



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:38 AM GMT

PDB ID : 3MFQ
Title : A Glance into the Metal Binding Specificity of TroA: Where Elaborate Behaviors Occur in the Active Center
Authors : Gao, G.F.; Zheng, B.; Zhang, Q.; Gao, J.; Han, H.; Li, M.
Deposited on : 2010-04-03
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

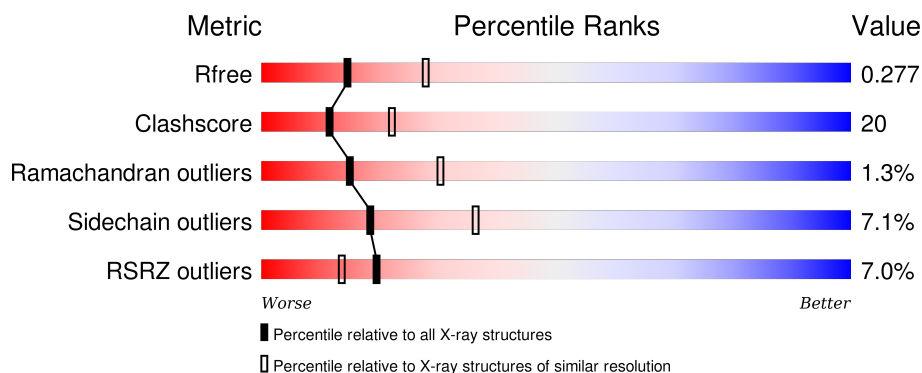
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 ≥ 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	282	<div> <div>7%</div> <div>55%</div> <div>38%</div> <div>5% •</div> </div>
1	B	282	<div> <div>2%</div> <div>62%</div> <div>33%</div> <div>• •</div> </div>
1	C	282	<div> <div>12%</div> <div>56%</div> <div>35%</div> <div>6% ••</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6826 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 High-affinity zinc uptake system protein znuA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2193	1397	353	435	8			
1	B	278	Total	C	N	O	S	0	0	0
			2193	1397	353	435	8			
1	C	278	Total	C	N	O	S	0	0	0
			2193	1397	353	435	8			

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

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

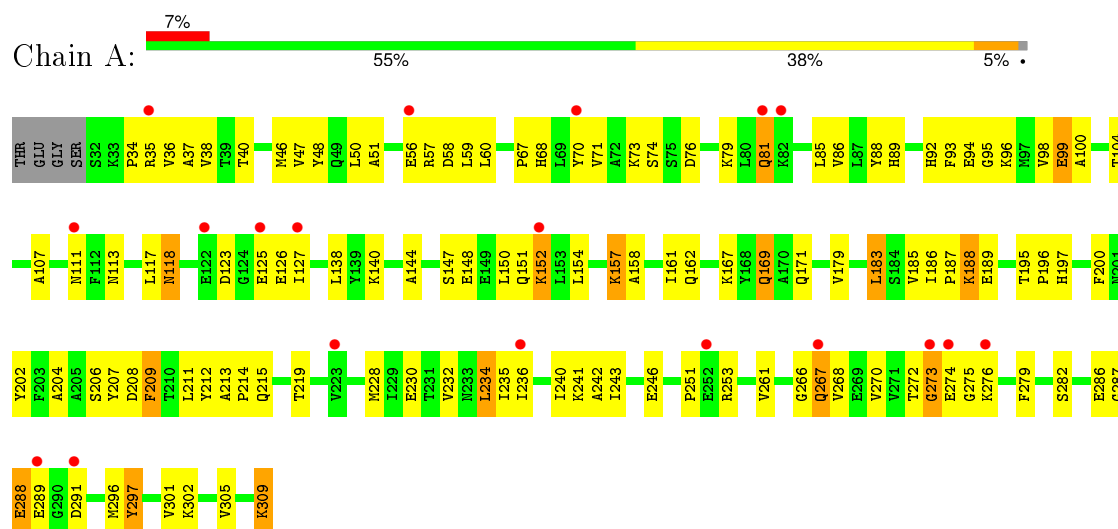
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	110	Total	O	0	0
			110	110		
3	C	32	Total	O	0	0
			32	32		

