



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 10:12 PM EDT

PDB ID : 3R6M  
Title : Crystal structure of *Vibrio parahaemolyticus* YeaZ  
Authors : Roujeinikova, A.; Aydin, I.  
Deposited on : 2011-03-21  
Resolution : 3.10 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 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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

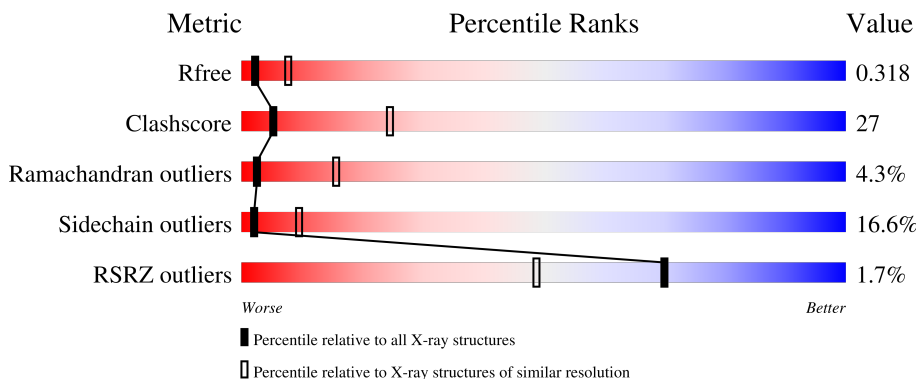
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	213	
1	B	213	
1	C	213	
1	D	213	

## 2 Entry composition

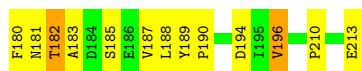
There is only 1 type of molecule in this entry. The entry contains 6162 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 YeaZ, resuscitation promoting factor.

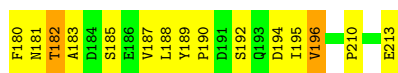
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1539	973	256	305	5	0	0	0
1	B	212	1539	973	256	305	5	0	0	0
1	C	212	1539	973	256	305	5	0	0	0
1	D	212	1545	976	259	305	5	0	0	0





- Molecule 1: YeaZ, resuscitation promoting factor

Chain D: 55% 35% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.73Å 63.84Å 82.27Å 90.00° 104.94° 90.00°	Depositor
Resolution (Å)	79.49 – 3.10 49.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.9 (79.49-3.10) 90.0 (49.78-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.12Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.239 , 0.294 0.262 , 0.318	Depositor DCC
$R_{free}$ test set	687 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.4	Xtrriage
Anisotropy	0.154	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 94.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.18% 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](#)

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	0.74	0/1565	0.85	0/2140
1	B	0.77	0/1565	0.86	0/2140
1	C	0.71	0/1565	0.84	0/2140
1	D	0.71	0/1571	0.84	0/2147
All	All	0.73	0/6266	0.85	0/8567

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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	PRO	Peptide
1	B	177	GLY	Peptide
1	B	179	PRO	Peptide
1	C	177	GLY	Peptide
1	C	179	PRO	Peptide
1	D	177	GLY	Peptide
1	D	179	PRO	Peptide

## 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	1539	0	1458	83	1
1	B	1539	0	1458	83	1
1	C	1539	0	1458	76	1
1	D	1545	0	1469	89	1
All	All	6162	0	5843	319	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 27.

All (319) 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:D:33:ARG:HG3	1:D:33:ARG:HH11	0.99	1.08
1:C:95:THR:HG22	1:C:190:PRO:HG3	1.40	1.03
1:A:95:THR:HG22	1:A:190:PRO:HG3	1.39	1.02
1:D:95:THR:HG22	1:D:190:PRO:HG3	1.41	0.97
1:A:119:ARG:HH11	1:A:119:ARG:HA	1.30	0.94
1:C:95:THR:CG2	1:C:190:PRO:HG3	1.98	0.94
1:D:33:ARG:HG3	1:D:33:ARG:NH1	1.74	0.94
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.32	0.92
1:B:95:THR:HG22	1:B:190:PRO:HG3	1.49	0.92
1:B:119:ARG:HA	1:B:119:ARG:HH11	1.36	0.91
1:C:127:ARG:HG3	1:C:127:ARG:HH11	1.34	0.91
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.35	0.90
1:C:119:ARG:HH11	1:C:119:ARG:HA	1.38	0.89
1:D:127:ARG:HG3	1:D:127:ARG:HH11	1.40	0.85
1:D:31:ALA:HB1	1:D:32:PRO:HD2	1.58	0.84
1:D:95:THR:CG2	1:D:190:PRO:HG3	2.07	0.84
1:D:119:ARG:HA	1:D:119:ARG:HH11	1.40	0.84
1:A:95:THR:CG2	1:A:190:PRO:HG3	2.09	0.83
1:D:101:GLN:CG	1:D:194:ASP:HB3	2.11	0.80
1:C:171:TYR:HB3	1:C:174:GLU:CG	2.12	0.80
1:B:31:ALA:HB1	1:B:32:PRO:HD2	1.64	0.79
1:D:31:ALA:HB1	1:D:32:PRO:CD	2.13	0.78
1:C:31:ALA:HB1	1:C:32:PRO:HD2	1.65	0.78

