



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 PM UTC

PDB ID : 4WD7 / pdb_00004wd7
Title : Crystal structure of a bacterial Bestrophin homolog from *Klebsiella pneumoniae* by Zn-SAD phasing
Authors : Yang, T.; Liu, Q.; Hendrickson, W.A.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : 2014-09-08
Resolution : 2.90 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

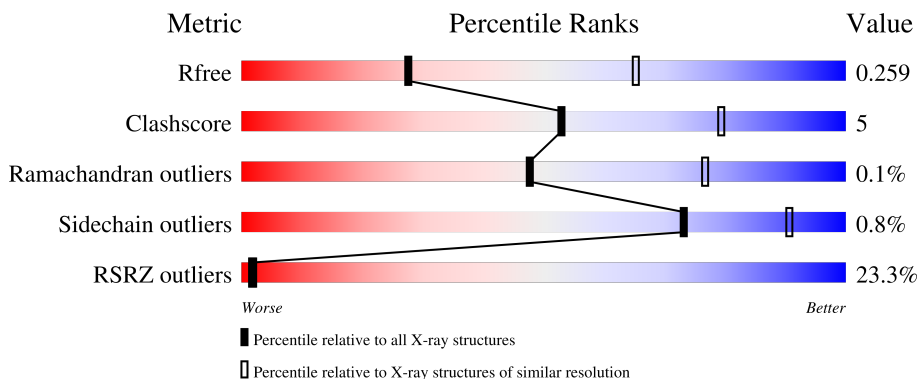
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	301	18% 76% 13% 11%
1	B	301	22% 78% 11% 10%
1	C	301	19% 81% 8% 11%
1	D	301	25% 77% 12% 11%
1	E	301	21% 75% 12% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10651 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 Bestrophin domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2120	1373	359	379	9			
1	B	270	Total	C	N	O	S	0	0	0
			2148	1391	364	384	9			
1	C	269	Total	C	N	O	S	0	0	0
			2110	1362	362	377	9			
1	D	268	Total	C	N	O	S	0	0	0
			2114	1367	359	379	9			
1	E	270	Total	C	N	O	S	0	0	0
			2144	1389	364	382	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP S7AS11
A	-1	ASN	-	expression tag	UNP S7AS11
A	0	ALA	-	expression tag	UNP S7AS11
B	-2	SER	-	expression tag	UNP S7AS11
B	-1	ASN	-	expression tag	UNP S7AS11
B	0	ALA	-	expression tag	UNP S7AS11
C	-2	SER	-	expression tag	UNP S7AS11
C	-1	ASN	-	expression tag	UNP S7AS11
C	0	ALA	-	expression tag	UNP S7AS11
D	-2	SER	-	expression tag	UNP S7AS11
D	-1	ASN	-	expression tag	UNP S7AS11
D	0	ALA	-	expression tag	UNP S7AS11
E	-2	SER	-	expression tag	UNP S7AS11
E	-1	ASN	-	expression tag	UNP S7AS11
E	0	ALA	-	expression tag	UNP S7AS11

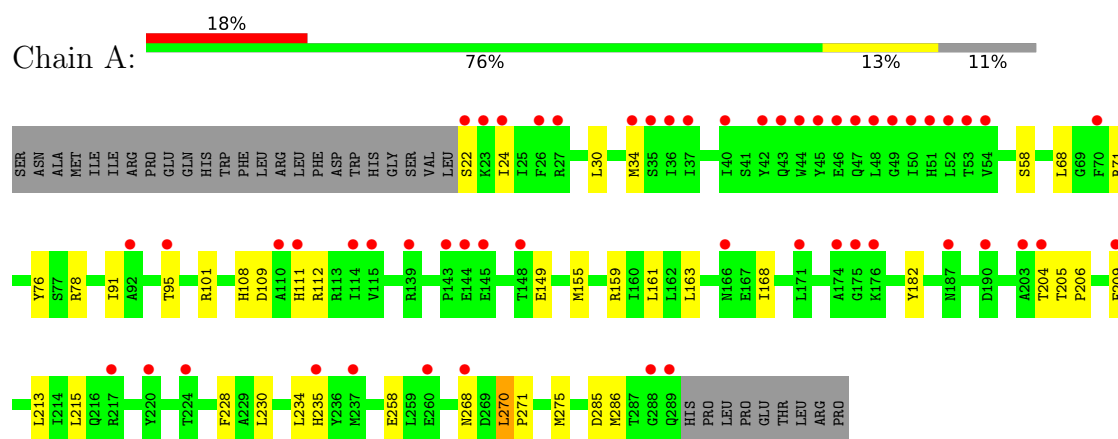
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Zn 4	0	0
2	B	3	Total 3	Zn 3	0	0
2	C	3	Total 3	Zn 3	0	0
2	D	3	Total 3	Zn 3	0	0
2	E	2	Total 2	Zn 2	0	0