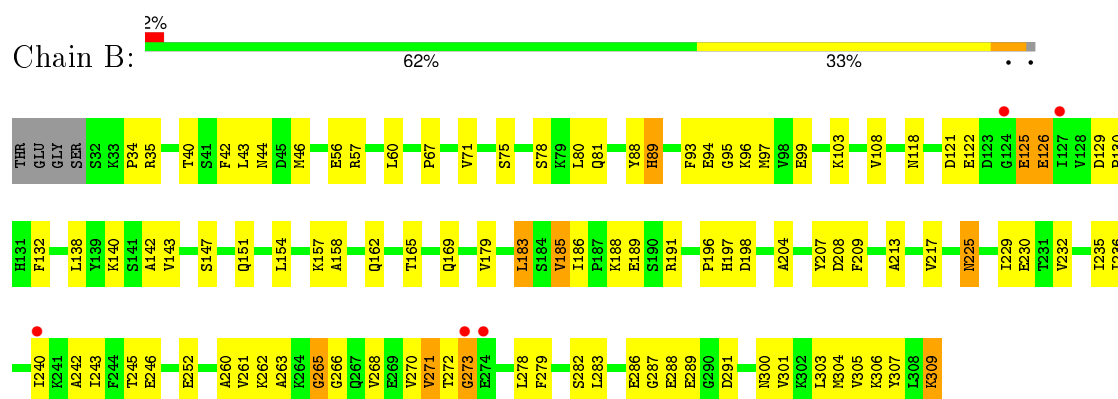
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

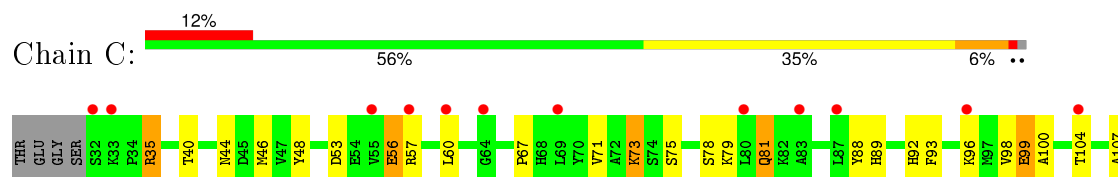
- Molecule 1: High-affinity zinc uptake system protein znuA

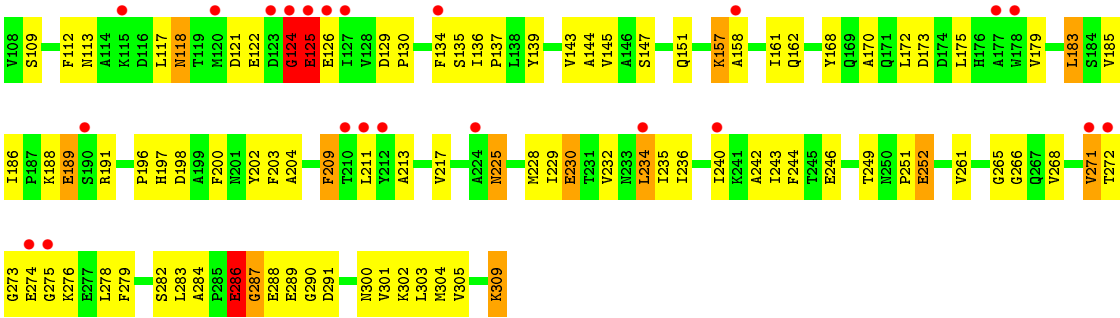


- Molecule 1: High-affinity zinc uptake system protein znuA



- Molecule 1: High-affinity zinc uptake system protein znuA





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	102.36Å 102.36Å 107.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.44 – 2.60 25.44 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.7 (25.44-2.60) 96.3 (25.44-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.226 , 0.256 0.237 , 0.277	Depositor DCC
R_{free} test set	1666 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
Estimated twinning fraction	0.502 for h,-k,-l 0.000 for -h,-l,-k 0.000 for -h,l,k 0.000 for l,-k,h 0.000 for -l,-k,-h 0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.502 for h,-k,-l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32873 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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 37.56 % 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 4.2082e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.25	0/2237	0.51	3/3028 (0.1%)
1	B	0.25	0/2237	0.51	4/3028 (0.1%)
1	C	0.23	0/2237	0.50	4/3028 (0.1%)
All	All	0.24	0/6711	0.50	11/9084 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLU	CB-CA-C	11.06	132.52	110.40
1	B	125	GLU	CB-CA-C	10.39	131.18	110.40
1	C	287	GLY	N-CA-C	9.05	135.73	113.10
1	C	125	GLU	N-CA-C	-7.04	91.98	111.00
1	B	126	GLU	N-CA-C	-6.67	93.00	111.00
1	B	89	HIS	CB-CA-C	-6.15	98.10	110.40
1	B	126	GLU	N-CA-CB	6.04	121.46	110.60
1	C	124	GLY	N-CA-C	5.76	127.49	113.10
1	A	125	GLU	N-CA-CB	-5.70	100.33	110.60
1	C	286	GLU	N-CA-C	5.23	125.12	111.00
1	A	152	LYS	CB-CA-C	-5.14	100.12	110.40

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	2193	0	2160	104	0
1	B	2193	0	2160	79	0
1	C	2193	0	2160	94	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	102	0	0	9	0
3	B	110	0	0	7	0
3	C	32	0	0	2	0
All	All	6826	0	6480	266	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 20.