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:HB3	1:A:174:GLU:CG	2.14	0.78
1:B:171:TYR:HB3	1:B:174:GLU:CG	2.14	0.78
1:A:101:GLN:CG	1:A:194:ASP:HB3	2.13	0.78
1:C:101:GLN:CG	1:C:194:ASP:HB3	2.14	0.78
1:B:171:TYR:HB3	1:B:174:GLU:HG2	1.66	0.77
1:D:101:GLN:HG2	1:D:194:ASP:HB3	1.67	0.77
1:C:101:GLN:HG2	1:C:194:ASP:HB3	1.68	0.76
1:D:171:TYR:HB3	1:D:174:GLU:CG	2.16	0.75
1:A:171:TYR:HB3	1:A:174:GLU:HG2	1.68	0.74
1:B:31:ALA:HB1	1:B:32:PRO:CD	2.18	0.74
1:C:76:ILE:HG22	1:C:80:GLN:NE2	2.02	0.74
1:A:31:ALA:HB1	1:A:32:PRO:HD2	1.70	0.74
1:A:119:ARG:HA	1:A:119:ARG:NH1	2.01	0.73
1:D:96:LEU:HD23	1:D:142:GLU:HG2	1.70	0.73
1:B:101:GLN:CG	1:B:194:ASP:HB3	2.18	0.73
1:A:107:HIS:NE2	1:A:185:SER:O	2.21	0.73
1:C:31:ALA:HB1	1:C:32:PRO:CD	2.19	0.73
1:B:96:LEU:HD23	1:B:142:GLU:HG2	1.70	0.72
1:B:119:ARG:HA	1:B:119:ARG:NH1	2.02	0.72
1:D:171:TYR:HB3	1:D:174:GLU:HG2	1.72	0.72
1:B:95:THR:CG2	1:B:190:PRO:HG3	2.19	0.72
1:C:171:TYR:HB3	1:C:174:GLU:HG2	1.71	0.72
1:C:119:ARG:HA	1:C:119:ARG:NH1	2.05	0.71
1:D:119:ARG:HA	1:D:119:ARG:NH1	2.07	0.69
1:C:96:LEU:HD23	1:C:142:GLU:HG2	1.75	0.69
1:D:34:ASP:OD2	1:D:35:HIS:N	2.27	0.68
1:D:68:SER:O	1:D:72:VAL:HG12	1.94	0.68
1:C:66:PRO:HB2	1:C:124:TYR:CD1	2.29	0.68
1:D:76:ILE:HG22	1:D:80:GLN:NE2	2.08	0.67
1:A:96:LEU:HD23	1:A:142:GLU:HG2	1.75	0.67
1:A:18:LEU:HD22	1:A:46:VAL:HG13	1.77	0.67
1:B:127:ARG:HG3	1:B:127:ARG:NH1	2.07	0.66
1:A:31:ALA:HB1	1:A:32:PRO:CD	2.25	0.66
1:B:127:ARG:HH11	1:B:127:ARG:CG	2.05	0.66
1:A:66:PRO:HB2	1:A:124:TYR:CD1	2.31	0.66
1:A:101:GLN:HG2	1:A:194:ASP:HB3	1.76	0.66
1:B:107:HIS:NE2	1:B:185:SER:O	2.27	0.66
1:D:54:LEU:H	1:D:54:LEU:HD22	1.60	0.66
1:C:116:ILE:HB	1:C:124:TYR:HB2	1.77	0.65
1:A:127:ARG:HG3	1:A:127:ARG:NH1	2.10	0.65
1:C:34:ASP:OD2	1:C:35:HIS:N	2.31	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASP:OD2	1:B:35:HIS:N	2.30	0.64
1:C:107:HIS:NE2	1:C:185:SER:O	2.28	0.64
1:B:66:PRO:HB2	1:B:124:TYR:CD1	2.33	0.64
1:C:76:ILE:HG22	1:C:80:GLN:HE21	1.62	0.63
1:B:101:GLN:HG2	1:B:194:ASP:HB3	1.78	0.63
1:A:34:ASP:OD2	1:A:35:HIS:N	2.31	0.63
1:A:127:ARG:HH11	1:A:127:ARG:CG	2.10	0.63
1:B:187:VAL:O	1:B:188:LEU:HD23	1.98	0.63
1:B:76:ILE:HG22	1:B:80:GLN:NE2	2.15	0.62
1:C:19:LEU:HB2	1:C:196:VAL:HG11	1.81	0.62
1:B:145:ILE:HG22	1:B:146:PRO:O	1.99	0.61
1:D:66:PRO:HB2	1:D:124:TYR:CD1	2.34	0.61
1:C:162:THR:HG22	1:C:183:ALA:HB3	1.81	0.61
1:A:145:ILE:HG22	1:A:146:PRO:O	2.00	0.61
1:A:76:ILE:HG22	1:A:80:GLN:NE2	2.15	0.61
1:D:107:HIS:NE2	1:D:185:SER:O	2.31	0.61
1:B:73:ARG:NH1	1:B:73:ARG:HG3	2.16	0.60
1:B:76:ILE:HG22	1:B:80:GLN:HE21	1.66	0.60
