression tag	UNP A9WBQ9
C	18	PRO	-	expression tag	UNP A9WBQ9
C	19	ARG	-	expression tag	UNP A9WBQ9
C	20	GLY	-	expression tag	UNP A9WBQ9
C	21	SER	-	expression tag	UNP A9WBQ9
C	22	HIS	-	expression tag	UNP A9WBQ9
C	23	MET	-	expression tag	UNP A9WBQ9

- Molecule 2 is a protein called Acetyl-coenzyme A carboxylase carboxyl transferase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			2038	1270	379	377	12			
2	D	264	Total	C	N	O	S	0	0	0
			2047	1275	380	380	12			

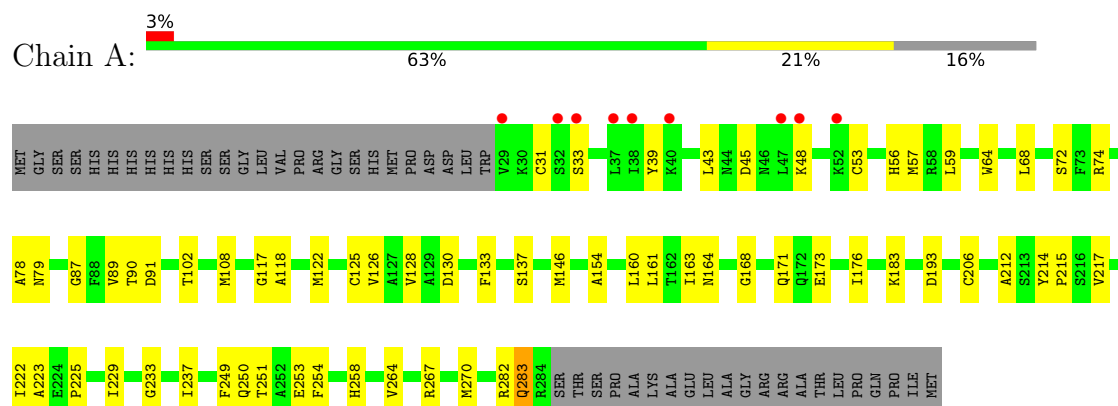
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

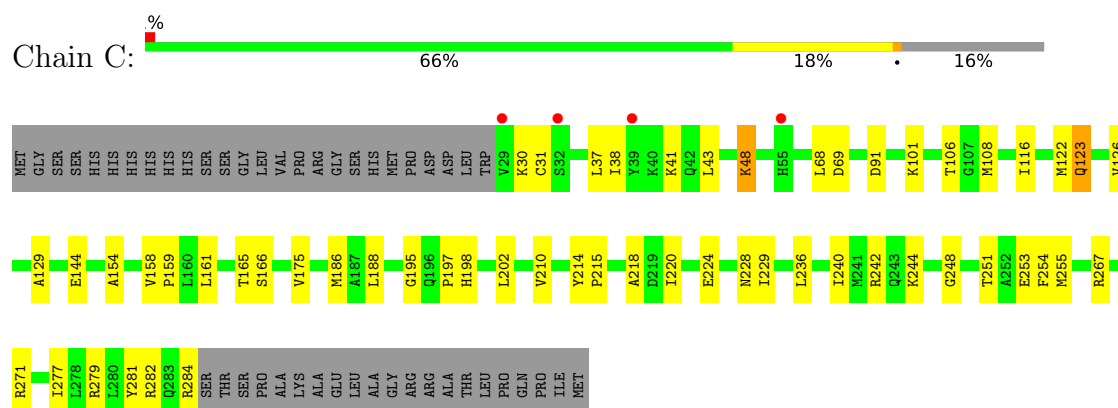
3 Residue-property plots [i](#)

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.