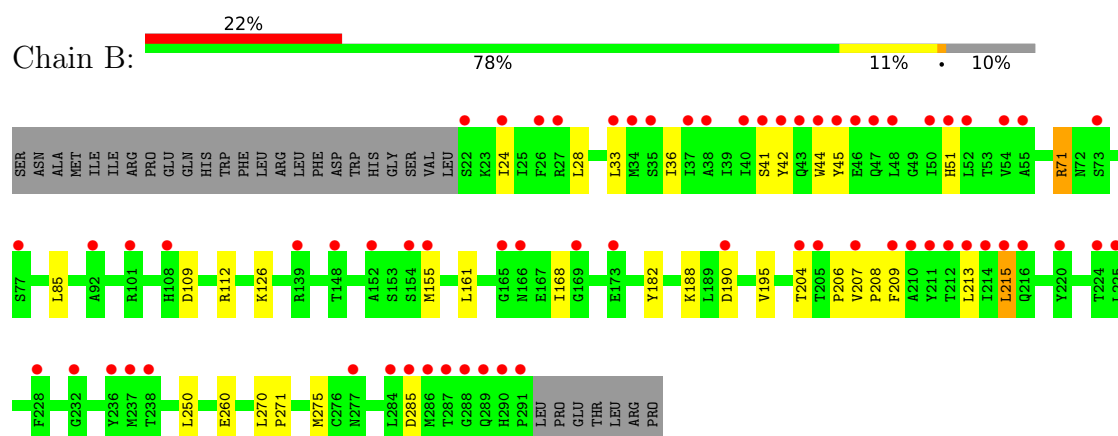
3 Residue-property plots [i](#)

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.

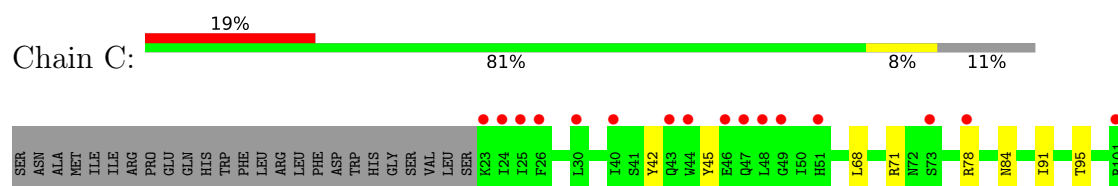
• Molecule 1: Bestrophin domain protein

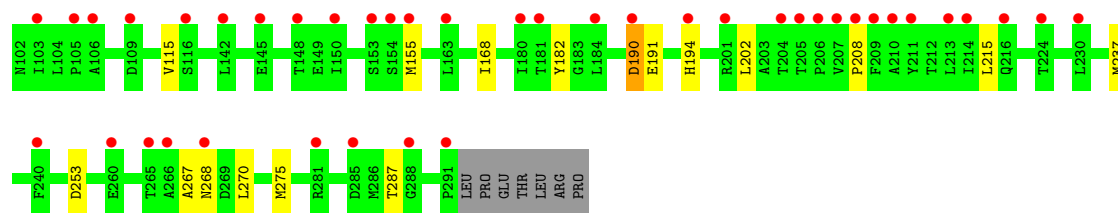


• Molecule 1: Bestrophin domain protein

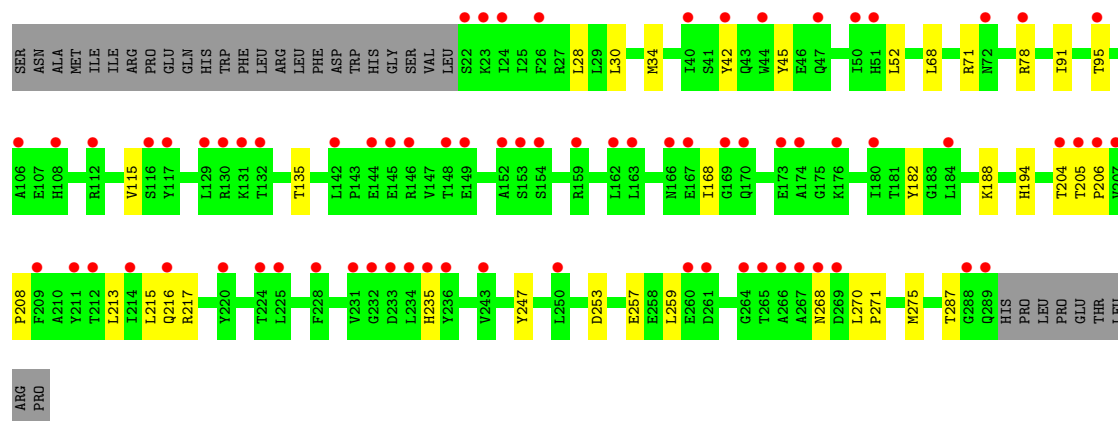
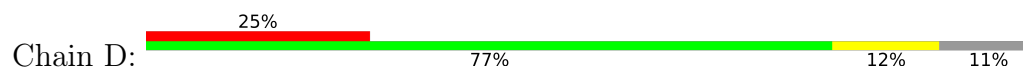


