



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:53 pm GMT

PDB ID : 3CK6  
Title : Crystal structure of ZntB cytoplasmic domain from *Vibrio parahaemolyticus* RIMD 2210633  
Authors : Tan, K.; Sather, A.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2008-03-14  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

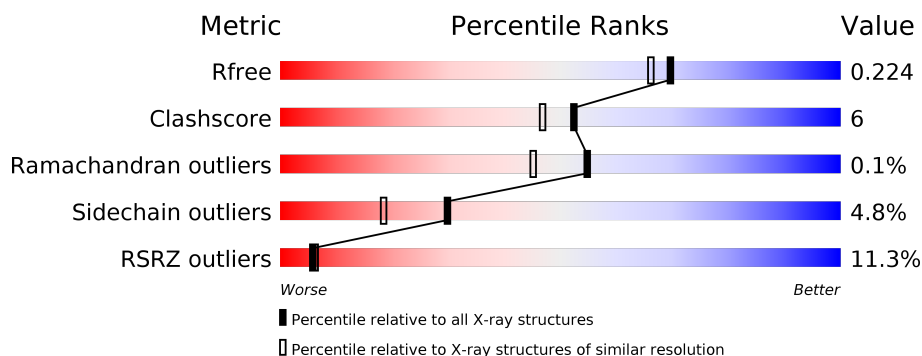
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	252	<div> <div>10%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div></div> </div> <div></div> </div>
1	B	252	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	C	252	<div> <div>12%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	D	252	<div> <div>12%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	E	252	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div></div> </div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	253	-	-	X	-
2	CL	C	252	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10739 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 Putative membrane transport protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total 2009	C 1265	N 354	O 381	S 1	Se 8	0	1	0
1	B	244	Total 2009	C 1265	N 354	O 381	S 1	Se 8	0	1	0
1	C	242	Total 2003	C 1261	N 352	O 382	S 1	Se 7	0	3	0
1	D	244	Total 2009	C 1265	N 354	O 381	S 1	Se 8	0	1	0
1	E	245	Total 2014	C 1268	N 355	O 382	S 1	Se 8	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q87M69
A	-1	ASN	-	EXPRESSION TAG	UNP Q87M69
A	0	ALA	-	EXPRESSION TAG	UNP Q87M69
A	42	GLY	SER	ENGINEERED	UNP Q87M69
B	-2	SER	-	EXPRESSION TAG	UNP Q87M69
B	-1	ASN	-	EXPRESSION TAG	UNP Q87M69
B	0	ALA	-	EXPRESSION TAG	UNP Q87M69
B	42	GLY	SER	ENGINEERED	UNP Q87M69
C	-2	SER	-	EXPRESSION TAG	UNP Q87M69
C	-1	ASN	-	EXPRESSION TAG	UNP Q87M69
C	0	ALA	-	EXPRESSION TAG	UNP Q87M69
C	42	GLY	SER	ENGINEERED	UNP Q87M69
D	-2	SER	-	EXPRESSION TAG	UNP Q87M69
D	-1	ASN	-	EXPRESSION TAG	UNP Q87M69
D	0	ALA	-	EXPRESSION TAG	UNP Q87M69
D	42	GLY	SER	ENGINEERED	UNP Q87M69
E	-2	SER	-	EXPRESSION TAG	UNP Q87M69
E	-1	ASN	-	EXPRESSION TAG	UNP Q87M69
E	0	ALA	-	EXPRESSION TAG	UNP Q87M69

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Chain	Residue	Modelled	Actual	Comment	Reference
E	42	GLY	SER	ENGINEERED	UNP Q87M69

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total Cl 5 5	0	0
2	A	5	Total Cl 5 5	0	0
2	D	5	Total Cl 5 5	0	0
2	C	5	Total Cl 5 5	0	0
2	E	5	Total Cl 5 5	0	0