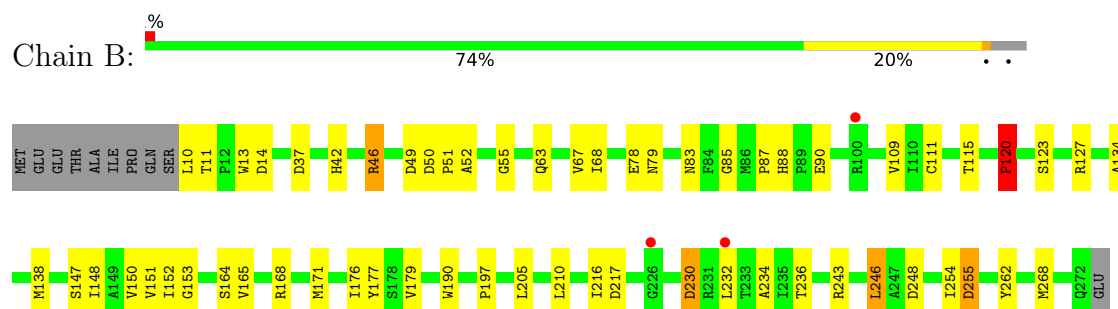
- Molecule 1: Acetyl-coenzyme A carboxylase carboxyl transferase subunit beta



- Molecule 1: Acetyl-coenzyme A carboxylase carboxyl transferase subunit beta



- Molecule 2: Acetyl-coenzyme A carboxylase carboxyl transferase subunit alpha



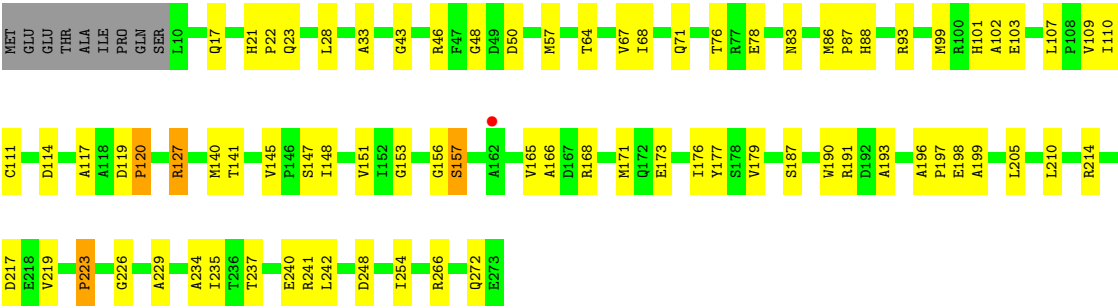
● Molecule 2: Acetyl-coenzyme A carboxylase carboxyl transferase subunit alpha

Chain D:

68%

27%

..



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.21Å 112.51Å 168.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.77 – 2.78 21.77 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.7 (21.77-2.78) 99.7 (21.77-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.79Å)	Xtriage
Refinement program	PHENIX 5.8.0267	Depositor
R, R_{free}	0.222 , 0.277 0.216 , 0.267	Depositor DCC
R_{free} test set	1746 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7957	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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	1.12	0/1964	1.54	7/2646 (0.3%)
1	C	1.12	0/1964	1.51	3/2646 (0.1%)
2	B	1.12	0/2078	1.57	10/2815 (0.4%)
2	D	1.09	0/2087	1.55	5/2827 (0.2%)
All	All	1.11	0/8093	1.54	25/10934 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ALA	CA-C-N	7.17	129.76	120.44
1	A	78	ALA	C-N-CA	7.17	129.76	120.44
2	D	76	THR	CA-C-O	-6.02	114.50	120.82
1	A	253	GLU	CB-CG-CD	5.82	122.49	112.60
2	B	120	PRO	N-CA-CB	-5.60	97.37	103.25
2	D	198	GLU	N-CA-C	-5.50	105.36	111.36
2	B	230	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	253	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	39	TYR	CA-C-N	5.38	127.75	120.38
1	A	39	TYR	C-N-CA	5.38	127.75	120.38
2	B	255	ASP	CA-CB-CG	5.35	117.95	112.60
2	B	234	ALA	CA-C-N	5.34	127.24	120.72
2	B	234	ALA	C-N-CA	5.34	127.24	120.72
1	A	154	ALA	CA-C-N	5.24	127.56	120.65
1	A	154	ALA	C-N-CA	5.24	127.56	120.65
2	D	248	ASP	CA-C-N	5.18	127.23	120.28
2	D	248	ASP	C-N-CA	5.18	127.23	120.28
2	B	78	GLU	CB-CA-C	5.18	118.94	110.96
2	B	262	TYR	N-CA-C	-5.18	105.53	111.07
1	C	154	ALA	CA-C-N	5.11	127.54	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154	ALA	C-N-CA	5.11	127.54	120.29
2	B	248	ASP	CA-C-N	5.09	127.11	120.28
2	B	248	ASP	C-N-CA	5.09	127.11	120.28
2	D	43	GLY	CA-C-O	-5.06	118.19	122.29
2	B	51	PRO	N-CA-CB	-5.01	98.80	103.46