• Molecule 1: Bestrophin domain protein

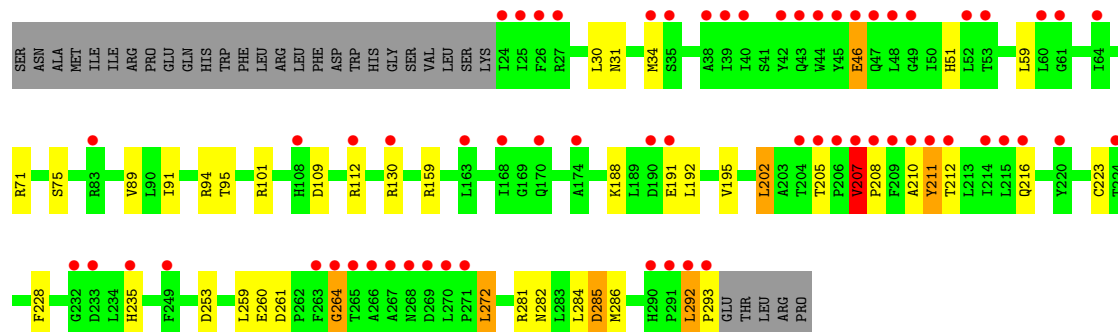
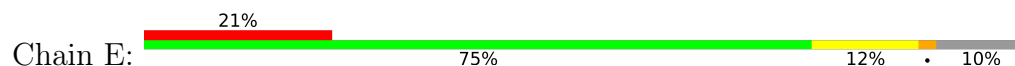




• Molecule 1: Bestrophin domain protein



• Molecule 1: Bestrophin domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.12Å 160.59Å 161.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.19 – 2.90 39.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.19-2.90) 99.9 (39.19-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.239 , 0.253 0.246 , 0.259	Depositor DCC
R_{free} test set	3279 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10651	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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	0.36	0/2166	0.78	4/2950 (0.1%)
1	B	0.35	0/2196	0.77	3/2991 (0.1%)
1	C	0.39	0/2155	0.76	0/2937
1	D	0.34	0/2159	0.78	3/2941 (0.1%)
1	E	0.40	0/2192	0.86	9/2987 (0.3%)
All	All	0.37	0/10868	0.79	19/14806 (0.1%)

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	E	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	LEU	N-CA-C	7.47	119.50	111.36
1	E	284	LEU	N-CA-C	-6.98	104.58	113.23
1	E	264	GLY	N-CA-C	6.58	123.32	112.66
1	E	191	GLU	N-CA-C	-6.16	104.57	111.28
1	E	211	TYR	N-CA-C	-5.68	106.19	113.01
1	A	155	MET	CA-C-N	5.57	125.23	119.05
1	A	155	MET	C-N-CA	5.57	125.23	119.05
1	B	155	MET	CA-C-N	5.32	124.95	119.05
1	B	155	MET	C-N-CA	5.32	124.95	119.05
1	D	135	THR	N-CA-C	5.22	116.66	111.07
1	E	207	VAL	CA-C-N	-5.19	114.57	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	207	VAL	C-N-CA	-5.19	114.57	119.76
1	D	270	LEU	CA-C-N	5.14	126.27	119.84
1	D	270	LEU	C-N-CA	5.14	126.27	119.84
1	E	46	GLU	N-CA-C	5.14	116.88	111.28
1	B	215	LEU	N-CA-C	5.08	116.90	111.36
1	A	270	LEU	CA-C-N	5.07	126.18	119.84
1	A	270	LEU	C-N-CA	5.07	126.18	119.84
1	E	235	HIS	CB-CA-C	-5.00	110.43	117.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	205	THR	Peptide

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	2120	0	2151	29	0
1	B	2148	0	2184	25	0
1	C	2110	0	2134	17	0
1	D	2114	0	2144	25	0
1	E	2144	0	2183	32	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
All	All	10651	0	10796	108	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 5.