1:A:163:THR:HB	1:A:168:TRP:CE2	2.36	0.60
1:D:116:ILE:HB	1:D:124:TYR:HB2	1.83	0.60
1:D:187:VAL:O	1:D:188:LEU:HD23	2.00	0.60
1:C:68:SER:O	1:C:72:VAL:HG12	2.01	0.59
1:D:27:ARG:NH1	1:D:28:SER:H	2.00	0.59
1:A:19:LEU:HB2	1:A:196:VAL:HG11	1.83	0.59
1:B:73:ARG:HG3	1:B:73:ARG:HH11	1.68	0.59
1:B:163:THR:HB	1:B:168:TRP:CE2	2.38	0.58
1:C:161:TRP:O	1:C:182:THR:HA	2.04	0.58
1:D:76:ILE:HG22	1:D:80:GLN:HE21	1.68	0.58
1:A:54:LEU:HD21	1:D:84:PHE:HE2	1.69	0.58
1:C:54:LEU:HD22	1:C:54:LEU:H	1.68	0.58
1:C:95:THR:HG22	1:C:190:PRO:CG	2.24	0.58
1:B:18:LEU:HD22	1:B:46:VAL:HG13	1.86	0.57
1:A:95:THR:HG22	1:A:190:PRO:CG	2.25	0.57
1:A:33:ARG:HA	1:B:172:GLN:NE2	2.20	0.57
1:C:25:ILE:HG12	1:C:49:GLU:OE1	2.04	0.57
1:D:95:THR:HG22	1:D:190:PRO:CG	2.28	0.57
1:C:18:LEU:HD22	1:C:46:VAL:HG13	1.86	0.57
1:C:27:ARG:NH1	1:C:28:SER:H	2.03	0.57
1:B:25:ILE:HG12	1:B:49:GLU:OE1	2.04	0.56
1:A:25:ILE:HG12	1:A:49:GLU:OE1	2.04	0.56
1:D:33:ARG:NH1	1:D:33:ARG:CG	2.57	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HB2	1:B:196:VAL:HG11	1.87	0.56
1:C:171:TYR:HB3	1:C:174:GLU:HG3	1.85	0.56
1:D:19:LEU:HB2	1:D:196:VAL:HG11	1.86	0.56
1:B:34:ASP:CG	1:B:35:HIS:H	2.09	0.56
1:C:125:TRP:C	1:C:125:TRP:CD1	2.79	0.56
1:C:127:ARG:HH11	1:C:127:ARG:CG	2.13	0.56
1:A:54:LEU:HD21	1:D:84:PHE:CE2	2.41	0.55
1:A:187:VAL:O	1:A:188:LEU:HD23	2.06	0.55
1:D:53:THR:O	1:D:56:ASP:HB2	2.06	0.55
1:D:162:THR:HG22	1:D:183:ALA:HB3	1.87	0.55
1:D:161:TRP:O	1:D:182:THR:HA	2.07	0.55
1:C:27:ARG:HH11	1:C:28:SER:H	1.53	0.55
1:D:54:LEU:HD22	1:D:54:LEU:N	2.22	0.55
1:D:14:CYS:SG	1:D:39:VAL:HG22	2.47	0.55
1:A:163:THR:HG22	1:A:168:TRP:CZ2	2.43	0.54
1:B:161:TRP:O	1:B:182:THR:HA	2.06	0.54
1:B:54:LEU:H	1:B:54:LEU:HD22	1.72	0.54
1:A:88:LEU:O	1:A:211:VAL:HG22	2.08	0.54
1:D:32:PRO:HG2	1:D:34:ASP:H	1.72	0.54
1:D:27:ARG:HH11	1:D:28:SER:H	1.54	0.53
1:A:119:ARG:HH22	1:B:119:ARG:HH12	1.56	0.53
1:B:160:THR:HA	1:B:181:ASN:HB2	1.89	0.53
1:D:178:LEU:HD22	1:D:180:PHE:CE2	2.44	0.53
1:D:39:VAL:O	1:D:43:VAL:HG23	2.08	0.53
1:D:192:SER:HA	1:D:195:ILE:HD12	1.90	0.53
1:B:5:LEU:HD21	1:B:43:VAL:HG13	1.89	0.53
1:C:5:LEU:HD21	1:C:43:VAL:HG13	1.89	0.53
1:C:14:CYS:SG	1:C:39:VAL:HG22	2.49	0.53
1:A:119:ARG:HH12	1:B:119:ARG:HH22	1.57	0.53
1:A:162:THR:HG22	1:A:183:ALA:HB3	1.91	0.53
1:B:27:ARG:HH11	1:B:28:SER:H	1.57	0.53
1:C:172:GLN:O	1:C:173:GLU:C	2.48	0.53
1:A:160:THR:HA	1:A:181:ASN:HB2	1.89	0.53
1:B:96:LEU:HA	1:B:114:VAL:HG11	1.89	0.52
1:A:35:HIS:O	1:A:39:VAL:HG23	2.10	0.52
1:B:84:PHE:CE2	1:C:54:LEU:HD21	2.44	0.52
1:B:27:ARG:NH1	1:B:28:SER:H	2.07	0.52