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	1935	0	1968	37	0
1	C	1935	0	1968	34	0
2	B	2038	0	2032	37	0
2	D	2047	0	2038	47	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	7957	0	8006	141	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 9.

All (141) 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:222:ILE:HG21	1:A:270:MET:HE1	1.59	0.85
1:C:186:MET:SD	2:D:141:THR:HB	2.24	0.77
2:D:83:ASN:ND2	2:D:119:ASP:OD2	2.20	0.73
2:D:147:SER:O	2:D:166:ALA:HB1	1.88	0.73
1:C:31:CYS:HB2	1:C:38:ILE:HD13	1.75	0.69
1:A:108:MET:HE1	1:A:130:ASP:OD2	1.92	0.69
2:D:57:MET:HE3	2:D:107:LEU:HD11	1.78	0.65
2:B:50:ASP:OD2	2:B:88:HIS:N	2.30	0.64
2:B:171:MET:HB2	2:B:216:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:TYR:O	1:C:284:ARG:NH1	2.32	0.62
1:A:173:GLU:O	1:A:176:ILE:HB	2.00	0.61
1:A:249:PHE:CE2	1:A:250:GLN:HG3	2.36	0.61
1:C:251:THR:O	1:C:254:PHE:HB3	2.01	0.60
2:D:68:ILE:O	2:D:111:CYS:HA	2.02	0.59
1:A:233:GLY:O	1:A:237:ILE:HG13	2.02	0.59
1:C:240:ILE:HD13	2:D:120:PRO:HG2	1.85	0.59
1:A:72:SER:O	1:A:117:GLY:HA2	2.03	0.58
2:B:168:ARG:HA	2:B:217:ASP:OD2	2.03	0.58
2:B:11:THR:O	2:B:14:ASP:HB2	2.02	0.58
1:C:144:GLU:OE2	2:D:266:ARG:NH2	2.32	0.58
1:A:57:MET:O	1:A:267:ARG:NH2	2.36	0.57
2:D:151:VAL:HB	2:D:171:MET:HG2	1.86	0.57
1:A:128:VAL:HG13	1:A:163:ILE:HB	1.87	0.57
1:A:146:MET:HE3	1:A:214:TYR:OH	2.04	0.56
1:C:214:TYR:CG	1:C:215:PRO:HD3	2.39	0.56
1:A:68:LEU:HD13	1:A:117:GLY:HA3	1.87	0.56
2:D:171:MET:SD	2:D:210:LEU:HD22	2.46	0.56
1:A:217:VAL:HB	2:B:138:MET:HE2	1.87	0.55
1:A:214:TYR:CG	1:A:215:PRO:HD3	2.41	0.55
1:A:90:THR:HA	2:B:190:TRP:CZ2	2.42	0.55
2:D:17:GLN:OE1	2:D:17:GLN:HA	2.07	0.54
2:D:177:TYR:HB3	2:D:210:LEU:HD21	1.88	0.54
1:A:59:LEU:HD12	1:A:64:TRP:CE2	2.43	0.54
2:D:205:LEU:C	2:D:205:LEU:HD12	2.33	0.54
1:A:122:MET:HG2	1:A:282:ARG:HD3	1.90	0.53
1:C:126:VAL:HA	1:C:161:LEU:O	2.08	0.53
2:D:168:ARG:HA	2:D:217:ASP:OD2	2.09	0.53
2:B:55:GLY:HA2	2:B:67:VAL:O	2.09	0.52
2:B:232:LEU:O	2:B:236:THR:HG23	2.09	0.52
2:B:68:ILE:O	2:B:111:CYS:HA	2.09	0.52
2:D:223:PRO:HD2	2:D:234:ALA:HB2	1.92	0.52
1:C:195:GLY:O	1:C:284:ARG:NH2	2.43	0.52
2:D:187:SER:O	2:D:191:ARG:HA	2.10	0.51
2:D:93:ARG:NH2	2:D:127:ARG:O	2.43	0.51
2:B:63:GLN:OE1	2:B:246:LEU:HD21	2.11	0.50
