



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:18 PM EDT

PDB ID : 1AW5 / pdb_00001aw5
Title : 5-AMINOLEVULINATE DEHYDRATASE FROM SACCHAROMYCES CEREVISIAE
Authors : Erskine, P.T.; Cooper, J.B.; Wood, S.P.
Deposited on : 1997-10-09
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
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

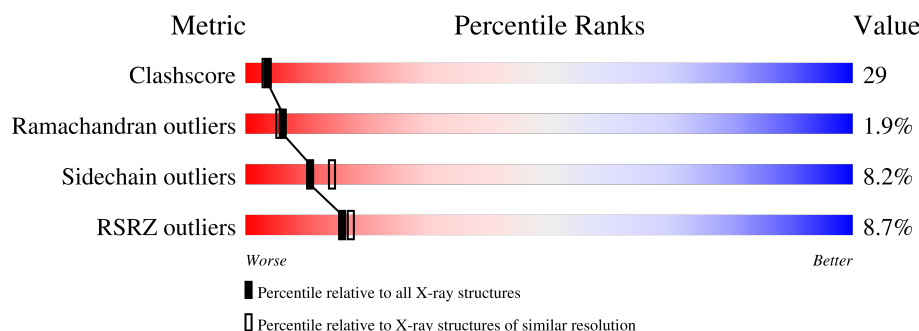
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	340	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2836 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 5-AMINOLEVULINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	Se	0	0	0
			2527	1611	437	466	8	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MSE	MET	engineered mutation	UNP P05373
A	60	ALA	LEU	conflict	UNP P05373
A	117	ARG	LYS	conflict	UNP P05373
A	122	LYS	TYR	conflict	UNP P05373
A	181	MSE	MET	engineered mutation	UNP P05373
A	219	ALA	PHE	conflict	UNP P05373
A	253	MSE	MET	engineered mutation	UNP P05373
A	272	VAL	MET	engineered mutation	UNP P05373
A	295	MSE	MET	engineered mutation	UNP P05373

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

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

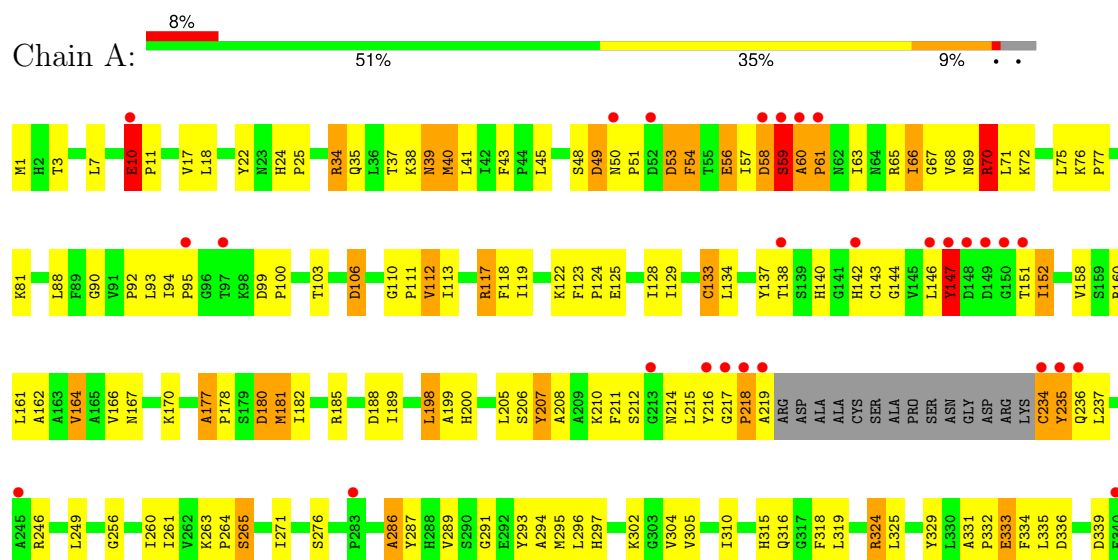
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	307	Total	O	0	0
			307	307		