1:D:34:ASP:CG	1:D:35:HIS:H	2.13	0.52
1:D:60:LEU:HD23	1:D:60:LEU:C	2.30	0.52
1:D:161:TRP:HD1	1:D:180:PHE:HB3	1.75	0.52
1:A:34:ASP:CG	1:A:35:HIS:H	2.13	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PHE:HE2	1:C:54:LEU:HD21	1.75	0.52
1:D:25:ILE:HG12	1:D:49:GLU:OE1	2.10	0.52
1:A:14:CYS:SG	1:A:39:VAL:HG22	2.49	0.52
1:C:161:TRP:HD1	1:C:180:PHE:HB3	1.75	0.52
1:D:35:HIS:O	1:D:39:VAL:HG23	2.10	0.52
1:B:161:TRP:HD1	1:B:180:PHE:HB3	1.75	0.51
1:A:172:GLN:O	1:A:173:GLU:C	2.48	0.51
1:B:160:THR:HG22	1:B:181:ASN:HB3	1.91	0.51
1:D:31:ALA:CB	1:D:32:PRO:CD	2.83	0.51
1:B:123:VAL:O	1:B:144:VAL:HA	2.10	0.51
1:A:84:PHE:CE2	1:D:54:LEU:HD21	2.46	0.51
1:B:60:LEU:HD23	1:B:60:LEU:C	2.31	0.51
1:D:73:ARG:NH1	1:D:73:ARG:HG3	2.26	0.51
1:C:34:ASP:CG	1:C:35:HIS:H	2.14	0.51
1:A:160:THR:HG22	1:A:181:ASN:HB3	1.92	0.51
1:A:76:ILE:HG22	1:A:80:GLN:HE21	1.76	0.51
1:A:161:TRP:O	1:A:182:THR:HA	2.10	0.51
1:C:60:LEU:C	1:C:60:LEU:HD23	2.32	0.51
1:D:125:TRP:CD1	1:D:125:TRP:C	2.84	0.50
1:B:162:THR:HG22	1:B:183:ALA:HB3	1.94	0.50
1:D:18:LEU:HD22	1:D:46:VAL:HG13	1.93	0.50
1:D:127:ARG:HH11	1:D:127:ARG:CG	2.17	0.50
1:D:172:GLN:O	1:D:173:GLU:C	2.50	0.50
1:A:84:PHE:HE2	1:D:54:LEU:HD21	1.76	0.50
1:B:35:HIS:O	1:B:39:VAL:HG23	2.12	0.50
1:B:116:ILE:HB	1:B:124:TYR:HB2	1.93	0.50
1:A:161:TRP:HD1	1:A:180:PHE:HB3	1.77	0.49
1:B:52:LEU:HD12	1:B:56:ASP:HB3	1.93	0.49
1:C:187:VAL:O	1:C:188:LEU:HD23	2.11	0.49
1:B:95:THR:HG22	1:B:190:PRO:CG	2.33	0.49
1:C:145:ILE:HG22	1:C:146:PRO:O	2.12	0.49
1:C:32:PRO:HG2	1:C:34:ASP:H	1.76	0.49
1:D:160:THR:HA	1:D:181:ASN:HB2	1.94	0.49
1:C:19:LEU:HB2	1:C:196:VAL:CG1	2.43	0.49
1:C:160:THR:HG22	1:C:181:ASN:HB3	1.94	0.49
1:D:54:LEU:H	1:D:54:LEU:CD2	2.25	0.49
1:C:127:ARG:HG3	1:C:127:ARG:NH1	2.13	0.49
1:D:5:LEU:HD21	1:D:43:VAL:HG13	1.93	0.49
1:B:34:ASP:CG	1:B:35:HIS:N	2.66	0.49
1:C:160:THR:HA	1:C:181:ASN:HB2	1.95	0.49
1:A:52:LEU:HD12	1:A:56:ASP:HB3	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:HD22	1:C:180:PHE:CE2	2.48	0.49
1:A:27:ARG:NH1	1:A:28:SER:H	2.11	0.48
1:B:163:THR:HG22	1:B:168:TRP:CZ2	2.48	0.48
1:D:52:LEU:HD12	1:D:56:ASP:HB3	1.95	0.48
1:D:171:TYR:HB3	1:D:174:GLU:HG3	1.94	0.48
1:A:18:LEU:CD2	1:A:46:VAL:HG13	2.42	0.48
1:A:5:LEU:HD21	1:A:43:VAL:HG13	1.94	0.48
1:A:50:ALA:O	1:A:52:LEU:HD22	2.13	0.48
1:A:27:ARG:HH11	1:A:28:SER:H	1.62	0.48
1:A:163:THR:HG22	1:A:168:TRP:CH2	2.48	0.48
1:B:3:LYS:HB2	1:B:57:LEU:HA	1.94	0.48
1:B:172:GLN:O	1:B:173:GLU:C	2.51	0.48
1:C:54:LEU:HD22	1:C:54:LEU:N	2.29	0.48
1:A:27:ARG:HG2	1:A:42:MET:HG2	1.94	0.48