All (108) 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:C:190:ASP:OD2	1:E:188:LYS:NZ	2.01	0.94
1:B:208:PRO:HB3	1:D:268:ASN:HD21	1.41	0.83
1:E:109:ASP:OD1	1:E:112:ARG:NH2	2.19	0.75
1:B:190:ASP:OD2	1:D:188:LYS:NZ	2.20	0.74
1:A:68:LEU:HD23	1:A:215:LEU:HD13	1.73	0.71
1:B:109:ASP:OD1	1:B:112:ARG:NH2	2.29	0.65
1:E:207:VAL:HG23	1:E:208:PRO:HD3	1.79	0.63
1:C:71:ARG:NH2	1:C:253:ASP:OD1	2.31	0.62
1:B:24:ILE:HD12	1:B:250:LEU:HB3	1.82	0.62
1:C:68:LEU:HD23	1:C:215:LEU:HD13	1.82	0.61
1:C:78:ARG:NH2	1:C:202:LEU:O	2.31	0.60
1:E:292:LEU:HD22	1:E:293:PRO:HD2	1.82	0.60
1:D:216:GLN:NE2	1:D:257:GLU:OE2	2.34	0.60
1:D:71:ARG:NH2	1:D:253:ASP:OD1	2.32	0.59
1:C:270:LEU:HD22	1:C:275:MET:HE1	1.84	0.59
1:A:22:SER:HB3	1:A:24:ILE:HG22	1.85	0.58
1:E:31:ASN:ND2	1:E:223:CYS:O	2.36	0.57
1:B:71:ARG:NH1	1:B:260:GLU:OE2	2.38	0.56
1:E:94:ARG:HH21	1:E:282:ASN:HD21	1.53	0.56
1:C:208:PRO:HG2	1:E:259:LEU:HD21	1.89	0.55
1:C:115:VAL:HG21	1:C:287:THR:HG21	1.88	0.54
1:B:207:VAL:HG21	1:B:260:GLU:CD	2.31	0.54
1:A:209:PHE:O	1:A:213:LEU:HD13	2.08	0.53
1:B:208:PRO:HG2	1:D:259:LEU:HD21	1.91	0.53
1:A:76:TYR:CE1	1:E:207:VAL:HG21	2.44	0.53
1:A:159:ARG:NH2	1:B:285:ASP:OD2	2.41	0.52
1:D:78:ARG:NH2	1:D:205:THR:O	2.43	0.52
1:A:78:ARG:NH1	1:A:205:THR:O	2.43	0.52
1:A:209:PHE:CZ	1:A:213:LEU:HD11	2.45	0.52
1:C:190:ASP:O	1:C:194:HIS:HD2	1.92	0.52
1:A:34:MET:HE3	1:A:228:PHE:HE1	1.74	0.52
1:A:109:ASP:OD1	1:A:112:ARG:NH2	2.43	0.52
1:D:115:VAL:HG21	1:D:287:THR:HG21	1.93	0.51
1:A:235:HIS:CD2	1:E:51:HIS:HD2	2.29	0.50
1:E:130:ARG:HH11	1:E:130:ARG:HG3	1.77	0.50
1:D:68:LEU:HD23	1:D:215:LEU:HD13	1.94	0.49
1:E:281:ARG:O	1:E:285:ASP:HB2	2.12	0.49
1:E:101:ARG:HD2	1:E:286:MET:O	2.13	0.49
1:D:271:PRO:HG2	1:D:275:MET:HE3	1.95	0.49
1:B:271:PRO:HG2	1:B:275:MET:HE3	1.93	0.49
1:B:33:LEU:O	1:B:36:ILE:HG12	2.14	0.48
1:E:34:MET:HE3	1:E:228:PHE:HE2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:LEU:O	1:E:34:MET:HG2	2.14	0.48
1:B:270:LEU:HD22	1:B:275:MET:HE1	1.96	0.47
1:E:71:ARG:NH2	1:E:253:ASP:OD1	2.47	0.47
1:E:188:LYS:HD3	1:E:188:LYS:HA	1.71	0.47
1:C:91:ILE:O	1:C:95:THR:HG23	2.14	0.47
1:A:270:LEU:HD22	1:A:275:MET:HE1	1.96	0.47
1:B:42:TYR:HA	1:B:45:TYR:CD1	2.50	0.47
1:C:155:MET:HE3	1:E:94:ARG:NH2	2.29	0.47
1:E:94:ARG:HH21	1:E:282:ASN:ND2	2.11	0.47
1:D:91:ILE:O	1:D:95:THR:HG23	2.15	0.47
1:B:41:SER:HA	1:B:44:TRP:HD1	1.79	0.46
1:E:71:ARG:HD3	1:E:260:GLU:OE2	2.15	0.46
1:E:130:ARG:HH22	1:E:272:LEU:HB2	1.80	0.46
1:C:191:GLU:OE2	1:D:194:HIS:CE1	2.67	0.46
1:E:75:SER:OG	1:E:260:GLU:HG3	2.16	0.46
1:E:261:ASP:OD2	1:E:264:GLY:HA3	2.16	0.46
1:A:204:THR:O	1:A:206:PRO:HD3	2.16	0.46