All (266) 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:284:ALA:HB3	1:C:290:GLY:O	1.39	1.19
1:C:284:ALA:CB	1:C:290:GLY:O	2.05	1.03
1:C:288:GLU:HG3	1:C:289:GLU:H	1.24	1.03
1:A:251:PRO:HB2	1:C:287:GLY:HA3	1.38	1.00
1:A:241:LYS:C	1:A:268:VAL:HG23	1.90	0.92
1:C:284:ALA:HB3	1:C:290:GLY:C	1.89	0.92
1:A:242:ALA:N	1:A:268:VAL:HG23	1.91	0.84
1:A:267:GLN:O	1:A:267:GLN:HG3	1.77	0.83
1:C:284:ALA:N	1:C:290:GLY:O	2.13	0.82
1:C:124:GLY:O	1:C:125:GLU:HG2	1.80	0.81
1:C:272:THR:O	1:C:276:LYS:HB2	1.80	0.81
1:A:267:GLN:O	1:A:267:GLN:CG	2.32	0.77
1:C:243:ILE:HG23	1:C:268:VAL:HG21	1.68	0.75
1:A:152:LYS:O	1:A:152:LYS:HG2	1.87	0.74
1:B:71:VAL:HG22	1:B:96:LYS:HD3	1.68	0.73
1:A:73:LYS:HD3	1:A:74:SER:N	2.04	0.72
1:A:151:GLN:O	1:A:152:LYS:HB3	1.86	0.72
1:C:284:ALA:CA	1:C:290:GLY:O	2.36	0.72
1:A:246:GLU:HB2	3:A:358:HOH:O	1.89	0.72
1:C:196:PRO:HG2	1:C:246:GLU:HG2	1.71	0.72
1:B:121:ASP:OD1	1:B:126:GLU:HG2	1.91	0.70
1:A:76:ASP:HA	1:A:79:LYS:HD2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ILE:HG23	1:B:268:VAL:HG21	1.74	0.69
1:B:288:GLU:CG	1:B:289:GLU:H	2.07	0.68
1:B:288:GLU:O	1:B:291:ASP:HB2	1.95	0.67
1:C:288:GLU:HG3	1:C:289:GLU:N	2.05	0.66
1:C:272:THR:HG23	1:C:273:GLY:H	1.60	0.65
1:C:305:VAL:O	1:C:309:LYS:HD2	1.97	0.65
1:C:186:ILE:HD11	1:C:305:VAL:HA	1.78	0.65
1:B:35:ARG:HH22	1:B:56:GLU:HG2	1.61	0.65
1:A:241:LYS:CA	1:A:268:VAL:HG23	2.26	0.65
1:C:96:LYS:O	3:C:335:HOH:O	2.15	0.65
1:A:273:GLY:O	1:C:288:GLU:HG2	1.98	0.64
1:B:204:ALA:HA	1:B:209:PHE:HB2	1.78	0.64
1:B:225:ASN:ND2	1:B:225:ASN:H	1.96	0.64
1:B:140:LYS:HE3	1:B:169:GLN:NE2	2.13	0.64
1:A:297:TYR:HE1	3:A:387:HOH:O	1.80	0.63
1:B:288:GLU:HA	1:B:288:GLU:OE1	1.98	0.63
1:B:186:ILE:HD11	1:B:305:VAL:HA	1.81	0.63
1:B:35:ARG:NH2	1:B:56:GLU:HG2	2.13	0.63
1:A:196:PRO:HG2	1:A:246:GLU:HG2	1.80	0.63
1:C:288:GLU:CG	1:C:289:GLU:H	2.05	0.62
1:C:204:ALA:HA	1:C:209:PHE:HB2	1.82	0.62
1:B:288:GLU:HG3	1:B:289:GLU:H	1.65	0.62
1:C:71:VAL:HG22	1:C:96:LYS:HD3	1.81	0.62
1:C:288:GLU:O	1:C:291:ASP:HB2	1.99	0.62
1:B:147:SER:O	1:B:151:GLN:HG3	2.00	0.62
1:B:243:ILE:HD11	1:B:270:VAL:HG22	1.81	0.61
1:C:200:PHE:HB2	1:C:211:LEU:HD22	1.83	0.61
1:A:305:VAL:O	1:A:309:LYS:HD2	2.01	0.61
1:A:152:LYS:O	1:A:152:LYS:CG	2.49	0.60
1:A:98:VAL:HG22	3:A:24:HOH:O	2.02	0.60
1:C:225:ASN:ND2	1:C:225:ASN:H	1.99	0.60
1:A:288:GLU:O	1:A:291:ASP:HB2	2.01	0.60