1:A:116:ILE:HB	1:A:124:TYR:HB2	1.96	0.48
1:A:70:THR:O	1:A:74:ILE:HG13	2.14	0.47
1:D:145:ILE:HG22	1:D:146:PRO:O	2.14	0.47
1:D:172:GLN:O	1:D:174:GLU:N	2.47	0.47
1:B:32:PRO:HG2	1:B:34:ASP:H	1.78	0.47
1:B:68:SER:O	1:B:72:VAL:HG12	2.14	0.47
1:B:125:TRP:CD1	1:B:125:TRP:C	2.87	0.47
1:A:54:LEU:HD22	1:A:54:LEU:H	1.79	0.47
1:C:39:VAL:O	1:C:43:VAL:HG23	2.13	0.47
1:D:160:THR:HG22	1:D:181:ASN:HB3	1.96	0.47
1:A:172:GLN:NE2	1:B:33:ARG:HA	2.29	0.47
1:A:3:LYS:HB2	1:A:57:LEU:HA	1.96	0.47
1:D:32:PRO:HB2	1:D:33:ARG:NH1	2.30	0.47
1:A:120:MET:SD	1:B:120:MET:SD	3.13	0.47
1:B:14:CYS:SG	1:B:39:VAL:HG22	2.55	0.47
1:B:169:SER:HA	1:B:172:GLN:HE21	1.79	0.47
1:C:5:LEU:O	1:C:60:LEU:HG	2.15	0.47
1:B:97:ALA:HB2	1:B:128:TYR:CZ	2.50	0.46
1:D:73:ARG:HG3	1:D:73:ARG:HH11	1.78	0.46
1:A:169:SER:HA	1:A:172:GLN:HE21	1.80	0.46
1:C:31:ALA:CB	1:C:32:PRO:CD	2.88	0.46
1:C:163:THR:HG22	1:C:168:TRP:CZ2	2.51	0.46
1:A:117:ASP:OD2	1:B:119:ARG:NH2	2.49	0.46
1:D:161:TRP:CD1	1:D:180:PHE:HB3	2.51	0.46
1:B:52:LEU:HA	1:B:56:ASP:OD2	2.14	0.46
1:C:52:LEU:HD12	1:C:56:ASP:HB3	1.97	0.46
1:D:34:ASP:CG	1:D:35:HIS:N	2.69	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD13	1:D:40:LEU:HA	1.77	0.46
1:D:69:PHE:CD2	1:D:69:PHE:C	2.89	0.46
1:A:19:LEU:HB2	1:A:196:VAL:CG1	2.45	0.46
1:A:125:TRP:CD1	1:A:125:TRP:C	2.88	0.46
1:A:34:ASP:CG	1:A:35:HIS:N	2.69	0.45
1:C:18:LEU:CD2	1:C:46:VAL:HG13	2.46	0.45
1:A:145:ILE:HG23	1:A:146:PRO:HD2	1.99	0.45
1:B:192:SER:HA	1:B:195:ILE:HD12	1.98	0.45
1:C:3:LYS:HB2	1:C:57:LEU:HA	1.98	0.45
1:A:171:TYR:HB3	1:A:174:GLU:HG3	1.95	0.45
1:C:178:LEU:HG	1:C:179:PRO:HD2	1.99	0.45
1:A:32:PRO:HG2	1:A:34:ASP:H	1.81	0.45
1:D:169:SER:HA	1:D:172:GLN:HE21	1.80	0.45
1:B:73:ARG:HH11	1:B:73:ARG:CG	2.30	0.45
1:B:96:LEU:O	1:B:114:VAL:HG21	2.16	0.45
1:D:5:LEU:O	1:D:60:LEU:HG	2.17	0.45
1:A:101:GLN:HG3	1:A:194:ASP:HB3	1.97	0.45
1:B:31:ALA:CB	1:B:32:PRO:CD	2.88	0.44
1:D:163:THR:HG22	1:D:168:TRP:CZ2	2.52	0.44
1:A:19:LEU:HD21	1:A:22:ASP:H	1.81	0.44
1:D:151:ALA:HB1	1:D:177:GLY:O	2.17	0.44
1:C:34:ASP:CG	1:C:35:HIS:N	2.71	0.44
1:A:39:VAL:O	1:A:43:VAL:HG23	2.17	0.44
1:A:198:LEU:O	1:A:201:GLN:HG2	2.18	0.44
1:B:171:TYR:HB3	1:B:174:GLU:HG3	1.95	0.44
1:C:163:THR:HB	1:C:168:TRP:CE2	2.52	0.44
1:A:125:TRP:CD2	1:A:150:LEU:HD11	2.52	0.44
1:D:96:LEU:HD12	1:D:114:VAL:CG1	2.48	0.44
1:D:96:LEU:HA	1:D:114:VAL:HG11	1.99	0.44
1:B:19:LEU:HB2	1:B:196:VAL:CG1	2.47	0.44
1:B:70:THR:O	1:B:74:ILE:HG13	2.17	0.44
1:D:70:THR:O	1:D:74:ILE:HG13	2.18	0.44
1:D:163:THR:HB	1:D:168:TRP:CE2	2.52	0.43
1:C:97:ALA:HB2	1:C:128:TYR:CZ	2.53	0.43