2:D:187:SER:HB2	2:D:193:ALA:HB2	1.92	0.50
1:C:224:GLU:OE2	1:C:267:ARG:NE	2.43	0.50
2:D:67:VAL:C	2:D:68:ILE:HG13	2.37	0.50
2:B:171:MET:HG3	2:B:216:ILE:HD13	1.93	0.50
2:D:223:PRO:CD	2:D:234:ALA:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:HE3	2:B:268:MET:O	2.11	0.49
2:D:147:SER:C	2:D:166:ALA:HB1	2.38	0.49
2:D:190:TRP:CH2	2:D:199:ALA:HA	2.47	0.49
2:B:42:HIS:CD2	2:B:49:ASP:OD2	2.66	0.49
2:B:150:VAL:HG12	2:B:152:ILE:HG23	1.96	0.48
1:C:69:ASP:OD1	1:C:271:ARG:NH2	2.47	0.48
1:A:171:GLN:HA	2:B:179:VAL:HG11	1.96	0.48
2:B:148:ILE:HG23	2:B:168:ARG:HB2	1.96	0.47
1:C:166:SER:CB	1:C:210:VAL:HG21	2.44	0.47
1:A:102:THR:HG22	1:A:133:PHE:CD2	2.50	0.47
2:B:171:MET:CG	2:B:216:ILE:HD13	2.44	0.47
1:C:202:LEU:HD21	1:C:215:PRO:HB2	1.97	0.47
2:D:176:ILE:HA	2:D:205:LEU:O	2.14	0.47
1:A:118:ALA:HA	1:A:122:MET:O	2.14	0.47
2:D:99:MET:HE1	2:D:140:MET:SD	2.54	0.47
1:C:248:GLY:HA2	1:C:251:THR:HG21	1.97	0.46
2:D:226:GLY:O	2:D:229:ALA:HB3	2.15	0.46
1:A:254:PHE:CE2	1:A:258:HIS:CE1	3.04	0.46
2:B:168:ARG:HD3	2:B:217:ASP:CG	2.40	0.46
1:C:122:MET:HE1	1:C:279:ARG:HA	1.97	0.46
2:D:78:GLU:HA	2:D:78:GLU:OE1	2.16	0.46
1:A:33:SER:HB2	1:A:53:CYS:SG	2.55	0.46
2:B:243:ARG:O	2:B:243:ARG:HG2	2.15	0.45
1:C:166:SER:HB2	1:C:210:VAL:HG21	1.99	0.45
2:B:85:GLY:O	2:B:115:THR:OG1	2.33	0.45
1:A:258:HIS:C	2:D:48:GLY:HA2	2.42	0.45
1:A:283:GLN:HB2	2:D:64:THR:OG1	2.16	0.45
2:D:102:ALA:O	2:D:103:GLU:C	2.60	0.45
1:C:214:TYR:CD1	1:C:215:PRO:HD3	2.52	0.45
2:B:151:VAL:HB	2:B:171:MET:HG2	1.99	0.44
2:B:10:LEU:HD22	2:B:14:ASP:HB3	1.98	0.44
2:B:13:TRP:HB2	2:B:197:PRO:HA	1.99	0.44
1:A:90:THR:HA	2:B:190:TRP:CE2	2.53	0.43
2:B:171:MET:HB2	2:B:216:ILE:CD1	2.47	0.43
2:D:237:THR:O	2:D:241:ARG:HG2	2.18	0.43
1:A:59:LEU:HB2	1:A:64:TRP:CD1	2.54	0.43
2:D:28:LEU:HD12	2:D:71:GLN:NE2	2.33	0.43
1:A:43:LEU:HG	1:A:48:LYS:HA	2.00	0.43
1:A:206:CYS:O	1:A:229:ILE:HA	2.18	0.43
2:B:46:ARG:HG2	2:D:46:ARG:HG2	2.01	0.43
2:B:165:VAL:HG12	2:B:165:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LEU:HD11	1:C:240:ILE:HD11	2.00	0.43
2:B:171:MET:CB	2:B:216:ILE:HD13	2.47	0.43
1:C:30:LYS:HG2	1:C:37:LEU:HD23	2.00	0.43
2:D:50:ASP:OD2	2:D:88:HIS:N	2.47	0.43
1:A:125:CYS:O	1:A:160:LEU:HA	2.18	0.43
1:A:137:SER:HA	1:A:168:GLY:O	2.18	0.43
2:B:90:GLU:H	2:B:90:GLU:CD	2.27	0.43