1:C:268:ASN:HD21	1:D:208:PRO:HB3	1.81	0.46
1:A:76:TYR:HE1	1:E:207:VAL:HG21	1.80	0.46
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.84	0.45
1:A:91:ILE:O	1:A:95:THR:HG23	2.16	0.45
1:C:168:ILE:HG22	1:C:182:TYR:CD1	2.51	0.45
1:E:261:ASP:CG	1:E:264:GLY:HA3	2.40	0.45
1:D:168:ILE:HG22	1:D:182:TYR:CD1	2.52	0.45
1:B:209:PHE:O	1:B:213:LEU:HD13	2.16	0.45
1:B:188:LYS:HD3	1:B:188:LYS:HA	1.69	0.45
1:E:46:GLU:OE2	1:E:51:HIS:HE1	1.99	0.45
1:E:212:THR:O	1:E:216:GLN:HG3	2.17	0.44
1:A:101:ARG:HD2	1:A:286:MET:O	2.17	0.44
1:B:71:ARG:HG3	1:B:215:LEU:HD12	1.98	0.44
1:C:42:TYR:HA	1:C:45:TYR:CD1	2.53	0.44
1:C:268:ASN:ND2	1:D:208:PRO:HB3	2.32	0.44
1:E:89:VAL:CG2	1:E:195:VAL:HG11	2.48	0.44
1:A:149:GLU:OE2	1:A:163:LEU:HD21	2.18	0.44
1:B:208:PRO:HB3	1:D:268:ASN:ND2	2.22	0.44
1:B:126:LYS:HE3	1:B:126:LYS:HB3	1.90	0.44
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.85	0.43
1:A:168:ILE:HG22	1:A:182:TYR:CD1	2.54	0.43
1:B:190:ASP:OD1	1:D:95:THR:HG21	2.19	0.42
1:A:108:HIS:HA	1:A:111:HIS:CG	2.53	0.42
1:C:268:ASN:HD21	1:D:208:PRO:CB	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ILE:O	1:E:95:THR:HG23	2.19	0.42
1:B:168:ILE:HG22	1:B:182:TYR:CD1	2.54	0.42
1:A:30:LEU:O	1:A:34:MET:HG2	2.20	0.42
1:B:204:THR:O	1:B:206:PRO:HD3	2.20	0.42
1:D:30:LEU:O	1:D:34:MET:HG2	2.20	0.42
1:D:42:TYR:HA	1:D:45:TYR:CD1	2.54	0.42
1:A:271:PRO:HG2	1:A:275:MET:HE3	2.01	0.42
1:D:213:LEU:HD11	1:D:217:ARG:NH2	2.35	0.42
1:E:202:LEU:HD12	1:E:202:LEU:HA	1.90	0.41
1:D:28:LEU:HD11	1:D:247:TYR:HD1	1.85	0.41
1:D:204:THR:O	1:D:206:PRO:HD3	2.19	0.41
1:A:108:HIS:HA	1:A:111:HIS:ND1	2.36	0.41
1:B:24:ILE:HG22	1:B:28:LEU:HG	2.02	0.41
1:A:34:MET:HE3	1:A:228:PHE:CE1	2.53	0.41
1:A:285:ASP:O	1:E:159:ARG:NH2	2.53	0.41
1:E:210:ALA:HA	1:E:212:THR:HG22	2.01	0.41
1:A:230:LEU:HB3	1:A:234:LEU:HD12	2.03	0.41
1:A:258:GLU:CD	1:A:268:ASN:HD22	2.28	0.41
1:B:51:HIS:HD2	1:D:235:HIS:HB2	1.85	0.41
1:A:58:SER:HA	1:E:59:LEU:HD13	2.02	0.41
1:A:71:ARG:HG3	1:A:215:LEU:HD12	2.04	0.40
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.90	0.40
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.93	0.40
1:C:237:MET:HE2	1:D:52:LEU:HD21	2.02	0.40
1:B:85:LEU:HD22	1:B:195:VAL:HA	2.04	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	266/301 (88%)	262 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	268/301 (89%)	265 (99%)	3 (1%)	0	100	100
1	C	267/301 (89%)	262 (98%)	4 (2%)	1 (0%)	30	59
1	D	266/301 (88%)	263 (99%)	3 (1%)	0	100	100
1	E	268/301 (89%)	263 (98%)	5 (2%)	0	100	100
All	All	1335/1505 (89%)	1315 (98%)	19 (1%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	267	ALA