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: 5-AMINOLEVULINATE DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.50Å 102.50Å 168.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 6.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (6.00-2.30) 93.7 (6.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.36 (at 2.30Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.198 , 0.270 0.285 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2836	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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	0.82	2/2579 (0.1%)	1.67	47/3493 (1.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	MSE	CG-SE	5.45	2.11	1.95
1	A	207	TYR	CA-C	5.12	1.59	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	SER	N-CA-C	8.12	122.13	109.96
1	A	43	PHE	CA-C-O	8.01	125.25	119.32
1	A	17	VAL	N-CA-C	7.55	118.71	107.15
1	A	70	ARG	CA-C-N	7.13	130.55	120.28
1	A	70	ARG	C-N-CA	7.13	130.55	120.28
1	A	256	GLY	N-CA-C	7.01	124.31	114.85
1	A	94	ILE	CA-C-N	7.01	128.60	119.84
1	A	94	ILE	C-N-CA	7.01	128.60	119.84
1	A	110	GLY	CA-C-N	6.95	126.20	118.97
1	A	110	GLY	C-N-CA	6.95	126.20	118.97
1	A	58	ASP	CA-C-N	6.72	134.37	121.54
1	A	58	ASP	C-N-CA	6.72	134.37	121.54
1	A	325	LEU	CA-C-N	-6.61	113.17	122.75
1	A	325	LEU	C-N-CA	-6.61	113.17	122.75
1	A	177	ALA	CA-C-O	-6.40	114.42	119.99
1	A	10	GLU	CA-C-N	-6.07	113.53	119.78
1	A	10	GLU	C-N-CA	-6.07	113.53	119.78
1	A	181	MSE	CG-SE-CE	6.07	112.27	98.92
1	A	88	LEU	N-CA-C	6.01	119.32	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	GLN	CA-C-N	6.00	126.60	120.00
1	A	316	GLN	C-N-CA	6.00	126.60	120.00
1	A	129	ILE	CB-CG1-CD1	-5.92	101.37	113.80
1	A	18	LEU	CA-C-N	5.78	128.81	120.38
1	A	18	LEU	C-N-CA	5.78	128.81	120.38
1	A	198	LEU	CA-C-N	5.76	128.00	120.28
1	A	198	LEU	C-N-CA	5.76	128.00	120.28
1	A	7	LEU	CA-C-N	-5.60	113.80	122.09
1	A	7	LEU	C-N-CA	-5.60	113.80	122.09
1	A	61	PRO	CA-C-N	5.57	131.46	121.15
1	A	61	PRO	C-N-CA	5.57	131.46	121.15
1	A	206	SER	CA-C-O	5.56	127.21	120.81
1	A	286	ALA	CA-C-N	-5.47	114.87	123.13
1	A	286	ALA	C-N-CA	-5.47	114.87	123.13
1	A	133	CYS	CA-C-O	-5.40	115.36	121.25
1	A	206	SER	CA-C-N	-5.39	113.64	122.26
1	A	206	SER	C-N-CA	-5.39	113.64	122.26
1	A	56	GLU	CA-CB-CG	5.38	124.86	114.10
1	A	246	ARG	CD-NE-CZ	5.31	131.84	124.40
1	A	58	ASP	N-CA-C	5.27	117.09	108.55
1	A	164	VAL	CA-CB-CG1	5.23	119.30	110.40
1	A	129	ILE	CA-C-N	-5.21	114.71	122.74
1	A	129	ILE	C-N-CA	-5.21	114.71	122.74
1	A	206	SER	O-C-N	-5.20	116.53	122.93
1	A	40	MSE	CG-SE-CE	-5.20	87.49	98.92
1	A	112	VAL	N-CA-C	5.14	115.29	110.30
1	A	40	MSE	CB-CG-SE	-5.10	97.40	112.70
1	A	147	TYR	CA-C-O	-5.01	115.81	121.72

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	2527	0	2520	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	307	0	0	11	2
All	All	2836	0	2520	147	2

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 29.