2:D:101:HIS:CD2	2:D:101:HIS:C	2.97	0.43
2:D:148:ILE:HG23	2:D:168:ARG:HB2	2.01	0.43
1:A:223:ALA:O	1:A:264:VAL:HA	2.19	0.43
1:C:122:MET:HE3	1:C:282:ARG:HD2	2.00	0.43
2:D:140:MET:HE1	2:D:165:VAL:H	1.83	0.43
1:A:126:VAL:HA	1:A:161:LEU:O	2.18	0.43
1:A:164:ASN:OD1	1:A:214:TYR:CE2	2.72	0.42
1:A:251:THR:O	1:A:254:PHE:HB3	2.19	0.42
1:C:126:VAL:HG13	1:C:126:VAL:O	2.18	0.42
2:D:109:VAL:O	2:D:147:SER:HA	2.19	0.42
1:C:68:LEU:HD11	1:C:126:VAL:HG11	2.01	0.42
2:D:33:ALA:HB3	2:D:235:ILE:HG21	2.02	0.42
2:D:242:LEU:HD23	2:D:242:LEU:HA	1.88	0.42
1:A:56:HIS:CD2	1:A:225:PRO:HD2	2.55	0.42
1:A:87:GLY:O	1:A:89:VAL:HG23	2.20	0.42
1:C:186:MET:HE1	2:D:141:THR:O	2.20	0.42
2:B:109:VAL:O	2:B:147:SER:HA	2.20	0.41
2:B:79:ASN:O	2:B:83:ASN:N	2.53	0.41
2:D:173:GLU:HA	2:D:219:VAL:HG13	2.02	0.41
1:C:198:HIS:O	1:C:218:ALA:HB1	2.21	0.41
1:C:240:ILE:CD1	2:D:120:PRO:HG2	2.49	0.41
1:C:248:GLY:HA2	1:C:251:THR:CG2	2.50	0.41
2:D:21:HIS:HA	2:D:22:PRO:HD3	1.95	0.41
2:D:140:MET:CE	2:D:165:VAL:H	2.33	0.41
1:A:122:MET:HE3	1:A:122:MET:HB2	1.97	0.41
1:C:123:GLN:HB3	1:C:158:VAL:HG11	2.01	0.41
1:C:129:ALA:HB3	1:C:165:THR:HG22	2.02	0.41
1:C:220:ILE:HD12	1:C:277:ILE:HG21	2.02	0.41
2:D:171:MET:O	2:D:219:VAL:HA	2.20	0.41
2:B:176:ILE:HA	2:B:205:LEU:O	2.21	0.41
1:C:228:ASN:C	1:C:229:ILE:HG13	2.45	0.41
1:A:212:ALA:C	2:B:134:ALA:HB2	2.46	0.41
2:B:90:GLU:CD	2:B:127:ARG:HH21	2.27	0.41
2:B:164:SER:OG	2:B:177:TYR:OH	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LEU:HG	1:C:48:LYS:HA	2.03	0.41
1:C:188:LEU:HD11	1:C:214:TYR:HB2	2.02	0.41
2:B:52:ALA:HB3	2:B:87:PRO:HA	2.04	0.41
2:D:86:MET:HA	2:D:87:PRO:HD3	1.92	0.40
2:D:157:SER:OG	2:D:179:VAL:O	2.29	0.40
2:D:196:ALA:N	2:D:197:PRO:CD	2.83	0.40
2:B:171:MET:SD	2:B:210:LEU:HD22	2.62	0.40
1:C:106:THR:O	1:C:108:MET:HG3	2.22	0.40
1:C:159:PRO:HB3	1:C:197:PRO:HG2	2.04	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	254/303 (84%)	230 (91%)	21 (8%)	3 (1%)	10	30
1	C	254/303 (84%)	237 (93%)	17 (7%)	0	100	100
2	B	261/273 (96%)	240 (92%)	17 (6%)	4 (2%)	8	25
2	D	262/273 (96%)	235 (90%)	21 (8%)	6 (2%)	5	16
All	All	1031/1152 (90%)	942 (91%)	76 (7%)	13 (1%)	9	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	CYS
1	A	283	GLN
2	B	37	ASP
2	B	230	ASP
2	D	114	ASP
2	D	120	PRO