1:D:163:THR:O	1:D:185:SER:HB2	2.18	0.43
1:B:160:THR:HG22	1:B:181:ASN:CB	2.49	0.43
1:A:118:ALA:HB3	1:A:122:GLU:O	2.19	0.43
1:B:54:LEU:HD22	1:B:54:LEU:N	2.34	0.43
1:B:161:TRP:CD1	1:B:180:PHE:HB3	2.54	0.43
1:B:163:THR:HG22	1:B:168:TRP:CH2	2.53	0.43
1:C:178:LEU:O	1:C:180:PHE:N	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:NH1	1:A:73:ARG:HG3	2.33	0.43
1:C:40:LEU:HA	1:C:40:LEU:HD13	1.72	0.43
1:D:19:LEU:HB2	1:D:196:VAL:CG1	2.49	0.43
1:C:70:THR:O	1:C:74:ILE:HG13	2.18	0.42
1:D:3:LYS:HB2	1:D:57:LEU:HA	2.01	0.42
1:B:53:THR:O	1:B:56:ASP:HB2	2.19	0.42
1:A:178:LEU:O	1:A:180:PHE:N	2.52	0.42
1:B:50:ALA:O	1:B:52:LEU:HD22	2.19	0.42
1:C:151:ALA:HB1	1:C:177:GLY:O	2.19	0.42
1:A:46:VAL:HG12	1:A:47:LEU:HG	2.01	0.42
1:C:96:LEU:HA	1:C:114:VAL:HG11	2.01	0.42
1:A:60:LEU:C	1:A:60:LEU:HD23	2.40	0.42
1:C:161:TRP:CD1	1:C:180:PHE:HB3	2.53	0.42
1:D:32:PRO:HD2	1:D:34:ASP:O	2.19	0.42
1:A:57:LEU:H	1:A:57:LEU:HG	1.67	0.42
1:B:53:THR:H	1:B:56:ASP:CG	2.22	0.42
1:D:52:LEU:HA	1:D:56:ASP:OD2	2.18	0.42
1:D:97:ALA:HB2	1:D:128:TYR:CZ	2.54	0.42
1:A:178:LEU:HD22	1:A:180:PHE:CE2	2.55	0.42
1:B:178:LEU:HG	1:B:179:PRO:HD2	2.02	0.42
1:C:73:ARG:HG3	1:C:73:ARG:NH1	2.35	0.42
1:D:127:ARG:HG3	1:D:127:ARG:NH1	2.18	0.42
1:D:178:LEU:O	1:D:180:PHE:N	2.53	0.42
1:A:161:TRP:CD1	1:A:180:PHE:HB3	2.55	0.42
1:D:125:TRP:CD2	1:D:150:LEU:HD11	2.54	0.42
1:C:125:TRP:CD2	1:C:150:LEU:HD11	2.55	0.41
1:D:53:THR:H	1:D:56:ASP:CG	2.24	0.41
1:C:32:PRO:HD2	1:C:34:ASP:O	2.20	0.41
1:C:50:ALA:O	1:C:52:LEU:HD22	2.20	0.41
1:D:73:ARG:O	1:D:74:ILE:C	2.58	0.41
1:D:128:TYR:HB3	1:D:136:TRP:HB3	2.02	0.41
1:B:146:PRO:HA	1:B:147:PRO:HD3	1.96	0.41
1:C:125:TRP:CE3	1:C:150:LEU:HD11	2.55	0.41
1:B:152:GLU:H	1:B:152:GLU:HG3	1.73	0.41
1:C:35:HIS:O	1:C:39:VAL:HG23	2.19	0.41
1:A:160:THR:HG22	1:A:181:ASN:CB	2.51	0.41
1:C:145:ILE:HG23	1:C:146:PRO:HD2	2.02	0.41
1:A:172:GLN:O	1:A:174:GLU:N	2.54	0.41
1:B:88:LEU:O	1:B:211:VAL:HG22	2.21	0.41
1:C:53:THR:O	1:C:56:ASP:HB2	2.20	0.41
1:C:69:PHE:CD2	1:C:69:PHE:C	2.95	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:CD2	1:B:46:VAL:HG13	2.49	0.41
1:D:27:ARG:HD2	1:D:27:ARG:HA	1.93	0.41
1:D:33:ARG:HH11	1:D:33:ARG:CG	1.91	0.40
1:D:101:GLN:HG3	1:D:194:ASP:HB3	1.97	0.40
1:A:146:PRO:HA	1:A:147:PRO:HD3	1.98	0.40
1:C:169:SER:HA	1:C:172:GLN:HE21	1.85	0.40
1:B:69:PHE:CD2	1:B:69:PHE:C	2.94	0.40
1:A:96:LEU:O	1:A:114:VAL:HG21	2.21	0.40
1:C:54:LEU:H	1:C:54:LEU:CD2	2.34	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:158:SER:OG	1:B:158:SER:OG[1_545]	1.79	0.41
1:C:189:TYR:OH	1:D:189:TYR:OH[2_646]	2.13	0.07

