



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:46 am BST

PDB ID : 3GYX  
Title : The ectoine binding protein of the TeaABC TRAP transporter TeaA in the Apo-State  
Authors : Kuhlmann, S.I.; Terwisscha Van Scheltinga, A.C.; Ziegler, C.  
Deposited on : 2009-04-06  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

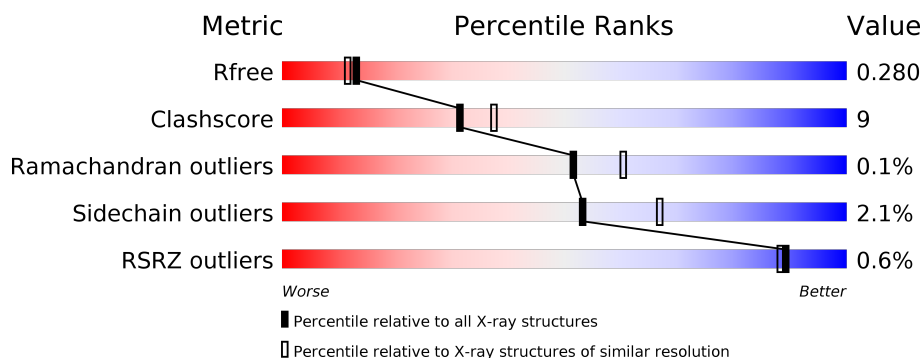
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	341	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 17%, orange 17%, yellow 17%, green 72%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>72%</span> <span>17%</span> <span>11%</span> </div> </div>
1	B	341	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 21%, green 68%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>68%</span> <span>21%</span> <span>10%</span> </div> </div>
1	C	341	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 20%, green 70%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>70%</span> <span>20%</span> <span>9%</span> </div> </div>
1	D	341	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 23%, green 68%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>68%</span> <span>23%</span> <span>9%</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	330	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10070 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 Periplasmic substrate binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	1	0
			2426	1545	380	491	10			
1	B	307	Total	C	N	O	S	0	0	0
			2451	1560	384	497	10			
1	C	309	Total	C	N	O	S	0	0	0
			2465	1567	386	502	10			
1	D	311	Total	C	N	O	S	0	0	0
			2478	1574	388	506	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	14	Total	Zn	0	0
			14	14		
2	A	7	Total	Zn	0	0
			7	7		
2	D	8	Total	Zn	0	0
			8	8		
2	C	7	Total	Zn	0	0
			7	7		

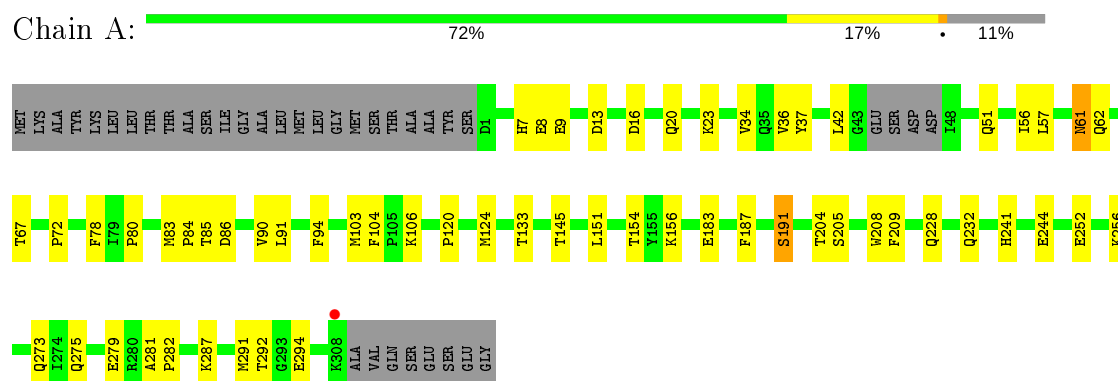
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	65	Total	O	0	0
			65	65		
3	C	48	Total	O	0	0
			48	48		
3	D	46	Total	O	0	0
			46	46		