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Mol	Chain	Res	Type
1	A	91	ASP
2	B	120	PRO
2	D	117	ALA
2	D	223	PRO
2	B	153	GLY
2	D	153	GLY
2	D	156	GLY

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	203/242 (84%)	199 (98%)	4 (2%)	48	77
1	C	203/242 (84%)	193 (95%)	10 (5%)	22	52
2	B	209/218 (96%)	203 (97%)	6 (3%)	37	70
2	D	210/218 (96%)	201 (96%)	9 (4%)	26	57
All	All	825/920 (90%)	796 (96%)	29 (4%)	32	64

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	74	ARG
1	A	79	ASN
1	A	193	ASP
2	B	46	ARG
2	B	120	PRO
2	B	123	SER
2	B	246	LEU
2	B	254	ILE
2	B	255	ASP
1	C	41	LYS
1	C	48	LYS
1	C	91	ASP
1	C	101	LYS

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Mol	Chain	Res	Type
1	C	116	ILE
1	C	123	GLN
1	C	175	VAL
1	C	242	ARG
1	C	244	LYS
1	C	255	MET
2	D	23	GLN
2	D	110	ILE
2	D	127	ARG
2	D	145	VAL
2	D	157	SER
2	D	214	ARG
2	D	240	GLU
2	D	254	ILE
2	D	272	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
2	B	17	GLN
2	B	23	GLN
2	B	83	ASN
1	C	42	GLN
2	D	63	GLN
2	D	70	HIS
2	D	74	ASN
2	D	172	GLN
2	D	250	GLN
2	D	272	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 [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 [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	256/303 (84%)	0.11	9 (3%)	47 40	45, 66, 145, 170	0
1	C	256/303 (84%)	0.04	4 (1%)	70 63	47, 66, 113, 141	0
2	B	263/273 (96%)	-0.07	3 (1%)	78 72	43, 60, 84, 115	0
2	D	264/273 (96%)	-0.08	1 (0%)	88 85	43, 62, 86, 106	0
All	All	1039/1152 (90%)	0.00	17 (1%)	70 63	43, 63, 106, 170	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	SER	4.6
1	A	29	VAL	4.4
1	A	47	LEU	3.9
1	C	55	HIS	2.8
1	A	38	ILE	2.5
1	A	40	LYS	2.5
2	B	100	ARG	2.4
1	A	37	LEU	2.4
1	A	33	SER	2.3
2	B	232	LEU	2.3
2	B	226	GLY	2.3
1	A	52	LYS	2.2
1	A	48	LYS	2.2
2	D	162	ALA	2.2
1	C	29	VAL	2.1
1	A	32	SER	2.1
1	C	39	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