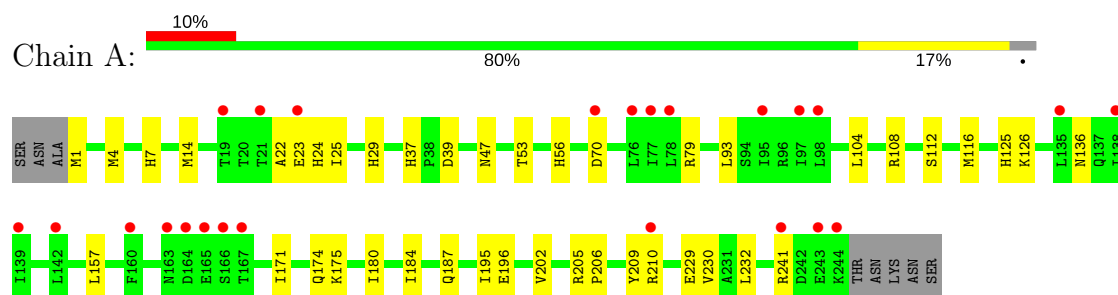
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	154	Total O 154 154	0	0
3	B	129	Total O 129 129	0	0
3	C	111	Total O 111 111	0	0
3	D	133	Total O 133 133	0	0
3	E	143	Total O 143 143	0	0

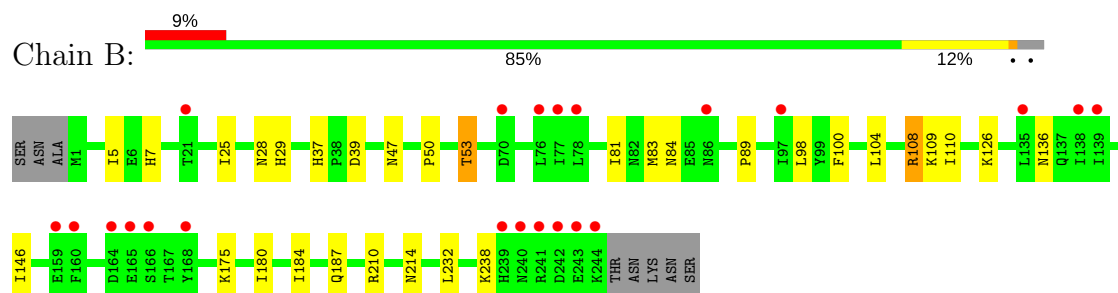
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

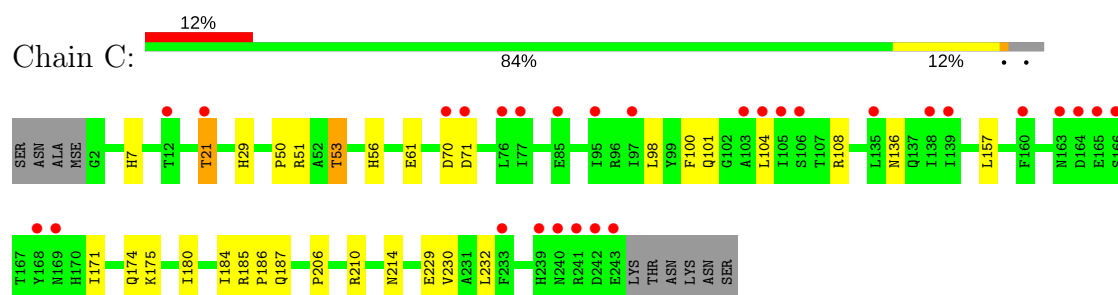
- Molecule 1: Putative membrane transport protein



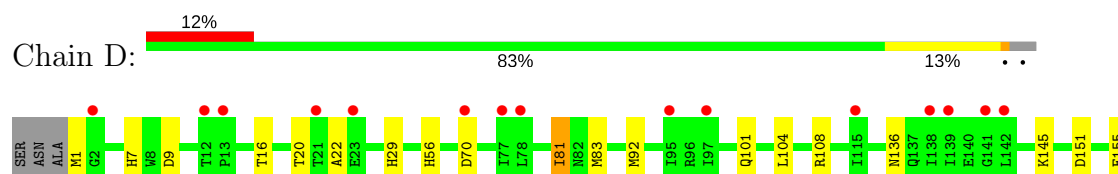
- Molecule 1: Putative membrane transport protein