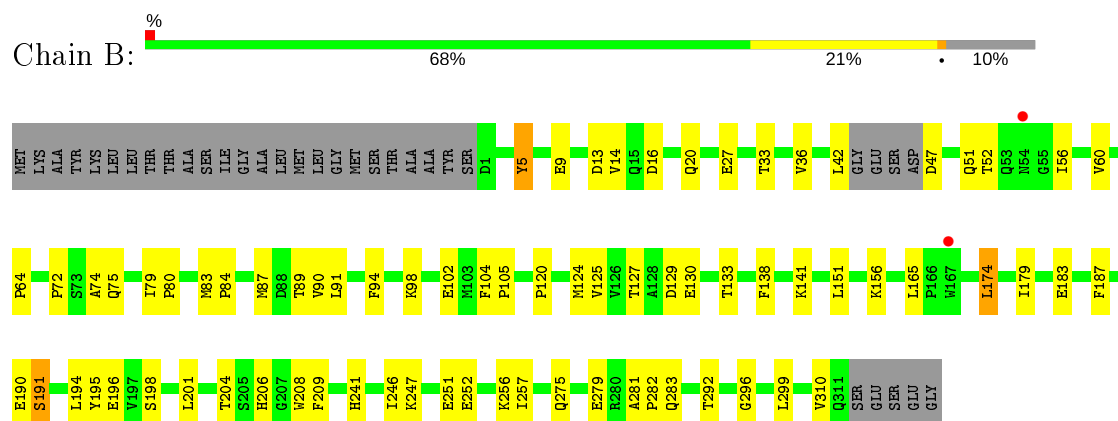
### 3 Residue-property plots [i](#)

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.

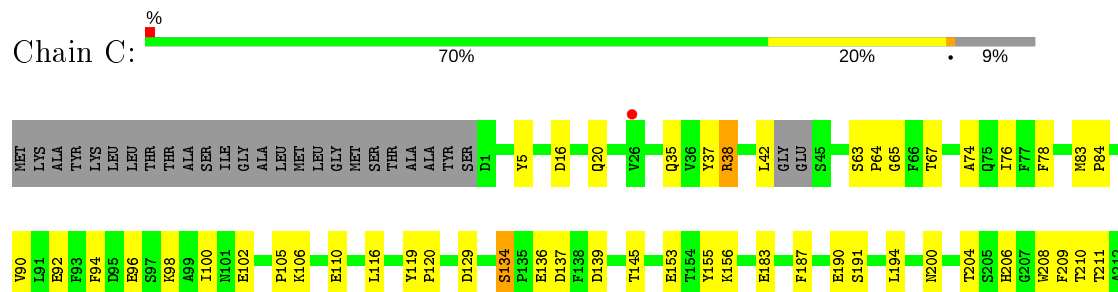
- Molecule 1: Periplasmic substrate binding protein



- Molecule 1: Periplasmic substrate binding protein

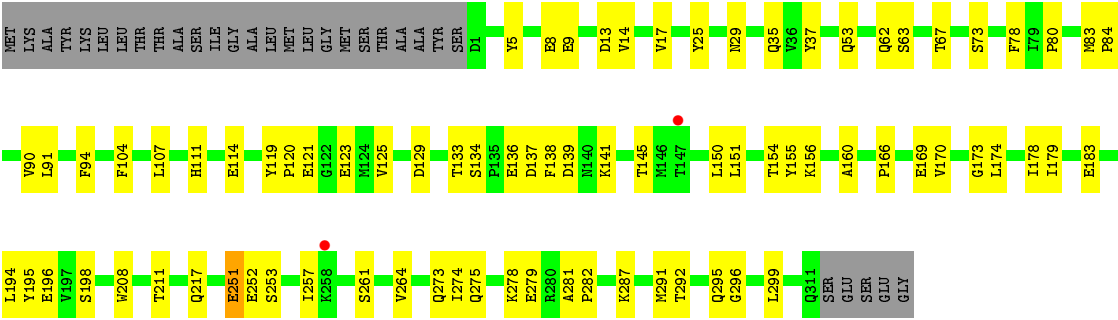


- Molecule 1: Periplasmic substrate binding protein





● Molecule 1: Periplasmic substrate binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.74Å 64.98Å 121.50Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	47.57 – 2.20 47.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.57-2.20) 97.3 (47.57-2.20)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.217 , 0.284 0.215 , 0.280	Depositor DCC
$R_{free}$ test set	2905 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6706e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	0.30	0/2478	0.44	0/3359
1	B	0.30	0/2509	0.46	0/3404
1	C	0.30	0/2523	0.46	0/3423
1	D	0.29	0/2537	0.45	0/3443
All	All	0.29	0/10047	0.45	0/13629