1:A:232:VAL:O	1:A:236:ILE:HG12	2.01	0.60
1:C:242:ALA:N	1:C:268:VAL:HG23	2.17	0.60
1:B:140:LYS:C	3:B:335:HOH:O	2.40	0.59
1:C:244:PHE:HA	1:C:271:VAL:HG23	1.84	0.59
1:A:215:GLN:NE2	1:A:253:ARG:HH12	1.99	0.59
1:A:169:GLN:HE21	1:A:169:GLN:HA	1.67	0.59
1:A:71:VAL:HG22	1:A:96:LYS:HD3	1.85	0.58
1:C:100:ALA:O	1:C:104:THR:HG22	2.03	0.58
1:C:75:SER:O	1:C:78:SER:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:NH2	1:A:56:GLU:HG2	2.18	0.58
1:A:36:VAL:HG22	1:A:85:LEU:HB3	1.86	0.58
1:A:35:ARG:HH22	1:A:56:GLU:HG2	1.69	0.58
1:A:67:PRO:HG2	1:A:93:PHE:CZ	2.39	0.58
1:B:67:PRO:HG2	1:B:93:PHE:CZ	2.39	0.58
1:C:168:TYR:CZ	1:C:172:LEU:HD21	2.37	0.58
1:C:67:PRO:HG2	1:C:93:PHE:CZ	2.39	0.57
1:A:158:ALA:O	1:A:162:GLN:HG3	2.04	0.57
1:A:235:ILE:HG23	1:A:240:ILE:HB	1.86	0.57
1:B:207:TYR:O	1:B:209:PHE:HD1	1.87	0.57
1:A:302:LYS:O	1:A:305:VAL:HG22	2.04	0.57
1:A:206:SER:HB2	1:A:207:TYR:CE2	2.40	0.56
1:B:300:ASN:O	1:B:304:MET:HG3	2.05	0.56
1:B:40:THR:OG1	1:B:89:HIS:HE1	1.88	0.56
1:C:113:ASN:O	1:C:117:LEU:HD13	2.06	0.56
1:C:124:GLY:O	1:C:125:GLU:CG	2.51	0.56
1:A:186:ILE:HD11	1:A:305:VAL:HA	1.88	0.55
1:A:279:PHE:CD2	1:A:296:MET:HG2	2.41	0.55
1:A:144:ALA:O	1:A:148:GLU:HG3	2.07	0.55
1:A:51:ALA:HB2	1:A:150:LEU:HD13	1.89	0.54
1:A:40:THR:OG1	1:A:89:HIS:HE1	1.89	0.54
1:A:242:ALA:N	1:A:268:VAL:CG2	2.67	0.54
1:B:143:VAL:N	3:B:335:HOH:O	2.41	0.54
1:A:279:PHE:HB3	1:A:282:SER:O	2.07	0.54
1:C:40:THR:OG1	1:C:89:HIS:HE1	1.91	0.54
1:A:273:GLY:HA3	1:A:276:LYS:HD2	1.89	0.54
1:C:179:VAL:HG12	1:C:183:LEU:HD22	1.88	0.54
1:A:243:ILE:HD11	1:A:270:VAL:HG22	1.90	0.54
1:C:279:PHE:HB3	1:C:282:SER:O	2.08	0.53
1:C:158:ALA:O	1:C:162:GLN:HG3	2.09	0.53
1:C:35:ARG:NH2	1:C:56:GLU:HG2	2.23	0.53
1:C:300:ASN:O	1:C:304:MET:HG3	2.08	0.53
1:B:169:GLN:HA	1:B:169:GLN:HE21	1.74	0.53
1:C:121:ASP:OD1	1:C:126:GLU:HG2	2.08	0.53
1:B:179:VAL:HG12	1:B:183:LEU:HD22	1.91	0.53
1:C:302:LYS:O	1:C:305:VAL:HG22	2.09	0.53
1:C:228:MET:O	1:C:232:VAL:HG23	2.09	0.53
1:C:147:SER:O	1:C:151:GLN:HG3	2.08	0.52
1:B:75:SER:O	1:B:78:SER:HB3	2.09	0.52
1:A:261:VAL:O	1:A:266:GLY:HA3	2.10	0.52
1:A:100:ALA:O	1:A:104:THR:HG22	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LYS:HE3	1:B:169:GLN:HE21	1.74	0.52
1:C:118:ASN:HB2	1:C:202:TYR:CZ	2.45	0.51
1:A:60:LEU:HD22	1:A:79:LYS:HD3	1.93	0.51
1:A:200:PHE:HB2	1:A:211:LEU:HD22	1.93	0.51