## 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	210/213 (99%)	173 (82%)	28 (13%)	9 (4%)	<b>2</b> <b>16</b>
1	B	210/213 (99%)	176 (84%)	25 (12%)	9 (4%)	<b>2</b> <b>16</b>
1	C	210/213 (99%)	172 (82%)	29 (14%)	9 (4%)	<b>2</b> <b>16</b>
1	D	210/213 (99%)	171 (81%)	30 (14%)	9 (4%)	<b>2</b> <b>16</b>
All	All	840/852 (99%)	692 (82%)	112 (13%)	36 (4%)	<b>2</b> <b>16</b>

All (36) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	154	ALA
1	B	50	ALA
1	B	154	ALA
1	C	50	ALA
1	C	154	ALA
1	D	50	ALA
1	D	154	ALA
1	A	50	ALA
1	A	210	PRO
1	B	210	PRO
1	C	210	PRO
1	D	32	PRO
1	D	74	ILE
1	D	173	GLU
1	D	210	PRO
1	A	32	PRO
1	A	173	GLU
1	B	32	PRO
1	B	173	GLU
1	B	184	ASP
1	C	32	PRO
1	C	173	GLU
1	A	179	PRO
1	B	179	PRO
1	D	81	GLY
1	D	179	PRO
1	A	74	ILE
1	A	184	ASP
1	B	118	ALA
1	C	74	ILE
1	C	179	PRO
1	A	46	VAL
1	B	46	VAL
1	D	46	VAL
1	C	46	VAL
1	C	81	GLY