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	2426	0	2280	31	1
1	B	2451	0	2303	44	1
1	C	2465	0	2312	44	1
1	D	2478	0	2322	53	1
2	A	7	0	0	0	0
2	B	14	0	0	0	0
2	C	7	0	0	0	0
2	D	8	0	0	0	0
3	A	55	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	65	0	0	1	0
3	C	48	0	0	0	0
3	D	46	0	0	0	0
All	All	10070	0	9217	172	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 9.

All (172) 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:38:ARG:CG	1:C:38:ARG:HH11	1.97	0.76
1:C:145:THR:HG22	1:C:183:GLU:HG2	1.66	0.76
1:D:133:THR:HG23	1:D:273:GLN:HE21	1.52	0.73
1:B:174:LEU:HD13	1:B:179:ILE:HG13	1.71	0.72
1:D:145:THR:HG22	1:D:183:GLU:HG2	1.72	0.71
1:D:251:GLU:HG3	1:D:252:GLU:N	2.07	0.70
1:D:136:GLU:OE1	1:D:139:ASP:OD2	2.11	0.69
1:B:127:THR:HG22	1:B:201:LEU:HG	1.74	0.68
1:C:94:PHE:CE2	1:C:120:PRO:HG3	2.28	0.68
1:D:123:GLU:HB2	1:D:208:TRP:CZ3	2.29	0.68
1:D:94:PHE:CE2	1:D:120:PRO:HG3	2.27	0.68
1:C:251:GLU:O	1:C:255:GLU:HG3	1.95	0.67
1:B:72:PRO:O	1:B:75:GLN:HG3	1.96	0.66
1:B:124:MET:CE	1:B:209:PHE:HB2	2.26	0.66
1:B:187:PHE:O	1:B:191:SER:HB3	1.96	0.65
1:A:145:THR:HG22	1:A:183:GLU:HG2	1.79	0.62
1:C:292:THR:OG1	1:C:296:GLY:HA3	2.00	0.62
1:D:170:VAL:O	1:D:174:LEU:HD13	1.99	0.61
1:D:133:THR:HG23	1:D:273:GLN:NE2	2.14	0.61
1:D:129:ASP:OD2	1:D:141:LYS:HE3	2.01	0.61
1:B:204:THR:HG1	1:B:206:HIS:HD1	1.49	0.61
1:D:261:SER:HB2	1:D:264:VAL:HG23	1.83	0.60
1:C:136:GLU:OE1	1:C:139:ASP:OD2	2.20	0.60
1:D:174:LEU:HD23	1:D:198:SER:HB2	1.83	0.60
1:C:35:GLN:HG2	1:C:37:TYR:CZ	2.37	0.60
1:A:94:PHE:CE2	1:A:120:PRO:HG3	2.37	0.60
1:C:204:THR:HA	1:C:269:LEU:HD12	1.83	0.59
1:B:195:TYR:CE1	1:B:196:GLU:HG3	2.37	0.59
1:C:38:ARG:HH11	1:C:38:ARG:HG2	1.68	0.59
1:D:174:LEU:CD1	1:D:179:ILE:HD11	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG21	1:A:208:TRP:CE2	2.40	0.57
1:D:114:GLU:OE1	1:D:217:GLN:HG3	2.04	0.57
1:A:16:ASP:O	1:A:20:GLN:HG2	2.05	0.57
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.69	0.56
1:C:90:VAL:HG21	1:C:208:TRP:CE2	2.40	0.56
1:D:174:LEU:HD12	1:D:179:ILE:HD11	1.86	0.56
1:B:129:ASP:O	1:B:130:GLU:HG2	2.06	0.56
1:B:275:GLN:O	1:B:279:GLU:HG3	2.07	0.55
1:B:94:PHE:CE2	1:B:120:PRO:HG3	2.42	0.55
1:D:35:GLN:HG3	1:D:37:TYR:CE2	2.42	0.55
1:B:283:GLN:HB2	3:B:352:HOH:O	2.06	0.54
1:B:129:ASP:C	1:B:130:GLU:HG2	2.28	0.54
1:D:107:LEU:HD21	1:D:295:GLN:NE2	2.23	0.54
1:D:145:THR:HG21	1:D:155:TYR:CE2	2.42	0.54
1:C:289:ILE:HD11	1:C:300:LEU:HD23	1.89	0.54
1:B:90:VAL:HG21	1:B:208:TRP:CE2	2.43	0.53
1:C:200:ASN:HA	1:C:265:THR:HB	1.91	0.53
1:A:133:THR:HG23	1:A:273:GLN:NE2	2.24	0.53
1:B:281:ALA:N	1:B:282:PRO:CD	2.71	0.52
1:D:292:THR:OG1	1:D:296:GLY:HA3	2.09	0.52
1:C:239:TYR:O	1:C:243:ILE:HG12	2.10	0.52