1:B:43:LEU:CD1	1:B:88:TYR:HA	2.41	0.51
1:B:279:PHE:HB3	1:B:282:SER:O	2.10	0.51
1:B:103:LYS:HB2	3:B:10:HOH:O	2.11	0.51
1:A:118:ASN:HB2	1:A:202:TYR:CZ	2.46	0.50
1:A:57:ARG:HB2	1:A:57:ARG:NH1	2.26	0.50
1:A:183:LEU:CD1	1:A:301:VAL:HG13	2.42	0.50
1:A:197:HIS:HB3	1:A:215:GLN:HE21	1.77	0.50
1:B:197:HIS:HA	1:B:213:ALA:HB1	1.94	0.50
1:B:288:GLU:CG	1:B:289:GLU:N	2.75	0.49
1:B:207:TYR:O	1:B:208:ASP:C	2.50	0.49
1:B:143:VAL:HB	3:B:335:HOH:O	2.12	0.49
1:B:60:LEU:HD11	1:B:80:LEU:HD21	1.95	0.49
1:A:111:ASN:HB2	3:A:8:HOH:O	2.13	0.49
1:B:278:LEU:HD23	1:B:303:LEU:HD23	1.94	0.48
1:C:197:HIS:HA	1:C:213:ALA:HB1	1.95	0.48
1:B:235:ILE:HG23	1:B:240:ILE:HB	1.95	0.48
1:B:43:LEU:HD11	1:B:88:TYR:HA	1.96	0.48
1:B:34:PRO:HG2	1:B:154:LEU:HD21	1.96	0.48
1:A:187:PRO:HG2	3:A:312:HOH:O	2.13	0.48
1:A:204:ALA:HA	1:A:209:PHE:HB2	1.96	0.48
1:C:88:TYR:O	1:C:107:ALA:HA	2.14	0.48
1:B:232:VAL:O	1:B:236:ILE:HG12	2.13	0.48
1:A:261:VAL:HG11	1:A:268:VAL:HG12	1.95	0.47
1:C:232:VAL:O	1:C:236:ILE:HG12	2.13	0.47
1:A:38:VAL:HG22	1:A:59:LEU:HA	1.97	0.47
1:C:143:VAL:HG21	1:C:172:LEU:HD11	1.96	0.47
1:A:179:VAL:HG12	1:A:183:LEU:HD22	1.96	0.47
1:A:275:GLY:HA3	1:C:274:GLU:HB3	1.96	0.47
1:B:188:LYS:HA	1:B:191:ARG:HG3	1.96	0.47
1:A:147:SER:O	1:A:151:GLN:HG3	2.15	0.47
1:C:183:LEU:HD13	1:C:301:VAL:HG13	1.96	0.47
1:A:167:LYS:O	1:A:171:GLN:HG3	2.15	0.47
1:A:36:VAL:HA	1:A:85:LEU:O	2.15	0.47
1:A:70:TYR:HB3	3:A:334:HOH:O	2.14	0.47
1:A:286:GLU:HA	1:A:287:GLY:HA2	1.50	0.47
1:A:287:GLY:H	1:C:251:PRO:HB2	1.80	0.47
1:A:169:GLN:NE2	1:A:169:GLN:HA	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASN:OD1	1:B:57:ARG:HD2	2.16	0.46
1:C:157:LYS:HD2	1:C:157:LYS:N	2.30	0.46
1:A:261:VAL:HG12	1:A:266:GLY:HA2	1.97	0.46
1:B:242:ALA:N	1:B:268:VAL:HG23	2.30	0.46
1:C:46:MET:SD	1:C:143:VAL:HA	2.55	0.46
1:B:183:LEU:HD13	1:B:301:VAL:HG13	1.97	0.46
1:C:198:ASP:OD1	1:C:213:ALA:HB3	2.15	0.46
1:C:157:LYS:O	1:C:161:ILE:HG13	2.15	0.46
1:C:278:LEU:HD23	1:C:303:LEU:HD23	1.98	0.46
1:A:127:ILE:HA	1:A:127:ILE:HD13	1.82	0.46
1:A:99:GLU:C	3:A:9:HOH:O	2.53	0.46
1:A:47:VAL:HB	1:A:57:ARG:HD3	1.97	0.46
1:A:113:ASN:O	1:A:117:LEU:HD13	2.15	0.46
1:B:288:GLU:CD	1:B:289:GLU:H	2.19	0.46
1:A:48:TYR:HA	3:A:21:HOH:O	2.16	0.46
1:B:225:ASN:O	1:B:229:ILE:HG13	2.16	0.46
1:B:305:VAL:O	1:B:309:LYS:HB3	2.16	0.46