All (147) 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:60:ALA:H	1:A:61:PRO:CD	1.30	1.34
1:A:60:ALA:H	1:A:61:PRO:HD2	1.05	1.13
1:A:60:ALA:N	1:A:61:PRO:HD2	1.63	1.12
1:A:60:ALA:N	1:A:61:PRO:CD	2.11	1.05
1:A:151:THR:HG22	1:A:152:ILE:H	1.27	0.96
1:A:60:ALA:H	1:A:61:PRO:HD3	1.28	0.95
1:A:304:VAL:HG12	1:A:305:VAL:HG13	1.50	0.94
1:A:61:PRO:HA	1:A:293:TYR:HE2	1.38	0.89
1:A:99:ASP:HB2	1:A:100:PRO:CD	2.03	0.89
1:A:72:LYS:HB2	1:A:118:PHE:HZ	1.39	0.87
1:A:61:PRO:HA	1:A:293:TYR:CE2	2.13	0.82
1:A:60:ALA:HB3	1:A:294:ALA:HA	1.62	0.81
1:A:177:ALA:HB1	1:A:207:TYR:HE1	1.49	0.78
1:A:51:PRO:HB2	1:A:69:ASN:ND2	1.98	0.77
1:A:218:PRO:O	1:A:219:ALA:HB2	1.84	0.76
1:A:151:THR:HG22	1:A:152:ILE:N	2.00	0.75
1:A:140:HIS:CE1	1:A:146:LEU:HD13	2.21	0.74
1:A:106:ASP:OD1	1:A:106:ASP:N	2.09	0.74
1:A:324:ARG:HH11	1:A:324:ARG:HG2	1.53	0.74
1:A:113:ILE:O	1:A:117:ARG:HG3	1.87	0.73
1:A:99:ASP:HB2	1:A:100:PRO:HD2	1.69	0.73
1:A:140:HIS:NE2	1:A:146:LEU:HD13	2.04	0.72
1:A:333:GLU:O	1:A:336:ASP:HB2	1.90	0.72
1:A:324:ARG:HG2	1:A:324:ARG:NH1	2.05	0.71
1:A:24:HIS:CG	1:A:25:PRO:HD2	2.25	0.71
1:A:162:ALA:O	1:A:166:VAL:HG23	1.91	0.71
1:A:177:ALA:HB1	1:A:207:TYR:CE1	2.27	0.69
1:A:336:ASP:O	1:A:339:ASP:HB2	1.93	0.69
1:A:208:ALA:HB2	1:A:260:ILE:HD12	1.73	0.69
1:A:216:TYR:HE1	1:A:263:LYS:HE2	1.57	0.69
1:A:180:ASP:O	1:A:181:MSE:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:O	1:A:189:ILE:HG13	1.94	0.68
1:A:181:MSE:HE2	1:A:237:LEU:HG	1.77	0.67
1:A:208:ALA:HB2	1:A:260:ILE:CD1	2.25	0.67
1:A:208:ALA:CB	1:A:260:ILE:HD12	2.27	0.64
1:A:218:PRO:O	1:A:219:ALA:CB	2.44	0.64
1:A:99:ASP:HB2	1:A:100:PRO:HD3	1.79	0.64
1:A:56:GLU:HG3	3:A:687:HOH:O	1.96	0.64
1:A:92:PRO:HG3	1:A:137:TYR:CE1	2.34	0.63
1:A:90:GLY:HA3	1:A:112:VAL:HG23	1.81	0.62
1:A:39:ASN:HD22	1:A:39:ASN:C	2.07	0.61
1:A:59:SER:HB3	1:A:61:PRO:HD3	1.82	0.61
1:A:166:VAL:HG12	1:A:170:LYS:HE3	1.80	0.61
1:A:54:PHE:HD2	1:A:66:ILE:HG23	1.66	0.61
1:A:216:TYR:HB2	3:A:626:HOH:O	2.01	0.60
1:A:111:PRO:HD2	3:A:534:HOH:O	2.00	0.60
1:A:24:HIS:CD2	1:A:25:PRO:HD2	2.36	0.60
1:A:134:LEU:HD12	1:A:144:GLY:HA2	1.83	0.60