1:D:287:LYS:O	1:D:291:MET:HG3	2.08	0.52
1:C:83:MET:HB3	1:C:84:PRO:HD2	1.91	0.52
1:B:104:PHE:CZ	1:B:299:LEU:HD21	2.45	0.52
1:B:47:ASP:O	1:B:51:GLN:HG3	2.10	0.52
1:C:35:GLN:HG2	1:C:37:TYR:CE2	2.44	0.51
1:D:104:PHE:CZ	1:D:299:LEU:HD21	2.45	0.51
1:C:288:PHE:CE1	1:C:292:THR:HG21	2.45	0.51
1:A:80:PRO:HG3	1:A:154:THR:HG23	1.93	0.51
1:D:53:GLN:NE2	1:D:111:HIS:HB3	2.26	0.51
1:D:134:SER:O	1:D:137:ASP:HB2	2.10	0.51
1:D:90:VAL:HG21	1:D:208:TRP:CE2	2.46	0.51
1:D:67:THR:O	1:D:67:THR:HG22	2.11	0.51
1:C:134:SER:O	1:C:137:ASP:HB2	2.10	0.50
1:B:124:MET:HE3	1:B:209:PHE:HB2	1.92	0.50
1:D:138:PHE:HB3	1:D:160:ALA:HB2	1.93	0.50
1:B:165:LEU:HD12	1:B:179:ILE:HD13	1.92	0.50
1:B:190:GLU:OE2	1:B:256:LYS:HD2	2.12	0.49
1:A:86:ASP:O	1:A:90:VAL:HG23	2.12	0.49
1:C:67:THR:HG22	1:C:67:THR:O	2.13	0.49
1:D:25:TYR:O	1:D:29:ASN:HB2	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:MET:O	1:A:106:LYS:HB2	2.13	0.48
1:C:38:ARG:HG3	1:C:38:ARG:NH1	2.27	0.48
1:D:14:VAL:HB	1:D:121:GLU:OE1	2.13	0.48
1:B:138:PHE:O	1:B:141:LYS:HB2	2.13	0.48
1:B:9:GLU:HB3	1:B:13:ASP:OD2	2.13	0.48
1:B:156:LYS:HE3	1:B:156:LYS:HB2	1.52	0.48
1:C:92:GLU:O	1:C:96:GLU:HG2	2.14	0.48
1:C:187:PHE:O	1:C:191:SER:HB3	2.13	0.48
1:D:53:GLN:HE21	1:D:111:HIS:HB3	1.77	0.48
1:A:252:GLU:O	1:A:256:LYS:HG2	2.13	0.48
1:C:63:SER:HA	1:C:211:THR:HA	1.94	0.48
1:B:16:ASP:O	1:B:20:GLN:HG2	2.14	0.48
1:A:8:GLU:OE2	1:A:62:GLN:HG3	2.14	0.48
1:B:174:LEU:HG	1:B:198:SER:HB2	1.96	0.48
1:C:20:GLN:OE1	1:C:20:GLN:HA	2.15	0.47
1:C:98:LYS:O	1:C:102:GLU:HB2	2.14	0.47
1:D:63:SER:HA	1:D:211:THR:HA	1.97	0.47
1:A:287:LYS:O	1:A:291:MET:HG3	2.14	0.47
1:D:195:TYR:CE1	1:D:196:GLU:HG3	2.49	0.47
1:A:83:MET:HB3	1:A:84:PRO:HD2	1.97	0.47
1:A:228:GLN:O	1:A:232:GLN:HG2	2.15	0.47
1:B:292:THR:OG1	1:B:296:GLY:HA3	2.15	0.46
1:C:145:THR:HG21	1:C:155:TYR:CE2	2.51	0.46
1:C:64:PRO:HD2	1:C:211:THR:HA	1.97	0.46
1:C:98:LYS:HE3	1:C:98:LYS:HB2	1.64	0.46
1:D:13:ASP:O	1:D:17:VAL:HG23	2.16	0.46
1:A:187:PHE:O	1:A:191:SER:HB3	2.16	0.46
1:C:254:LEU:HG	1:C:258:LYS:HE3	1.98	0.46
1:C:74:ALA:C	1:C:76:ILE:H	2.19	0.46
1:A:204:THR:O	1:A:205:SER:HB2	2.16	0.46
1:D:275:GLN:O	1:D:279:GLU:HG3	2.16	0.45
1:C:65:GLY:HA3	1:C:78:PHE:CZ	2.50	0.45
1:C:204:THR:OG1	1:C:206:HIS:ND1	2.46	0.45
1:B:87:MET:O	1:B:91:LEU:HD13	2.17	0.45
1:D:281:ALA:N	1:D:282:PRO:CD	2.79	0.44
1:C:153:GLU:OE2	1:C:283:GLN:HG2	2.17	0.44
1:B:5:TYR:O	1:B:36:VAL:HA	2.16	0.44
1:D:173:GLY:HA2	1:D:178:ILE:HD12	2.00	0.44
1:D:145:THR:HG21	1:D:155:TYR:CD2	2.53	0.44
1:B:190:GLU:HB2	1:B:257:ILE:HD11	1.98	0.44
1:B:52:THR:OG1	1:B:60:VAL:HB	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ILE:O	1:C:278:LYS:HG3	2.17	0.44