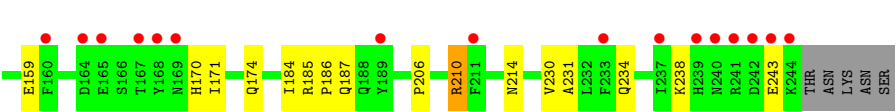


- Molecule 1: Putative membrane transport protein

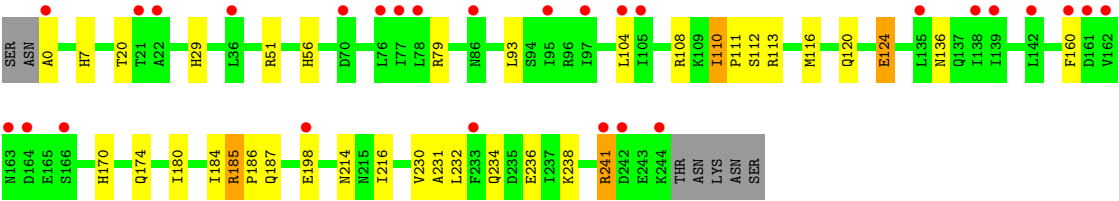
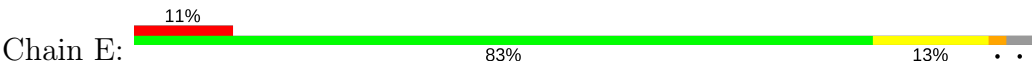


- Molecule 1: Putative membrane transport protein





● Molecule 1: Putative membrane transport protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.39Å 130.21Å 79.39Å 90.00° 103.41° 90.00°	Depositor
Resolution (Å)	30.80 – 1.90 30.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.80-1.90) 97.9 (30.79-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.223 0.184 , 0.224	Depositor DCC
$R_{free}$ test set	4875 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.63	0/2052	0.69	0/2770
1	B	0.56	0/2052	0.64	0/2770
1	C	0.56	0/2052	0.61	0/2772
1	D	0.56	0/2052	0.61	0/2770
1	E	0.59	0/2056	0.63	0/2774
All	All	0.58	0/10264	0.64	0/13856

There are no bond length outliers.

There are no bond angle outliers.

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	2009	0	1952	33	0
1	B	2009	0	1952	29	0
1	C	2003	0	1939	23	0
1	D	2009	0	1952	22	0
1	E	2014	0	1957	32	0
2	A	5	0	0	0	0
2	B	5	0	0	3	0
2	C	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	0	0
2	E	5	0	0	1	0
3	A	154	0	0	0	0
3	B	129	0	0	4	0
3	C	111	0	0	2	0
3	D	133	0	0	1	0
3	E	143	0	0	4	0
All	All	10739	0	9752	124	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 6.