1:A:207:TYR:HA	1:A:261:ILE:HB	1.82	0.60
1:A:265:SER:HB3	1:A:318:PHE:CE1	2.37	0.60
1:A:59:SER:H	1:A:61:PRO:HD2	1.68	0.59
1:A:151:THR:CG2	1:A:152:ILE:H	2.08	0.58
1:A:158:VAL:HG11	1:A:188:ASP:OD2	2.04	0.58
1:A:324:ARG:HH11	1:A:324:ARG:CG	2.13	0.58
1:A:296:LEU:HD21	3:A:563:HOH:O	2.04	0.57
1:A:75:LEU:HB2	1:A:123:PHE:CE2	2.39	0.57
1:A:106:ASP:CB	1:A:167:ASN:HD22	2.17	0.57
1:A:146:LEU:HD12	1:A:146:LEU:N	2.20	0.56
1:A:332:PRO:HG2	3:A:683:HOH:O	2.03	0.56
1:A:216:TYR:CE1	1:A:263:LYS:HE2	2.39	0.56
1:A:68:VAL:HG23	3:A:592:HOH:O	2.04	0.56
1:A:99:ASP:O	1:A:138:THR:HA	2.06	0.56
1:A:265:SER:OG	1:A:286:ALA:HB1	2.06	0.56
1:A:160:ARG:O	1:A:164:VAL:HG23	2.06	0.55
1:A:61:PRO:CA	1:A:293:TYR:HE2	2.16	0.55
1:A:152:ILE:CD1	1:A:234:CYS:HA	2.38	0.54
1:A:35:GLN:O	1:A:40:MSE:HE1	2.07	0.54
1:A:199:ALA:HB3	3:A:738:HOH:O	2.07	0.54
1:A:208:ALA:HB3	1:A:260:ILE:HG23	1.90	0.54
1:A:77:PRO:HG2	3:A:700:HOH:O	2.07	0.54
1:A:1:MSE:O	1:A:3:THR:HG23	2.08	0.54
1:A:119:ILE:HG22	1:A:128:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PRO:HB2	1:A:69:ASN:HD21	1.68	0.53
1:A:34:ARG:HG3	1:A:319:LEU:HD23	1.89	0.53
1:A:59:SER:N	1:A:61:PRO:HD2	2.23	0.53
1:A:99:ASP:CB	1:A:100:PRO:CD	2.75	0.53
1:A:143:CYS:O	1:A:182:ILE:HD11	2.08	0.53
1:A:53:ASP:O	1:A:54:PHE:HB2	2.10	0.52
1:A:45:LEU:HD11	1:A:75:LEU:HD21	1.91	0.52
1:A:215:LEU:O	1:A:291:GLY:HA3	2.10	0.52
1:A:177:ALA:CB	1:A:207:TYR:HE1	2.21	0.52
1:A:178:PRO:HG3	1:A:189:ILE:HD12	1.93	0.51
1:A:182:ILE:O	1:A:185:ARG:HD2	2.11	0.51
1:A:38:LYS:HD3	1:A:335:LEU:HD23	1.92	0.51
1:A:92:PRO:HG3	1:A:137:TYR:HE1	1.76	0.50
1:A:50:ASN:OD1	1:A:50:ASN:C	2.55	0.50
1:A:147:TYR:HE1	3:A:607:HOH:O	1.93	0.50
1:A:152:ILE:HD12	1:A:234:CYS:HA	1.94	0.50
1:A:59:SER:C	1:A:61:PRO:HD2	2.34	0.50
1:A:50:ASN:O	1:A:53:ASP:HB2	2.12	0.49
1:A:57:ILE:HG22	1:A:58:ASP:N	2.27	0.48
1:A:287:TYR:CD1	1:A:287:TYR:C	2.91	0.48
1:A:331:ALA:N	1:A:332:PRO:CD	2.77	0.48
1:A:113:ILE:O	1:A:113:ILE:HG22	2.13	0.48
1:A:263:LYS:HG3	1:A:289:VAL:CG1	2.44	0.47
1:A:51:PRO:O	1:A:69:ASN:HB2	2.14	0.47
1:A:123:PHE:C	1:A:125:GLU:H	2.22	0.47
1:A:287:TYR:C	1:A:287:TYR:HD1	2.23	0.47