1:D:83:MET:HB3	1:D:84:PRO:HD2	2.00	0.44
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.78	0.43
1:B:125:VAL:O	1:B:183:GLU:HA	2.19	0.43
1:A:72:PRO:CB	1:A:292:THR:HG22	2.48	0.43
1:C:190:GLU:HB2	1:C:257:ILE:HD11	2.01	0.43
1:B:102:GLU:C	1:B:105:PRO:HD2	2.39	0.43
1:C:116:LEU:HB2	1:C:213:MET:HE3	2.00	0.43
1:D:166:PRO:HG2	1:D:169:GLU:OE2	2.18	0.43
1:D:80:PRO:HG3	1:D:154:THR:HG23	2.01	0.43
1:C:100:ILE:O	1:C:105:PRO:HD3	2.19	0.43
1:C:156:LYS:HE3	1:C:156:LYS:HB2	1.52	0.43
1:D:174:LEU:HD12	1:D:179:ILE:CD1	2.49	0.43
1:A:51:GLN:OE1	1:A:57:LEU:HD11	2.20	0.42
1:C:16:ASP:O	1:C:20:GLN:HG2	2.19	0.42
1:A:67:THR:O	1:A:67:THR:HG22	2.18	0.42
1:A:156:LYS:HE3	1:A:156:LYS:HB2	1.60	0.42
1:B:14:VAL:HG11	1:B:246:ILE:HD11	2.01	0.42
1:C:208:TRP:O	1:C:210:THR:N	2.52	0.42
1:D:253:SER:O	1:D:257:ILE:HG13	2.19	0.42
1:A:37:TYR:CD1	1:A:42:LEU:HG	2.55	0.42
1:A:56:ILE:HD12	1:A:56:ILE:N	2.34	0.42
1:B:14:VAL:CG1	1:B:246:ILE:HD11	2.50	0.42
1:B:89:THR:CG2	1:B:310:VAL:HG13	2.50	0.42
1:C:281:ALA:N	1:C:282:PRO:CD	2.82	0.42
1:D:251:GLU:CG	1:D:252:GLU:N	2.81	0.42
1:A:80:PRO:HG3	1:A:154:THR:CG2	2.50	0.42
1:B:27:GLU:HG2	1:B:33:THR:HA	2.02	0.42
1:B:64:PRO:HB3	1:B:74:ALA:HB1	2.01	0.42
1:D:119:TYR:HA	1:D:120:PRO:HD3	1.82	0.42
1:A:124:MET:HE1	1:A:209:PHE:HB2	2.02	0.42
1:B:124:MET:HE2	1:B:209:PHE:HB2	1.98	0.42
1:C:106:LYS:O	1:C:110:GLU:HG3	2.20	0.42
1:C:129:ASP:N	1:C:129:ASP:OD2	2.50	0.42
1:D:150:LEU:HD23	1:D:150:LEU:HA	1.86	0.42
1:D:274:ILE:O	1:D:278:LYS:HG3	2.20	0.42
1:A:85:THR:HB	1:A:205:SER:HB3	2.02	0.42
1:C:119:TYR:HA	1:C:120:PRO:HD3	1.85	0.41
1:D:78:PHE:CD1	1:D:151:LEU:HD21	2.55	0.41
1:D:8:GLU:OE2	1:D:62:GLN:HG3	2.20	0.41
1:A:275:GLN:O	1:A:279:GLU:HG3	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:MET:HB3	1:B:84:PRO:HD2	2.01	0.41
1:B:98:LYS:HE2	1:B:98:LYS:HB3	1.88	0.41
1:D:9:GLU:HB3	1:D:13:ASP:OD2	2.20	0.41
1:D:156:LYS:HE3	1:D:156:LYS:HB2	1.78	0.41
1:A:281:ALA:N	1:A:282:PRO:CD	2.84	0.41
1:A:78:PHE:CD1	1:A:151:LEU:HD21	2.56	0.41
1:B:251:GLU:CG	1:B:252:GLU:N	2.83	0.41
1:D:83:MET:HB3	1:D:84:PRO:CD	2.51	0.41
1:A:9:GLU:HB3	1:A:13:ASP:OD2	2.21	0.41
1:D:195:TYR:HA	1:D:198:SER:O	2.21	0.41
1:A:23:LYS:HG3	1:A:34:VAL:HB	2.02	0.41
1:D:136:GLU:O	1:D:139:ASP:HB2	2.21	0.41
1:A:23:LYS:HD2	1:A:36:VAL:HG23	2.03	0.40
1:B:79:ILE:HA	1:B:80:PRO:HD3	1.92	0.40
1:D:125:VAL:O	1:D:183:GLU:HA	2.21	0.40
1:B:56:ILE:N	1:B:56:ILE:HD12	2.36	0.40
1:A:7:HIS:CB	1:A:61:ASN:HB3	2.52	0.40
1:D:73:SER:HA	1:D:292:THR:HG21	2.04	0.40
1:B:91:LEU:HD21	1:B:247:LYS:HE3	2.03	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)
1:A:241:HIS:ND1	1:D:136:GLU:OE1[2_444]	2.07	0.13
1:B:241:HIS:ND1	1:C:136:GLU:OE1[2_445]	2.08	0.12