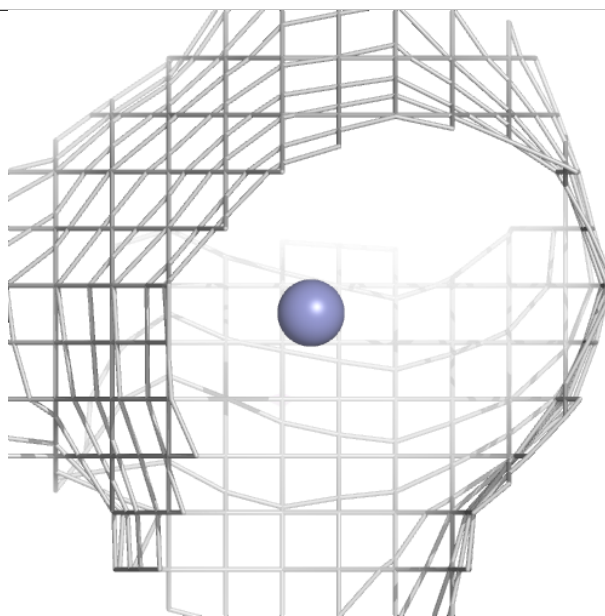
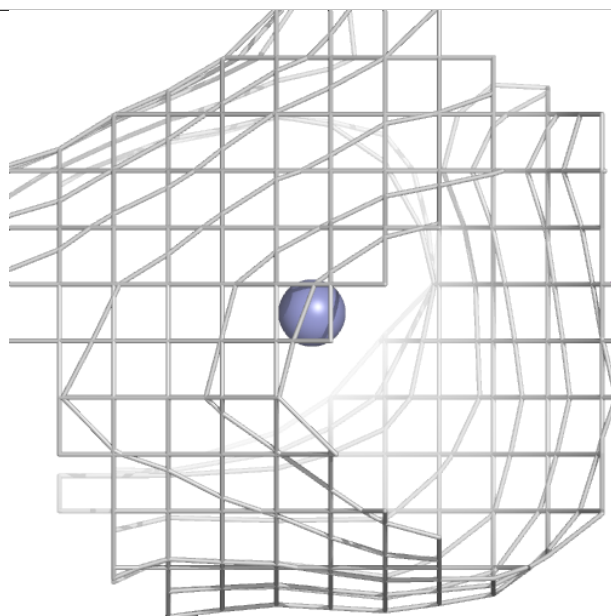
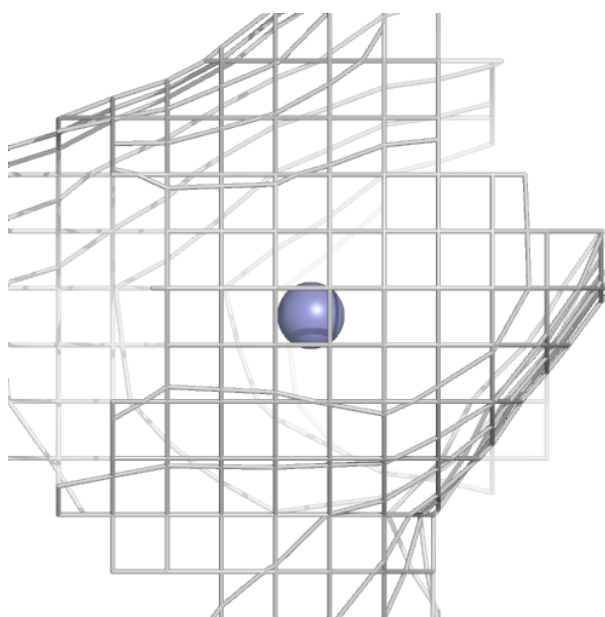
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	A	401	1/1	0.91	0.08	170,170,170,170	0
3	ZN	C	401	1/1	0.98	0.09	115,115,115,115	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