1:A:57:ILE:HG22	1:A:58:ASP:H	1.79	0.47
1:A:66:ILE:HG22	1:A:67:GLY:N	2.30	0.47
1:A:66:ILE:HG22	1:A:67:GLY:H	1.79	0.47
1:A:212:SER:HA	1:A:236:GLN:NE2	2.29	0.47
1:A:77:PRO:O	1:A:81:LYS:HG3	2.16	0.47
1:A:214:ASN:HD21	1:A:218:PRO:HA	1.79	0.47
1:A:99:ASP:OD2	1:A:103:THR:HB	2.15	0.46
1:A:310:ILE:HD12	1:A:310:ILE:HA	1.83	0.46
1:A:119:ILE:CG2	1:A:128:ILE:HD11	2.45	0.46
1:A:133:CYS:HA	1:A:161:LEU:HD21	1.98	0.46
1:A:177:ALA:HA	1:A:205:LEU:O	2.16	0.46
1:A:142:HIS:HB2	1:A:146:LEU:HD11	1.98	0.45
1:A:215:LEU:HD12	1:A:264:PRO:HG2	1.98	0.45
1:A:39:ASN:C	1:A:39:ASN:ND2	2.75	0.45
1:A:212:SER:CA	1:A:236:GLN:HE21	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TYR:O	1:A:236:GLN:HG3	2.17	0.45
1:A:66:ILE:CG2	1:A:70:ARG:HB2	2.47	0.45
1:A:212:SER:HA	1:A:236:GLN:HE21	1.82	0.45
1:A:60:ALA:HB3	1:A:294:ALA:CA	2.39	0.44
1:A:41:LEU:HD11	1:A:334:PHE:HB3	1.98	0.44
1:A:146:LEU:N	1:A:146:LEU:CD1	2.79	0.44
1:A:48:SER:HB2	1:A:65:ARG:HG2	2.00	0.43
1:A:63:ILE:HG21	1:A:329:TYR:CD1	2.52	0.43
1:A:249:LEU:CD2	1:A:260:ILE:HG21	2.48	0.43
1:A:331:ALA:O	1:A:332:PRO:C	2.60	0.43
1:A:60:ALA:HB1	1:A:297:HIS:HB3	2.00	0.43
1:A:212:SER:HB3	1:A:236:GLN:NE2	2.33	0.43
1:A:217:GLY:O	1:A:218:PRO:C	2.60	0.43
1:A:118:PHE:C	1:A:118:PHE:CD1	2.97	0.43
1:A:302:LYS:O	1:A:302:LYS:HG3	2.19	0.43
1:A:170:LYS:HG3	1:A:198:LEU:HD11	2.01	0.43
1:A:37:THR:OG1	1:A:40:MSE:HE3	2.19	0.42
1:A:59:SER:CA	1:A:61:PRO:HD2	2.50	0.42
1:A:211:PHE:CZ	1:A:271:ILE:HG13	2.54	0.42
1:A:260:ILE:HG22	1:A:261:ILE:N	2.33	0.42
1:A:49:ASP:HB2	1:A:93:LEU:H	1.84	0.42
1:A:212:SER:HB3	1:A:236:GLN:HE21	1.85	0.42
1:A:214:ASN:O	1:A:214:ASN:CG	2.63	0.42
1:A:10:GLU:HB3	1:A:11:PRO:CD	2.50	0.41
1:A:180:ASP:OD1	1:A:180:ASP:N	2.50	0.41
1:A:113:ILE:O	1:A:113:ILE:CG2	2.68	0.41
1:A:235:TYR:HD1	1:A:235:TYR:H	1.67	0.41
1:A:22:TYR:O	1:A:22:TYR:CG	2.74	0.41
1:A:200:HIS:CD2	1:A:200:HIS:H	2.39	0.41
1:A:295:MSE:O	1:A:295:MSE:HG2	2.19	0.41
1:A:235:TYR:CD1	1:A:235:TYR:N	2.89	0.40
1:A:324:ARG:HG2	3:A:575:HOH:O	2.21	0.40
1:A:124:PRO:HA	3:A:805:HOH:O	2.21	0.40
1:A:315:HIS:HA	1:A:318:PHE:CD2	2.55	0.40