All (124) 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:180:ILE:CG2	1:C:184:ILE:HD12	1.59	1.31
1:A:180:ILE:CG2	1:A:184:ILE:HD12	1.65	1.26
2:B:250:CL:CL	3:B:287:HOH:O	1.87	1.22
1:A:180:ILE:HG22	1:A:184:ILE:HD12	1.17	1.16
1:B:180:ILE:CG2	1:B:184:ILE:HD12	1.75	1.15
1:A:232:LEU:HD21	1:B:175:LYS:HG2	1.12	1.08
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.23	1.08
1:E:180:ILE:CG2	1:E:184:ILE:HD12	1.90	1.01
1:B:180:ILE:HG22	1:B:184:ILE:HD12	1.37	0.99
1:A:232:LEU:CD2	1:B:175:LYS:HG2	1.98	0.93
1:C:180:ILE:CG2	1:C:184:ILE:CD1	2.46	0.92
1:A:232:LEU:HD21	1:B:175:LYS:CG	2.01	0.90
1:A:180:ILE:CG2	1:A:184:ILE:CD1	2.50	0.89
1:D:101:GLN:HG2	3:D:370:HOH:O	1.72	0.88
1:C:7:HIS:NE2	1:C:29:HIS:HD2	1.71	0.87
2:B:253:CL:CL	3:B:354:HOH:O	2.31	0.85
1:B:180:ILE:CG2	1:B:184:ILE:CD1	2.55	0.83
1:B:83[B]:MSE:CE	1:B:89:PRO:HB3	2.10	0.81
1:D:7:HIS:NE2	1:D:29:HIS:HD2	1.79	0.81
1:E:7:HIS:NE2	1:E:29:HIS:HD2	1.79	0.81
1:A:37:HIS:HD2	1:A:39:ASP:H	1.29	0.80
1:E:180:ILE:HG22	1:E:184:ILE:HD12	1.64	0.79
1:C:180:ILE:HG23	1:C:184:ILE:HD12	1.63	0.79
1:D:81:ILE:HD11	1:D:145:LYS:HB3	1.64	0.79
1:E:120:GLN:O	1:E:124:GLU:HG2	1.87	0.73
1:A:7:HIS:NE2	1:A:29:HIS:HD2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:HG3	1:E:232:LEU:HD21	1.72	0.72
1:B:37:HIS:HD2	1:B:39:ASP:H	1.39	0.71
1:C:21:THR:HG23	1:C:21:THR:O	1.90	0.71
1:E:111:PRO:HB3	1:E:116:MSE:HE2	1.72	0.70
1:E:116:MSE:HE1	3:E:392:HOH:O	1.91	0.69
1:E:111:PRO:CB	1:E:116:MSE:HE2	2.22	0.69
1:B:7:HIS:NE2	1:B:29:HIS:HD2	1.91	0.67
2:E:250:CL:CL	3:E:296:HOH:O	2.48	0.67
1:B:83[B]:MSE:HE3	1:B:89:PRO:HB3	1.77	0.67
1:C:180:ILE:HG23	1:C:184:ILE:CD1	2.23	0.66
1:E:180:ILE:HG23	1:E:184:ILE:HD12	1.74	0.65
1:A:23:GLU:HG3	1:A:24:HIS:H	1.64	0.63
1:A:171:ILE:HG22	1:A:175:LYS:HE3	1.81	0.63
1:A:175:LYS:CG	1:E:232:LEU:HD21	2.28	0.62
1:C:7:HIS:NE2	1:C:29:HIS:CD2	2.62	0.61
1:A:23:GLU:HG3	1:A:24:HIS:N	2.16	0.61
1:B:83[B]:MSE:HE2	1:B:83[B]:MSE:HA	1.81	0.61
1:C:214:ASN:HD22	1:D:56:HIS:HE1	1.49	0.60
1:E:113:ARG:HH21	1:E:116:MSE:SE	2.34	0.60
1:D:185:ARG:HB3	1:D:186:PRO:HD3	1.83	0.59
1:B:109:LYS:HB3	2:B:253:CL:CL	2.40	0.58
1:B:83[B]:MSE:HE1	1:B:89:PRO:HB3	1.86	0.57
1:B:180:ILE:HG23	1:B:184:ILE:CD1	2.33	0.57
1:E:185:ARG:HB3	1:E:186:PRO:HD3	1.87	0.57
1:E:7:HIS:NE2	1:E:29:HIS:CD2	2.68	0.56
1:A:112:SER:O	1:A:116[B]:MSE:HG3	2.05	0.56
1:D:92:MSE:HE1	1:D:184:ILE:HD11	1.86	0.56
1:B:37:HIS:CD2	1:B:39:ASP:H	2.23	0.56
1:A:180:ILE:HG23	1:A:184:ILE:CD1	2.36	0.56
1:A:206:PRO:O	1:A:210:ARG:HG2	2.06	0.56
1:E:93:LEU:HB3	1:E:110:ILE:HD11	1.88	0.55
2:C:252:CL:CL	3:C:291:HOH:O	2.55	0.55
1:A:37:HIS:CD2	1:A:39:ASP:H	2.17	0.54
1:A:171:ILE:HG21	1:E:236:GLU:HG3	1.88	0.53
1:A:1:MSE:HE2	1:A:22:ALA:N	2.24	0.53
1:A:25:ILE:HD12	1:A:47:ASN:HB3	1.91	0.52
1:E:184:ILE:HG23	1:E:216:ILE:HD11	1.90	0.52
1:C:21:THR:CG2	1:C:21:THR:O	2.57	0.52
1:C:214:ASN:HD22	1:D:56:HIS:CE1	2.28	0.52
1:C:29:HIS:HE1	3:C:305:HOH:O	1.92	0.52
1:C:100:PHE:CD2	1:C:101:GLN:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLU:O	1:D:159:GLU:HG2	2.11	0.51
1:C:206:PRO:O	1:C:210:ARG:HG2	2.11	0.51