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	229/264 (87%)	229 (100%)	0	100	100
1	B	234/264 (89%)	233 (100%)	1 (0%)	84	94
1	C	226/264 (86%)	224 (99%)	2 (1%)	70	90
1	D	228/264 (86%)	228 (100%)	0	100	100
1	E	233/264 (88%)	227 (97%)	6 (3%)	40	73
All	All	1150/1320 (87%)	1141 (99%)	9 (1%)	73	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	ARG
1	C	84	ASN
1	C	190	ASP
1	E	202	LEU
1	E	207	VAL
1	E	211	TYR
1	E	272	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	285	ASP
1	E	292	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	99	GLN
1	A	158	ASN
1	A	166	ASN
1	A	235	HIS
1	A	268	ASN
1	B	43	GLN
1	B	51	HIS
1	B	166	ASN
1	C	51	HIS
1	C	102	ASN
1	C	166	ASN
1	C	235	HIS
1	C	268	ASN
1	D	99	GLN
1	D	166	ASN
1	D	268	ASN
1	E	51	HIS
1	E	99	GLN
1	E	166	ASN
1	E	282	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 15 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	268/301 (89%)	1.08	54 (20%) 3 2	49, 81, 145, 225	0
1	B	270/301 (89%)	1.27	66 (24%) 2 1	51, 89, 149, 253	0
1	C	269/301 (89%)	1.21	57 (21%) 2 2	52, 86, 164, 217	0
1	D	268/301 (89%)	1.51	74 (27%) 1 1	54, 90, 144, 217	0
1	E	270/301 (89%)	1.28	63 (23%) 2 2	48, 80, 161, 301	0
All	All	1345/1505 (89%)	1.27	314 (23%) 2 2	48, 85, 154, 301	0