All (2) 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)
3:A:726:HOH:O	3:A:726:HOH:O[16_555]	0.94	1.26
3:A:675:HOH:O	3:A:675:HOH:O[5_555]	1.52	0.68

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	322/340 (95%)	292 (91%)	24 (8%)	6 (2%)	6 5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	PHE
1	A	60	ALA
1	A	95	PRO
1	A	53	ASP
1	A	59	SER
1	A	218	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	268/273 (98%)	246 (92%)	22 (8%)	10 14

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	34	ARG
1	A	39	ASN
1	A	49	ASP
1	A	59	SER

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Mol	Chain	Res	Type
1	A	66	ILE
1	A	70	ARG
1	A	71	LEU
1	A	76	LYS
1	A	106	ASP
1	A	117	ARG
1	A	122	LYS
1	A	147	TYR
1	A	152	ILE
1	A	180	ASP
1	A	210	LYS
1	A	234	CYS
1	A	235	TYR
1	A	265	SER
1	A	276	SER
1	A	324	ARG
1	A	333	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	29	GLN
1	A	39	ASN
1	A	64	ASN
1	A	69	ASN
1	A	140	HIS
1	A	167	ASN
1	A	214	ASN
1	A	236	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 ⓘ

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	321/340 (94%)	0.83	28 (8%) 16 17	0, 0, 1, 1	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	SER	7.6
1	A	150	GLY	6.9
1	A	60	ALA	6.5
1	A	219	ALA	5.9
1	A	148	ASP	5.3
1	A	217	GLY	5.1
1	A	149	ASP	5.0
1	A	151	THR	5.0
1	A	61	PRO	4.8
1	A	234	CYS	4.4
1	A	146	LEU	4.4
1	A	58	ASP	4.2
1	A	218	PRO	4.1
1	A	213	GLY	4.0
1	A	216	TYR	4.0
1	A	235	TYR	3.1
1	A	97	THR	2.8
1	A	147	TYR	2.8
1	A	236	GLN	2.7
1	A	52	ASP	2.6
1	A	95	PRO	2.6
1	A	245	ALA	2.5
1	A	142	HIS	2.5
1	A	50	ASN	2.3
1	A	340	GLU	2.3
1	A	10	GLU	2.2
1	A	138	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	283	PRO	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($\text{\AA}^2$)	Q<0.9
2	ZN	A	400	1/1	0.97	0.04	0,0,0,0	0
2	ZN	A	401	1/1	0.99	0.25	0,0,0,0	0

6.5 Other polymers [i](#)

There are no such residues in this entry.