1:D:214:ASN:HD22	1:E:56:HIS:CE1	2.29	0.51
1:E:231:ALA:HA	1:E:234:GLN:HE21	1.76	0.50
1:B:29:HIS:HE1	3:B:258:HOH:O	1.94	0.50
1:D:243:GLU:HG2	1:E:241:ARG:NH2	2.27	0.49
1:E:111:PRO:HB2	1:E:116:MSE:HE2	1.94	0.49
1:B:214:ASN:HD22	1:C:56:HIS:HE1	1.60	0.49
1:C:50:PRO:HB2	1:C:53:THR:HG23	1.93	0.49
1:B:214:ASN:HD22	1:C:56:HIS:CE1	2.31	0.48
1:C:98:LEU:HG	1:C:100:PHE:HB2	1.96	0.48
1:D:9:ASP:HB3	1:D:16:THR:HG23	1.95	0.48
1:E:180:ILE:HG23	1:E:184:ILE:CD1	2.41	0.48
1:C:157:LEU:HD23	1:C:229:GLU:OE2	2.14	0.48
1:B:25:ILE:HD12	1:B:47:ASN:HB3	1.96	0.47
1:D:151:ASP:O	1:D:155:GLU:HG3	2.14	0.47
1:B:53:THR:HG21	3:B:355:HOH:O	2.14	0.47
1:D:174:GLN:HB2	1:D:230:VAL:HG11	1.97	0.47
1:D:1:MSE:HE2	1:D:22:ALA:N	2.30	0.47
1:D:92:MSE:HE1	1:D:184:ILE:CD1	2.45	0.46
1:D:81:ILE:HD13	1:D:83:MSE:HE3	1.98	0.46
1:E:170:HIS:HB2	1:E:230:VAL:HG13	1.99	0.45
1:D:231:ALA:HA	1:D:234:GLN:HE21	1.81	0.45
1:E:160:PHE:CZ	1:E:170:HIS:HB3	2.51	0.45
1:C:185:ARG:HB3	1:C:186:PRO:HD3	1.98	0.45
1:B:180:ILE:HG22	1:B:184:ILE:CD1	2.25	0.45
1:A:175:LYS:HG2	1:E:232:LEU:CD2	2.47	0.45
1:A:56:HIS:HE1	1:E:214:ASN:HD22	1.64	0.45
1:B:50:PRO:HB2	1:B:53:THR:HG23	1.98	0.44
1:E:79:ARG:HA	1:E:93:LEU:O	2.16	0.44
1:A:1:MSE:HE3	1:A:4:MSE:HE3	1.98	0.44
1:D:206:PRO:O	1:D:210:ARG:HD2	2.18	0.44
1:D:81:ILE:HG13	1:D:81:ILE:H	1.69	0.44
1:B:180:ILE:HG21	1:B:184:ILE:HD12	1.87	0.44
1:D:214:ASN:HD22	1:E:56:HIS:HE1	1.64	0.43
1:E:0:ALA:N	3:E:376:HOH:O	2.51	0.43
1:D:170:HIS:CD2	1:D:170:HIS:H	2.36	0.43
1:A:56:HIS:CE1	1:E:214:ASN:HD22	2.36	0.42
1:A:157:LEU:HD23	1:A:229:GLU:OE2	2.19	0.42
1:B:232:LEU:HD11	1:C:171:ILE:HG23	2.01	0.42
1:B:81:ILE:CG2	1:B:83[B]:MSE:HE3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:HB2	1:A:230:VAL:HG11	2.02	0.42
1:A:175:LYS:CG	1:E:232:LEU:CD2	2.98	0.42
1:D:7:HIS:NE2	1:D:29:HIS:CD2	2.71	0.41
1:B:146:ILE:HG21	1:B:184:ILE:HD13	2.02	0.41
1:A:14:MSE:HE1	1:A:125:HIS:HB3	2.03	0.41
1:C:174[B]:GLN:HB2	1:C:230:VAL:HG11	2.02	0.41
1:A:1:MSE:HE1	1:A:22:ALA:O	2.20	0.41
1:A:195:ILE:HA	1:A:202:VAL:HG11	2.02	0.41
1:A:205:ARG:HG3	1:A:209:TYR:CE1	2.56	0.41
1:B:84:ASN:ND2	1:B:110:ILE:HG12	2.36	0.41
1:E:116:MSE:CE	3:E:392:HOH:O	2.59	0.41
1:A:171:ILE:HG23	1:E:232:LEU:HD11	2.03	0.41
1:B:98:LEU:HG	1:B:100:PHE:HB2	2.02	0.41
1:C:174[A]:GLN:HB2	1:C:230:VAL:HG11	2.03	0.41
1:A:79:ARG:HA	1:A:93:LEU:O	2.21	0.40
1:B:5:ILE:HD13	1:B:108:ARG:CZ	2.51	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	243/252 (96%)	236 (97%)	7 (3%)	0	100	100
1	B	243/252 (96%)	239 (98%)	4 (2%)	0	100	100
1	C	243/252 (96%)	236 (97%)	6 (2%)	1 (0%)	38	26
1	D	243/252 (96%)	237 (98%)	6 (2%)	0	100	100
1	E	244/252 (97%)	240 (98%)	4 (2%)	0	100	100
All	All	1216/1260 (96%)	1188 (98%)	27 (2%)	1 (0%)	55	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	71	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	221/220 (100%)	212 (96%)	9 (4%)	35	24
1	B	221/220 (100%)	212 (96%)	9 (4%)	35	24
1	C	221/220 (100%)	210 (95%)	11 (5%)	28	17
1	D	221/220 (100%)	211 (96%)	10 (4%)	32	21
1	E	221/220 (100%)	207 (94%)	14 (6%)	21	10
All	All	1105/1100 (100%)	1052 (95%)	53 (5%)	30	18