## 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	300/341 (88%)	294 (98%)	6 (2%)	0	100 100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	303/341 (89%)	301 (99%)	2 (1%)	0	100	100
1	C	305/341 (89%)	296 (97%)	8 (3%)	1 (0%)	41	46
1	D	309/341 (91%)	302 (98%)	7 (2%)	0	100	100
All	All	1217/1364 (89%)	1193 (98%)	23 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	209	PHE

### 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	259/289 (90%)	253 (98%)	6 (2%)	50	63
1	B	263/289 (91%)	257 (98%)	6 (2%)	50	63
1	C	265/289 (92%)	259 (98%)	6 (2%)	50	63
1	D	266/289 (92%)	262 (98%)	4 (2%)	65	78
All	All	1053/1156 (91%)	1031 (98%)	22 (2%)	53	67

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	91	LEU
1	A	104	PHE
1	A	191	SER
1	A	244	GLU
1	A	294	GLU
1	B	5	TYR
1	B	42	LEU
1	B	133	THR
1	B	174	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	191	SER
1	B	194	LEU
1	C	5	TYR
1	C	38	ARG
1	C	42	LEU
1	C	134	SER
1	C	194	LEU
1	C	265	THR
1	D	5	TYR
1	D	91	LEU
1	D	194	LEU
1	D	251	GLU