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	GLN	15.2
1	A	47	GLN	11.6
1	B	287	THR	9.6
1	B	220	TYR	9.3
1	E	269	ASP	8.8
1	D	170	GLN	8.5
1	E	266	ALA	8.2
1	D	173	GLU	8.1
1	D	265	THR	8.0
1	E	270	LEU	8.0
1	D	145	GLU	8.0
1	D	233	ASP	7.9
1	E	293	PRO	7.9
1	A	175	GLY	7.8
1	E	47	GLN	7.1
1	B	291	PRO	7.0
1	E	265	THR	6.8
1	E	292	LEU	6.6
1	D	154	SER	6.5
1	C	291	PRO	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	51	HIS	6.2
1	D	131	LYS	5.9
1	A	204	THR	5.8
1	D	166	ASN	5.8
1	B	288	GLY	5.8
1	D	232	GLY	5.6
1	B	211	TYR	5.6
1	E	42	TYR	5.6
1	A	48	LEU	5.5
1	D	146	ARG	5.5
1	E	49	GLY	5.5
1	B	216	GLN	5.5
1	D	130	ARG	5.4
1	D	163	LEU	5.3
1	B	47	GLN	5.2
1	D	266	ALA	5.1
1	E	45	TYR	5.1
1	C	49	GLY	4.9
1	A	145	GLU	4.9
1	E	61	GLY	4.9
1	B	210	ALA	4.8
1	D	148	THR	4.8
1	D	264	GLY	4.8
1	A	260	GLU	4.7
1	D	289	GLN	4.7
1	E	48	LEU	4.7
1	B	37	ILE	4.7
1	D	42	TYR	4.7
1	C	46	GLU	4.7
1	D	209	PHE	4.6
1	E	26	PHE	4.6
1	E	130	ARG	4.6
1	D	117	TYR	4.6
1	C	207	VAL	4.6
1	D	268	ASN	4.6
1	E	108	HIS	4.5
1	D	224	THR	4.5
1	E	204	THR	4.5
1	D	132	THR	4.4
1	E	264	GLY	4.4
1	B	46	GLU	4.4
1	B	139	ARG	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	26	PHE	4.4
1	E	215	LEU	4.4
1	C	184	LEU	4.3
1	B	214	ILE	4.3
1	E	206	PRO	4.3
1	A	44	TRP	4.2
1	E	64	ILE	4.2
1	C	210	ALA	4.1
1	D	236	TYR	4.1
1	E	209	PHE	4.1
1	C	208	PRO	4.0
1	E	210	ALA	4.0
1	B	41	SER	4.0
1	D	144	GLU	4.0
1	E	211	TYR	4.0
1	D	24	ILE	3.9
1	B	48	LEU	3.9
1	A	268	ASN	3.9
1	E	268	ASN	3.9
1	A	143	PRO	3.9
1	C	44	TRP	3.8
1	E	290	HIS	3.8
1	C	213	LEU	3.8
1	A	209	PHE	3.8
1	C	154	SER	3.7
1	A	46	GLU	3.7
1	B	35	SER	3.7
1	B	286	MET	3.7
1	C	48	LEU	3.7
1	B	289	GLN	3.7
1	D	235	HIS	3.7
1	C	180	ILE	3.7
1	E	207	VAL	3.6
1	B	207	VAL	3.6
1	B	290	HIS	3.6
1	D	159	ARG	3.6
1	C	214	ILE	3.6
1	B	190	ASP	3.5
1	B	277	ASN	3.5
1	E	291	PRO	3.5
1	B	77	SER	3.5
1	E	205	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	3.5
1	B	285	ASP	3.5
1	D	108	HIS	3.5
1	C	211	TYR	3.5
1	A	36	ILE	3.4
1	D	23	LYS	3.4
1	B	73	SER	3.4
1	A	235	HIS	3.4
1	E	235	HIS	3.4
1	E	220	TYR	3.4
1	C	24	ILE	3.4
1	C	150	ILE	3.4
1	C	106	ALA	3.4
1	D	269	ASP	3.4
1	E	60	LEU	3.4
1	D	112	ARG	3.4
1	B	155	MET	3.4
1	B	51	HIS	3.3
1	E	44	TRP	3.3
1	E	83	ARG	3.3
1	A	51	HIS	3.3
1	C	109	ASP	3.3
1	D	174	ALA	3.3
1	B	43	GLN	3.3
1	B	224	THR	3.3
1	D	116	SER	3.3
1	E	190	ASP	3.2
1	C	268	ASN	3.2
1	E	25	ILE	3.2
1	E	267	ALA	3.2
1	D	142	LEU	3.2
1	D	212	THR	3.2
1	B	173	GLU	3.2
1	D	47	GLN	3.2
1	C	285	ASP	3.2
1	E	212	THR	3.2
1	D	206	PRO	3.2
1	E	43	GLN	3.2
1	A	53	THR	3.2
1	C	145	GLU	3.1
1	D	169	GLY	3.1
1	A	35	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	22	SER	3.1
1	A	43	GLN	3.1
1	A	49	GLY	3.1
1	A	144	GLU	3.1
1	A	92	ALA	3.0
1	D	288	GLY	3.0
1	E	46	GLU	3.0
1	C	204	THR	3.0
1	B	40	ILE	3.0
1	A	54	VAL	3.0
1	B	232	GLY	3.0
1	A	174	ALA	3.0
1	C	148	THR	3.0
1	D	167	GLU	2.9
1	B	22	SER	2.9
1	C	155	MET	2.9
1	C	181	THR	2.9
1	A	24	ILE	2.9
1	D	220	TYR	2.9
1	A	23	LYS	2.9
1	B	284	LEU	2.9
1	D	214	ILE	2.9
1	E	39	ILE	2.9
1	C	260	GLU	2.8
1	B	152	ALA	2.8
1	A	52	LEU	2.8
1	B	205	THR	2.8
1	C	26	PHE	2.8
1	D	261	ASP	2.8
1	D	149	GLU	2.8
1	A	220	TYR	2.8