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	THR
1	A	70	ASP
1	A	104	LEU
1	A	108	ARG
1	A	126	LYS
1	A	136	ASN
1	A	187	GLN
1	A	196	GLU
1	A	241	ARG
1	B	28	ASN
1	B	53	THR
1	B	104	LEU
1	B	108	ARG
1	B	126	LYS
1	B	136	ASN
1	B	187	GLN
1	B	210	ARG
1	B	238	LYS
1	C	21	THR

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Mol	Chain	Res	Type
1	C	51	ARG
1	C	53	THR
1	C	61	GLU
1	C	70	ASP
1	C	104	LEU
1	C	108	ARG
1	C	136	ASN
1	C	175	LYS
1	C	187	GLN
1	C	232	LEU
1	D	20	THR
1	D	70	ASP
1	D	81	ILE
1	D	104	LEU
1	D	108	ARG
1	D	136	ASN
1	D	171	ILE
1	D	187	GLN
1	D	210	ARG
1	D	238	LYS
1	E	20	THR
1	E	51	ARG
1	E	104	LEU
1	E	108	ARG
1	E	110	ILE
1	E	112	SER
1	E	124	GLU
1	E	136	ASN
1	E	174	GLN
1	E	185	ARG
1	E	187	GLN
1	E	198	GLU
1	E	238	LYS
1	E	241	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	29	HIS
1	A	37	HIS
1	A	56	HIS