1:C:183:LEU:CD1	1:C:301:VAL:HG13	2.45	0.46
1:A:37:ALA:HB3	1:A:86:VAL:HG22	1.97	0.46
1:C:136:ILE:HB	1:C:137:PRO:HD3	1.98	0.46
1:B:169:GLN:HA	1:B:169:GLN:NE2	2.31	0.46
1:C:175:LEU:O	1:C:179:VAL:HG23	2.16	0.46
1:C:235:ILE:HG23	1:C:240:ILE:HB	1.98	0.46
1:B:240:ILE:HG22	1:B:242:ALA:H	1.81	0.46
1:A:228:MET:O	1:A:232:VAL:HG23	2.15	0.46
1:B:286:GLU:HA	1:B:287:GLY:HA2	1.56	0.45
1:B:260:ALA:O	1:B:263:ALA:HB3	2.16	0.45
1:C:272:THR:HG23	1:C:273:GLY:N	2.29	0.45
1:B:97:MET:HA	3:B:347:HOH:O	2.16	0.45
1:A:286:GLU:CG	1:C:252:GLU:HG2	2.47	0.45
1:A:195:THR:O	1:A:214:PRO:HD2	2.17	0.45
1:A:286:GLU:HG3	1:C:252:GLU:HG2	1.98	0.45
1:A:140:LYS:NZ	1:A:169:GLN:NE2	2.65	0.45
1:A:240:ILE:O	1:A:268:VAL:HB	2.17	0.45
1:B:305:VAL:HG23	1:B:306:LYS:N	2.31	0.45
1:B:118:ASN:HB3	1:B:129:ASP:HB3	1.98	0.45
1:C:249:THR:O	1:C:251:PRO:HD3	2.17	0.44
1:B:108:VAL:HB	1:B:142:ALA:HB1	2.00	0.44
1:C:230:GLU:O	1:C:234:LEU:HD22	2.17	0.44
1:A:34:PRO:HG2	1:A:154:LEU:HD21	1.98	0.44
1:C:225:ASN:H	1:C:225:ASN:HD22	1.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:HD2	1:B:217:VAL:CG1	2.47	0.44
1:C:93:PHE:HB2	1:C:130:PRO:HB2	1.99	0.44
1:B:165:THR:O	1:B:169:GLN:HG2	2.17	0.44
1:B:225:ASN:HD22	1:B:225:ASN:H	1.63	0.44
1:A:241:LYS:HA	1:A:268:VAL:HG23	2.00	0.44
1:B:60:LEU:HA	1:B:60:LEU:HD23	1.86	0.44
1:C:189:GLU:CD	1:C:189:GLU:H	2.18	0.44
1:C:145:VAL:HG21	3:C:312:HOH:O	2.17	0.44
1:A:40:THR:OG1	1:A:89:HIS:CE1	2.69	0.44
1:B:108:VAL:O	1:B:142:ALA:HA	2.17	0.44
1:A:274:GLU:HB3	1:C:275:GLY:HA3	2.00	0.44
1:B:288:GLU:OE1	1:B:288:GLU:CA	2.64	0.43
1:B:196:PRO:HG2	1:B:246:GLU:HG2	1.99	0.43
1:A:297:TYR:CE1	3:A:387:HOH:O	2.56	0.43
1:C:135:SER:HB2	1:C:202:TYR:HB3	2.00	0.43
1:A:272:THR:O	1:A:273:GLY:C	2.56	0.43
1:A:186:ILE:HA	1:A:187:PRO:HD3	1.90	0.43
1:B:183:LEU:CD1	1:B:301:VAL:HG13	2.49	0.43
1:B:99:GLU:C	3:B:10:HOH:O	2.56	0.43
1:C:60:LEU:HD22	1:C:79:LYS:HD2	2.00	0.43
1:B:158:ALA:O	1:B:162:GLN:HG3	2.19	0.43
1:A:272:THR:HG23	1:A:273:GLY:N	2.34	0.43
1:B:94:GLU:O	1:B:96:LYS:N	2.46	0.43
1:A:289:GLU:HG3	1:C:274:GLU:CG	2.49	0.43
1:C:139:TYR:O	1:C:143:VAL:HG23	2.19	0.43
1:A:206:SER:HB2	1:A:207:TYR:CD2	2.54	0.43
1:B:198:ASP:OD1	1:B:213:ALA:HB3	2.19	0.43
1:C:44:ASN:OD1	1:C:57:ARG:HD2	2.19	0.43
1:C:109:SER:HB2	1:C:112:PHE:CD2	2.53	0.43
1:B:262:LYS:C	1:B:265:GLY:H	2.22	0.43
1:C:118:ASN:HB3	1:C:129:ASP:HB3	2.01	0.43