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

Mol	Chain	Res	Type
1	A	61	ASN
1	B	61	ASN
1	B	217	GLN
1	B	302	GLN
1	C	2	ASN
1	C	229	GLN
1	C	295	GLN
1	D	53	GLN
1	D	295	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 36 ligands modelled in this entry, 36 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	304/341 (89%)	-0.22	1 (0%) 94 93	15, 31, 54, 83	2 (0%)
1	B	307/341 (90%)	-0.27	2 (0%) 87 86	14, 30, 52, 71	1 (0%)
1	C	309/341 (90%)	-0.10	3 (0%) 82 81	18, 34, 59, 79	2 (0%)
1	D	311/341 (91%)	-0.22	2 (0%) 89 88	18, 34, 56, 82	1 (0%)
All	All	1231/1364 (90%)	-0.20	8 (0%) 89 88	14, 32, 56, 83	6 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	VAL	3.5
1	C	26	VAL	3.0
1	C	299	LEU	2.8
1	A	308	LYS	2.7
1	B	54	ASN	2.4
1	B	167	TRP	2.4
1	D	147	THR	2.2
1	D	258	LYS	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 ⓘ

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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	B	330	1/1	0.17	0.61	233,233,233,233	0
2	ZN	B	328	1/1	0.50	0.10	123,123,123,123	0
2	ZN	B	317	1/1	0.62	0.10	122,122,122,122	0
2	ZN	A	323	1/1	0.64	0.10	127,127,127,127	0
2	ZN	C	318	1/1	0.79	0.09	94,94,94,94	0
2	ZN	D	321	1/1	0.88	0.12	84,84,84,84	0
2	ZN	D	322	1/1	0.89	0.05	94,94,94,94	0
2	ZN	B	327	1/1	0.89	0.09	88,88,88,88	0
2	ZN	D	317	1/1	0.92	0.12	61,61,61,61	0
2	ZN	B	325	1/1	0.92	0.07	68,68,68,68	0
2	ZN	D	320	1/1	0.92	0.06	58,58,58,58	0
2	ZN	C	319	1/1	0.93	0.09	62,62,62,62	0
2	ZN	B	329	1/1	0.95	0.15	85,85,85,85	0
2	ZN	C	322	1/1	0.95	0.07	101,101,101,101	0
2	ZN	D	323	1/1	0.95	0.08	51,51,51,51	0
2	ZN	B	326	1/1	0.96	0.05	79,79,79,79	0
2	ZN	A	317	1/1	0.96	0.06	75,75,75,75	0
2	ZN	B	321	1/1	0.96	0.07	61,61,61,61	0
2	ZN	A	320	1/1	0.97	0.07	53,53,53,53	0
2	ZN	D	319	1/1	0.97	0.09	59,59,59,59	0
2	ZN	A	322	1/1	0.97	0.07	47,47,47,47	0
2	ZN	B	322	1/1	0.97	0.09	55,55,55,55	0
2	ZN	B	320	1/1	0.97	0.09	58,58,58,58	0
2	ZN	B	323	1/1	0.97	0.12	45,45,45,45	0
2	ZN	C	323	1/1	0.98	0.10	86,86,86,86	0
2	ZN	B	318	1/1	0.98	0.12	42,42,42,42	0
2	ZN	B	319	1/1	0.98	0.10	39,39,39,39	0
2	ZN	C	320	1/1	0.98	0.04	64,64,64,64	0
2	ZN	D	318	1/1	0.98	0.05	65,65,65,65	0
2	ZN	A	324	1/1	0.99	0.11	34,34,34,34	0
2	ZN	A	321	1/1	0.99	0.08	37,37,37,37	0
2	ZN	D	324	1/1	0.99	0.10	38,38,38,38	0
2	ZN	B	324	1/1	0.99	0.08	29,29,29,29	0
2	ZN	C	321	1/1	0.99	0.07	48,48,48,48	0
2	ZN	C	317	1/1	0.99	0.12	55,55,55,55	0
2	ZN	A	318	1/1	1.00	0.09	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.