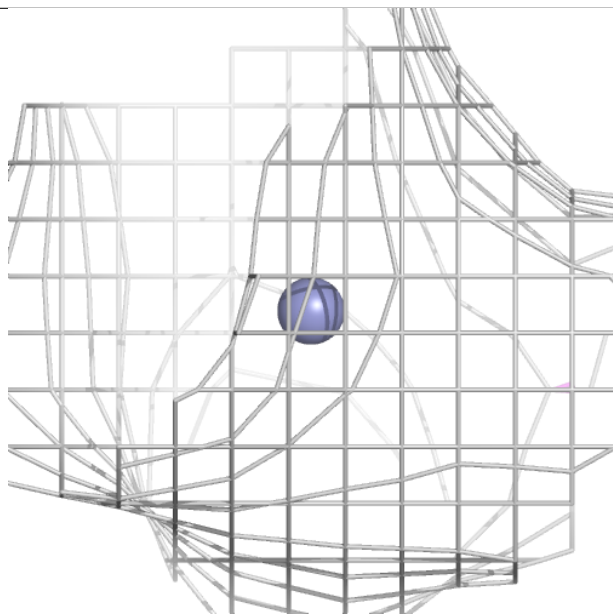
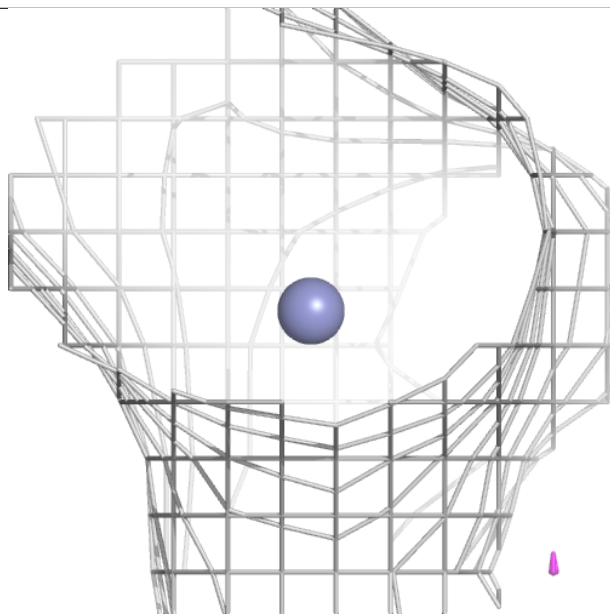
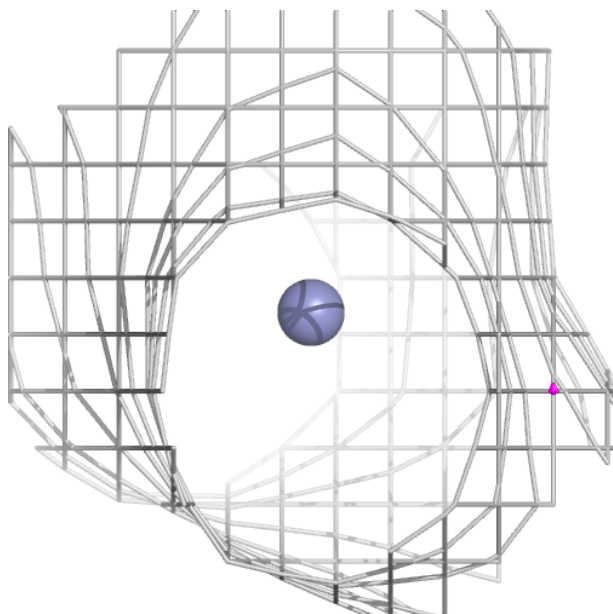
Electron density around ZN A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.