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Mol	Chain	Res	Type
1	A	170	HIS
1	A	174	GLN
1	B	28	ASN
1	B	29	HIS
1	B	37	HIS
1	B	56	HIS
1	B	170	HIS
1	B	174	GLN
1	B	234	GLN
1	C	29	HIS
1	C	56	HIS
1	C	125	HIS
1	C	234	GLN
1	D	17	GLN
1	D	28	ASN
1	D	29	HIS
1	D	56	HIS
1	D	170	HIS
1	D	174	GLN
1	D	234	GLN
1	D	239	HIS
1	E	26	GLN
1	E	28	ASN
1	E	29	HIS
1	E	56	HIS
1	E	101	GLN
1	E	234	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 carbohydrates in this entry.



## 5.6 Ligand geometry

Of 25 ligands modelled in this entry, 25 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/252 (94%)	0.63	24 (10%) 8 8	24, 30, 44, 54	0
1	B	237/252 (94%)	0.60	22 (9%) 9 10	24, 32, 44, 67	0
1	C	236/252 (93%)	0.66	29 (12%) 5 5	26, 32, 46, 72	0
1	D	237/252 (94%)	0.73	31 (13%) 4 4	26, 32, 45, 66	0
1	E	238/252 (94%)	0.73	28 (11%) 5 5	25, 31, 43, 59	0
All	All	1185/1260 (94%)	0.67	134 (11%) 6 6	24, 32, 44, 72	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	ASP	5.8
1	C	21	THR	5.7
1	E	244	LYS	5.6
1	C	243	GLU	5.3
1	B	242	ASP	5.2
1	A	243	GLU	5.1
1	E	77	ILE	5.0
1	C	166	SER	4.8
1	A	244	LYS	4.7
1	E	22	ALA	4.6
1	B	244	LYS	4.5
1	D	244	LYS	4.5
1	B	241	ARG	4.4
1	E	242	ASP	4.4
1	D	242	ASP	4.2
1	D	139	ILE	4.2
1	A	21	THR	4.0
1	A	241	ARG	4.0
1	E	0	ALA	4.0
1	B	21	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	243	GLU	3.9
1	C	241	ARG	3.9
1	E	166	SER	3.8
1	D	21	THR	3.8
1	D	142	LEU	3.8
1	C	239	HIS	3.7
1	E	70	ASP	3.7
1	C	164	ASP	3.7
1	E	163	ASN	3.6
1	A	166	SER	3.6
1	B	243	GLU	3.5
1	C	240	ASN	3.4
1	D	239	HIS	3.4
1	D	77	ILE	3.3
1	B	165	GLU	3.3
1	B	239	HIS	3.2
1	A	164	ASP	3.2
1	B	166	SER	3.2
1	E	160	PHE	3.2
1	E	76	LEU	3.2
1	E	78	LEU	3.2
1	B	168	TYR	3.2
1	E	164	ASP	3.2
1	B	160	PHE	3.2
1	C	160	PHE	3.2
1	E	21	THR	3.1
1	C	233	PHE	3.1
1	D	78	LEU	3.1
1	C	139	ILE	3.1
1	D	164	ASP	3.0
1	E	241	ARG	3.0
1	C	77	ILE	3.0
1	D	95	ILE	3.0
1	D	97	ILE	3.0
1	D	13	PRO	3.0
1	D	241	ARG	2.9
1	C	163	ASN	2.9
1	B	135	LEU	2.9
1	C	12	THR	2.9
1	B	139	ILE	2.9
1	C	97	ILE	2.9
1	D	12	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	76	LEU	2.8
1	A	97	ILE	2.8
1	E	138	ILE	2.8
1	D	233	PHE	2.8
1	C	138	ILE	2.8
1	E	105	ILE	2.8
1	B	164	ASP	2.8
1	D	70	ASP	2.8
1	E	86	ASN	2.8
1	C	71	ASP	2.7
1	D	240	ASN	2.7