1:A:274:GLU:C	1:C:275:GLY:HA3	2.38	0.42
1:A:94:GLU:O	1:A:96:LYS:N	2.46	0.42
1:C:144:ALA:O	1:C:147:SER:HB3	2.19	0.42
1:C:81:GLN:HB3	1:C:81:GLN:HE21	1.71	0.42
1:C:73:LYS:HG2	1:C:73:LYS:H	1.60	0.42
1:A:157:LYS:HD2	1:A:157:LYS:N	2.34	0.42
1:B:245:THR:HG23	3:B:367:HOH:O	2.18	0.42
1:A:195:THR:HG21	1:A:200:PHE:CE1	2.55	0.42
1:B:283:LEU:HD23	1:B:291:ASP:O	2.20	0.42
1:A:305:VAL:O	1:A:309:LYS:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TYR:HB2	1:A:94:GLU:OE2	2.20	0.42
1:A:289:GLU:HG3	1:C:274:GLU:HG3	2.01	0.42
1:A:287:GLY:N	1:C:251:PRO:HB2	2.34	0.42
1:C:98:VAL:HG23	1:C:99:GLU:N	2.35	0.42
1:B:261:VAL:O	1:B:266:GLY:HA3	2.19	0.42
1:A:46:MET:O	1:A:50:LEU:HG	2.20	0.42
1:A:188:LYS:NZ	1:A:208:ASP:OD2	2.53	0.42
1:A:81:GLN:HE21	1:A:81:GLN:HB3	1.72	0.42
1:C:288:GLU:HA	1:C:288:GLU:OE2	2.20	0.42
1:C:225:ASN:O	1:C:229:ILE:HG13	2.20	0.42
1:A:68:HIS:CD2	1:A:219:THR:HG23	2.55	0.42
1:A:212:TYR:CZ	1:A:234:LEU:HG	2.55	0.42
1:B:71:VAL:CG2	1:B:96:LYS:HD3	2.43	0.41
1:B:169:GLN:CA	1:B:169:GLN:HE21	2.32	0.41
1:A:197:HIS:HA	1:A:213:ALA:HB1	2.01	0.41
1:C:170:ALA:O	1:C:173:ASP:HB2	2.20	0.41
1:C:289:GLU:C	1:C:291:ASP:H	2.23	0.41
1:B:185:VAL:HG13	1:B:309:LYS:HB2	2.02	0.41
1:B:40:THR:OG1	1:B:42:PHE:HB2	2.20	0.41
1:B:130:PRO:HD2	1:B:217:VAL:HG13	2.02	0.41
1:C:261:VAL:O	1:C:266:GLY:HA3	2.21	0.41
1:A:36:VAL:O	1:A:38:VAL:HG13	2.20	0.41
1:B:271:VAL:HG11	1:B:307:TYR:CD2	2.55	0.41
1:B:46:MET:SD	1:B:143:VAL:HA	2.61	0.41
1:B:132:PHE:HB2	1:B:138:LEU:HD23	2.03	0.41
1:C:134:PHE:HB3	1:C:203:PHE:HB2	2.02	0.41
1:A:140:LYS:HZ2	1:A:169:GLN:HE21	1.68	0.41
1:A:189:GLU:CD	1:A:189:GLU:H	2.22	0.41
1:C:191:ARG:HD3	1:C:209:PHE:CE1	2.56	0.41
1:C:278:LEU:CD2	1:C:303:LEU:HD23	2.51	0.41
1:C:234:LEU:HD12	1:C:234:LEU:HA	1.84	0.41
1:B:140:LYS:HE2	1:B:140:LYS:HB3	1.84	0.40
1:C:188:LYS:HA	1:C:191:ARG:HG3	2.03	0.40
1:A:157:LYS:O	1:A:161:ILE:HG13	2.21	0.40
1:A:88:TYR:O	1:A:107:ALA:HA	2.22	0.40
1:B:272:THR:O	1:B:273:GLY:C	2.59	0.40
1:C:283:LEU:HD23	1:C:291:ASP:O	2.21	0.40
1:A:140:LYS:NZ	1:A:169:GLN:HE21	2.19	0.40
1:C:48:TYR:HE1	1:C:53:ASP:OD1	2.05	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	276/282 (98%)	250 (91%)	23 (8%)	3 (1%)	17	36
1	B	276/282 (98%)	248 (90%)	24 (9%)	4 (1%)	14	28
1	C	276/282 (98%)	246 (89%)	26 (9%)	4 (1%)	14	28
All	All	828/846 (98%)	744 (90%)	73 (9%)	11 (1%)	15	30