1	B	228	PHE	2.8
1	D	162	LEU	2.8
1	A	95	THR	2.8
1	C	266	ALA	2.7
1	C	205	THR	2.7
1	C	201	ARG	2.7
1	C	265	THR	2.7
1	D	204	THR	2.7
1	E	224	THR	2.7
1	C	288	GLY	2.7
1	B	24	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	240	PHE	2.7
1	D	267	ALA	2.7
1	B	45	TYR	2.7
1	E	27	ARG	2.7
1	B	108	HIS	2.7
1	D	207	VAL	2.7
1	B	50	ILE	2.6
1	B	213	LEU	2.7
1	D	152	ALA	2.6
1	A	45	TYR	2.6
1	C	224	THR	2.6
1	B	209	PHE	2.6
1	E	24	ILE	2.6
1	C	190	ASP	2.6
1	A	110	ALA	2.6
1	A	148	THR	2.6
1	C	163	LEU	2.6
1	C	103	ILE	2.6
1	A	289	GLN	2.6
1	D	216	GLN	2.6
1	E	170	GLN	2.6
1	C	30	LEU	2.5
1	D	250	LEU	2.5
1	A	203	ALA	2.5
1	C	209	PHE	2.5
1	B	154	SER	2.5
1	C	105	PRO	2.5
1	D	225	LEU	2.5
1	E	271	PRO	2.5
1	B	236	TYR	2.5
1	D	231	VAL	2.5
1	B	204	THR	2.5
1	B	101	ARG	2.5
1	D	78	ARG	2.5
1	E	233	ASP	2.5
1	B	54	VAL	2.5
1	B	212	THR	2.5
1	A	187	ASN	2.5
1	B	166	ASN	2.5
1	C	194	HIS	2.5
1	C	40	ILE	2.5
1	A	27	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	215	LEU	2.4
1	A	50	ILE	2.4
1	D	153	SER	2.4
1	B	44	TRP	2.4
1	A	26	PHE	2.4
1	B	55	ALA	2.4
1	E	38	ALA	2.4
1	D	95	THR	2.4
1	B	237	MET	2.4
1	B	38	ALA	2.4
1	A	237	MET	2.4
1	C	230	LEU	2.4
1	E	52	LEU	2.4
1	E	232	GLY	2.4
1	E	216	GLN	2.4
1	E	163	LEU	2.4
1	D	106	ALA	2.3
1	C	153	SER	2.3
1	E	35	SER	2.3
1	D	211	TYR	2.3
1	C	206	PRO	2.3
1	E	249	PHE	2.3
1	E	191	GLU	2.3
1	C	142	LEU	2.3
1	D	234	LEU	2.3
1	E	53	THR	2.3
1	B	169	GLY	2.3
1	D	260	GLU	2.3
1	A	190	ASP	2.3
1	B	148	THR	2.3
1	E	208	PRO	2.3
1	A	70	PHE	2.2
1	E	174	ALA	2.2
1	E	34	MET	2.2
1	E	263	PHE	2.2
1	C	281	ARG	2.2
1	C	73	SER	2.2
1	A	34	MET	2.2
1	A	176	LYS	2.2
1	A	166	ASN	2.2
1	A	37	ILE	2.2
1	D	180	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	40	ILE	2.2
1	A	111	HIS	2.2
1	B	42	TYR	2.2
1	A	171	LEU	2.2
1	B	33	LEU	2.2
1	A	139	ARG	2.2
1	C	25	ILE	2.2
1	A	224	THR	2.2
1	B	225	LEU	2.2
1	A	114	ILE	2.1
1	C	216	GLN	2.1
1	B	238	THR	2.1
1	D	22	SER	2.1
1	C	78	ARG	2.1
1	E	214	ILE	2.1
1	D	129	LEU	2.1
1	C	116	SER	2.1
1	D	40	ILE	2.1
1	D	51	HIS	2.1
1	A	115	VAL	2.1
1	B	34	MET	2.1
1	D	184	LEU	2.1
1	D	26	PHE	2.1
1	D	205	THR	2.1
1	C	101	ARG	2.1
1	E	112	ARG	2.1
1	E	168	ILE	2.1
1	A	288	GLY	2.1
1	B	165	GLY	2.1
1	A	217	ARG	2.1
1	A	40	ILE	2.1
1	A	42	TYR	2.1
1	C	43	GLN	2.0
1	D	243	VAL	2.0
1	B	27	ARG	2.0
1	D	228	PHE	2.0
1	B	92	ALA	2.0
1	D	44	TRP	2.0
1	C	23	LYS	2.0
1	D	72	ASN	2.0
1	D	50	ILE	2.0
1	D	176	LYS	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	E	302	1/1	0.43	0.31	227,227,227,227	0
2	ZN	A	302	1/1	0.60	0.25	96,96,96,96	0
2	ZN	C	301	1/1	0.61	0.27	88,88,88,88	0
2	ZN	A	304	1/1	0.64	0.17	168,168,168,168	0
2	ZN	D	302	1/1	0.73	0.16	129,129,129,129	0
2	ZN	D	303	1/1	0.74	0.19	189,189,189,189	0
2	ZN	B	301	1/1	0.75	0.30	140,140,140,140	0
2	ZN	C	303	1/1	0.78	0.20	97,97,97,97	0
2	ZN	A	301	1/1	0.80	0.18	84,84,84,84	0
2	ZN	D	301	1/1	0.83	0.22	117,117,117,117	0
2	ZN	A	303	1/1	0.83	0.19	102,102,102,102	0
2	ZN	B	302	1/1	0.86	0.14	92,92,92,92	0
2	ZN	C	302	1/1	0.90	0.12	107,107,107,107	0
2	ZN	B	303	1/1	0.91	0.15	101,101,101,101	0
2	ZN	E	301	1/1	0.94	0.18	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.