### 5.3.2 Protein sidechains [i](#)

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	146/167 (87%)	123 (84%)	23 (16%)	2	11
1	B	146/167 (87%)	124 (85%)	22 (15%)	3	12
1	C	146/167 (87%)	121 (83%)	25 (17%)	2	9
1	D	147/167 (88%)	120 (82%)	27 (18%)	1	7
All	All	585/668 (88%)	488 (83%)	97 (17%)	2	9

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	23	GLN
1	A	30	VAL
1	A	36	THR
1	A	55	GLN
1	A	68	SER
1	A	95	THR
1	A	96	LEU
1	A	112	VAL
1	A	119	ARG
1	A	120	MET
1	A	123	VAL
1	A	127	ARG
1	A	129	SER
1	A	149	ARG
1	A	150	LEU
1	A	152	GLU
1	A	166	THR
1	A	173	GLU
1	A	178	LEU
1	A	182	THR
1	A	196	VAL
1	A	213	GLU
1	B	23	GLN
1	B	30	VAL
1	B	36	THR
1	B	55	GLN
1	B	57	LEU
1	B	68	SER
1	B	73	ARG
1	B	95	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	96	LEU
1	B	112	VAL
1	B	119	ARG
1	B	123	VAL
1	B	127	ARG
1	B	129	SER
1	B	149	ARG
1	B	150	LEU
1	B	152	GLU
1	B	166	THR
1	B	173	GLU
1	B	178	LEU
1	B	196	VAL
1	B	213	GLU
1	C	7	ILE
1	C	20	VAL
1	C	23	GLN
1	C	25	ILE
1	C	30	VAL
1	C	36	THR
1	C	46	VAL
1	C	55	GLN
1	C	57	LEU
1	C	68	SER
1	C	95	THR
1	C	96	LEU
1	C	112	VAL
1	C	119	ARG
1	C	123	VAL
1	C	127	ARG
1	C	129	SER
1	C	150	LEU
1	C	152	GLU
1	C	166	THR
1	C	173	GLU
1	C	178	LEU
1	C	182	THR
1	C	196	VAL
1	C	213	GLU
1	D	7	ILE
1	D	20	VAL
1	D	23	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	25	ILE
1	D	30	VAL
1	D	33	ARG
1	D	36	THR
1	D	46	VAL
1	D	55	GLN
1	D	57	LEU
1	D	68	SER
1	D	73	ARG
1	D	95	THR
1	D	96	LEU
1	D	112	VAL
1	D	119	ARG
1	D	123	VAL
1	D	127	ARG
1	D	129	SER
1	D	150	LEU
1	D	152	GLU
1	D	166	THR
1	D	173	GLU
1	D	178	LEU
1	D	182	THR
1	D	196	VAL
1	D	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	80	GLN
1	A	172	GLN
1	B	35	HIS
1	B	80	GLN
1	B	172	GLN
1	C	35	HIS
1	C	80	GLN
1	C	172	GLN
1	D	35	HIS
1	D	80	GLN
1	D	172	GLN
1	D	193	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	212/213 (99%)	-0.11	4 (1%) 66 46	51, 88, 137, 160	0
1	B	212/213 (99%)	-0.14	3 (1%) 75 56	51, 88, 138, 158	0
1	C	212/213 (99%)	0.05	6 (2%) 53 30	52, 102, 164, 213	0
1	D	212/213 (99%)	-0.09	1 (0%) 91 81	49, 94, 148, 180	0
All	All	848/852 (99%)	-0.07	14 (1%) 70 49	49, 92, 150, 213	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	59	ALA	3.6
1	C	103	SER	3.0
1	C	4	ILE	2.9
1	B	32	PRO	2.9
1	C	111	ASP	2.5
1	A	32	PRO	2.4
1	A	4	ILE	2.4
1	D	4	ILE	2.3
1	C	36	THR	2.3
1	C	30	VAL	2.1
1	B	202	GLU	2.0
1	B	207	ASN	2.0
1	A	213	GLU	2.0
1	A	33	ARG	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.