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	273	GLY
1	B	125	GLU
1	B	273	GLY
1	C	125	GLU
1	C	286	GLU
1	B	95	GLY
1	C	265	GLY
1	B	265	GLY
1	A	95	GLY
1	C	124	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/244 (99%)	222 (92%)	19 (8%)	15	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	241/244 (99%)	230 (95%)	11 (5%)	33	61
1	C	241/244 (99%)	220 (91%)	21 (9%)	13	24
All	All	723/732 (99%)	672 (93%)	51 (7%)	18	36

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	81	GLN
1	A	92	HIS
1	A	99	GLU
1	A	118	ASN
1	A	123	ASP
1	A	126	GLU
1	A	138	LEU
1	A	157	LYS
1	A	169	GLN
1	A	183	LEU
1	A	185	VAL
1	A	188	LYS
1	A	209	PHE
1	A	230	GLU
1	A	234	LEU
1	A	288	GLU
1	A	297	TYR
1	A	309	LYS
1	B	81	GLN
1	B	122	GLU
1	B	157	LYS
1	B	183	LEU
1	B	185	VAL
1	B	189	GLU
1	B	225	ASN
1	B	230	GLU
1	B	252	GLU
1	B	271	VAL
1	B	309	LYS
1	C	35	ARG
1	C	56	GLU
1	C	73	LYS
1	C	81	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	92	HIS
1	C	99	GLU
1	C	118	ASN
1	C	122	GLU
1	C	157	LYS
1	C	183	LEU
1	C	185	VAL
1	C	189	GLU
1	C	209	PHE
1	C	217	VAL
1	C	225	ASN
1	C	230	GLU
1	C	234	LEU
1	C	252	GLU
1	C	271	VAL
1	C	286	GLU
1	C	309	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	89	HIS
1	A	169	GLN
1	A	171	GLN
1	A	215	GLN
1	A	239	ASN
1	B	81	GLN
1	B	89	HIS
1	B	169	GLN
1	B	171	GLN
1	B	201	ASN
1	B	225	ASN
1	B	233	ASN
1	B	239	ASN
1	C	81	GLN
1	C	89	HIS
1	C	169	GLN
1	C	171	GLN
1	C	215	GLN
1	C	225	ASN
1	C	233	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	239	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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	278/282 (98%)	0.48	19 (6%) 20 15	33, 52, 88, 219	0
1	B	278/282 (98%)	0.36	5 (1%) 71 66	18, 40, 67, 152	0
1	C	278/282 (98%)	0.92	34 (12%) 5 3	43, 71, 130, 375	0
All	All	834/846 (98%)	0.59	58 (6%) 19 13	18, 54, 105, 375	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	ASP	9.3
1	C	120	MET	9.1
1	C	124	GLY	7.3
1	A	223	VAL	6.3
1	B	273	GLY	6.1
1	C	178	TRP	6.0
1	C	125	GLU	5.6
1	C	57	ARG	5.5
1	C	275	GLY	5.5
1	C	33	LYS	5.2
1	C	127	ILE	4.9
1	C	115	LYS	4.8
1	B	274	GLU	4.4
1	C	211	LEU	4.3
1	C	224	ALA	4.1
1	C	177	ALA	3.8
1	C	55	VAL	3.8
1	A	291	ASP	3.7
1	A	125	GLU	3.6
1	B	127	ILE	3.6
1	A	289	GLU	3.5
1	C	234	LEU	3.2
1	C	274	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	96	LYS	3.1
1	A	82	LYS	3.0
1	C	104	THR	2.9
1	A	127	ILE	2.9
1	A	122	GLU	2.8
1	C	126	GLU	2.8
1	C	210	THR	2.7
1	A	81	GLN	2.7
1	C	240	ILE	2.6
1	A	35	ARG	2.6
1	C	134	PHE	2.6
1	A	56	GLU	2.5
1	A	276	LYS	2.5
1	C	80	LEU	2.5
1	C	272	THR	2.5
1	A	274	GLU	2.4
1	C	271	VAL	2.4
1	A	152	LYS	2.4
1	A	273	GLY	2.3
1	A	236	ILE	2.3
1	C	69	LEU	2.3
1	C	212	TYR	2.3
1	C	60	LEU	2.3
1	C	64	GLY	2.3
1	C	32	SER	2.3
1	C	190	SER	2.3
1	B	124	GLY	2.3
1	A	70	TYR	2.1
1	A	267	GLN	2.1
1	A	252	GLU	2.1
1	C	87	LEU	2.1
1	C	83	ALA	2.0
1	C	158	ALA	2.0
1	B	240	ILE	2.0
1	A	111	ASN	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 [i](#)

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	401	1/1	0.99	0.18	0.28	41,41,41,41	0
2	ZN	A	401	1/1	0.98	0.15	-0.72	48,48,48,48	0
2	ZN	C	401	1/1	0.88	0.14	-0.85	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.