1	A	160	PHE	2.7
1	C	135	LEU	2.7
1	B	97	ILE	2.7
1	A	135	LEU	2.7
1	E	95	ILE	2.7
1	C	168	TYR	2.7
1	E	139	ILE	2.6
1	B	76	LEU	2.6
1	B	77	ILE	2.6
1	A	77	ILE	2.5
1	A	76	LEU	2.5
1	D	141	GLY	2.5
1	A	142	LEU	2.5
1	B	78	LEU	2.5
1	E	142	LEU	2.5
1	A	78	LEU	2.5
1	E	161	ASP	2.5
1	A	138	ILE	2.4
1	A	98	LEU	2.4
1	E	97	ILE	2.4
1	A	19	THR	2.4
1	A	23	GLU	2.4
1	D	168	TYR	2.3
1	D	23	GLU	2.3
1	B	159	GLU	2.3
1	C	169	ASN	2.3
1	C	165	GLU	2.3
1	A	95	ILE	2.3
1	E	233	PHE	2.3
1	C	70	ASP	2.3
1	C	95	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	105	ILE	2.3
1	C	103	ALA	2.3
1	A	165	GLU	2.3
1	E	162	VAL	2.3
1	E	104	LEU	2.3
1	D	2	GLY	2.2
1	D	160	PHE	2.2
1	D	211	PHE	2.2
1	B	138	ILE	2.2
1	D	169	ASN	2.2
1	A	139	ILE	2.2
1	D	115	ILE	2.2
1	D	138	ILE	2.1
1	D	165	GLU	2.1
1	D	167	THR	2.1
1	D	189	TYR	2.1
1	B	86	ASN	2.1
1	C	104	LEU	2.1
1	E	36	LEU	2.1
1	E	198	GLU	2.1
1	B	240	ASN	2.1
1	E	135	LEU	2.1
1	A	70	ASP	2.1
1	A	163	ASN	2.1
1	C	106	SER	2.1
1	D	237	ILE	2.1
1	A	167	THR	2.0
1	B	70	ASP	2.0
1	A	210	ARG	2.0
1	C	85	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	C	252	1/1	0.98	0.19	2.25	33,33,33,33	0
2	CL	B	250	1/1	0.97	0.17	1.21	36,36,36,36	0
2	CL	C	250	1/1	0.98	0.12	0.09	27,27,27,27	0
2	CL	B	252	1/1	0.95	0.12	-0.29	33,33,33,33	0
2	CL	A	250	1/1	0.99	0.11	-0.45	23,23,23,23	0
2	CL	D	250	1/1	0.99	0.11	-0.53	27,27,27,27	0
2	CL	E	252	1/1	0.99	0.12	-0.54	27,27,27,27	0
2	CL	B	251	1/1	0.99	0.13	-0.68	23,23,23,23	0
2	CL	A	252	1/1	0.97	0.10	-0.95	30,30,30,30	0
2	CL	D	252	1/1	0.98	0.10	-1.36	32,32,32,32	0
2	CL	E	250	1/1	0.90	0.09	-1.54	37,37,37,37	0
2	CL	D	251	1/1	0.99	0.09	-1.82	23,23,23,23	0
2	CL	E	251	1/1	0.99	0.08	-1.91	21,21,21,21	0
2	CL	C	251	1/1	0.99	0.09	-2.20	24,24,24,24	0
2	CL	A	251	1/1	0.99	0.06	-2.91	22,22,22,22	0
2	CL	E	254	1/1	0.97	0.12	-	36,36,36,36	0
2	CL	D	253	1/1	0.99	0.12	-	26,26,26,26	0
2	CL	D	254	1/1	0.98	0.20	-	33,33,33,33	0
2	CL	C	253	1/1	1.00	0.06	-	27,27,27,27	0
2	CL	B	254	1/1	0.98	0.23	-	34,34,34,34	0
2	CL	E	253	1/1	0.91	0.10	-	53,53,53,53	0
2	CL	C	254	1/1	0.98	0.20	-	40,40,40,40	0
2	CL	B	253	1/1	0.98	0.22	-	45,45,45,45	0
2	CL	A	253	1/1	0.97	0.08	-	24,24,24,24	0
2	CL	A	254	1/1	0.98	0.22	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.