



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 09:08 AM EST

PDB ID : 2P3Y  
Title : Crystal structure of VPA0735 from *Vibrio parahaemolyticus*. NorthEast Structural Genomics target VpR109  
Authors : Seetharaman, J.; Neely, H.; Forouhar, F.; Wang, D.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xia, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2007-03-10  
Resolution : 1.80 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.

---

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	:	rb-20030736
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)	:	rb-20030736

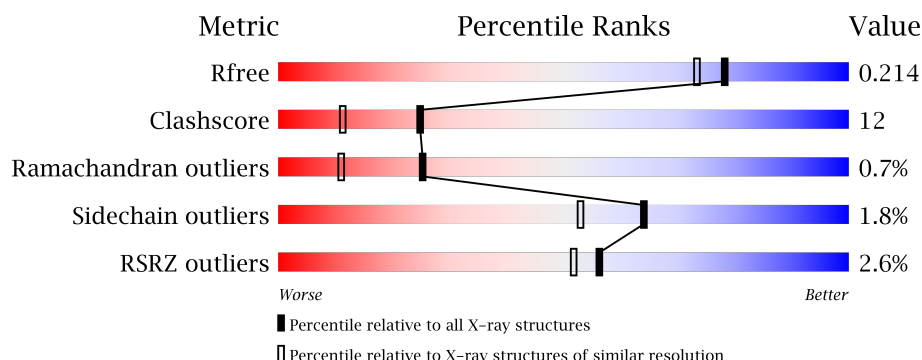
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	491	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	B	491	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8142 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 Hypothetical protein VPA0735.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	Se	0	0	0
			3726	2387	625	700	14			
1	B	461	Total	C	N	O	Se	0	0	0
			3726	2387	625	700	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	13	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	45	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	48	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	52	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	71	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	88	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	131	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	134	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	135	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	263	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	297	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	352	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	407	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	469	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	476	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
A	484	LEU	-	CLONING ARTIFACT	UNP Q87I71
A	485	GLU	-	CLONING ARTIFACT	UNP Q87I71
A	486	HIS	-	CLONING ARTIFACT	UNP Q87I71
A	487	HIS	-	CLONING ARTIFACT	UNP Q87I71
A	488	HIS	-	CLONING ARTIFACT	UNP Q87I71
A	489	HIS	-	CLONING ARTIFACT	UNP Q87I71
A	490	HIS	-	CLONING ARTIFACT	UNP Q87I71
A	491	HIS	-	CLONING ARTIFACT	UNP Q87I71
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q87I71

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	45	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	48	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	52	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	71	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	88	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	131	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	134	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	135	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	263	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	297	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	352	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	407	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	469	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	476	MSE	MET	MODIFIED RESIDUE	UNP Q87I71
B	484	LEU	-	CLONING ARTIFACT	UNP Q87I71
B	485	GLU	-	CLONING ARTIFACT	UNP Q87I71
B	486	HIS	-	CLONING ARTIFACT	UNP Q87I71
B	487	HIS	-	CLONING ARTIFACT	UNP Q87I71
B	488	HIS	-	CLONING ARTIFACT	UNP Q87I71
B	489	HIS	-	CLONING ARTIFACT	UNP Q87I71
B	490	HIS	-	CLONING ARTIFACT	UNP Q87I71
B	491	HIS	-	CLONING ARTIFACT	UNP Q87I71

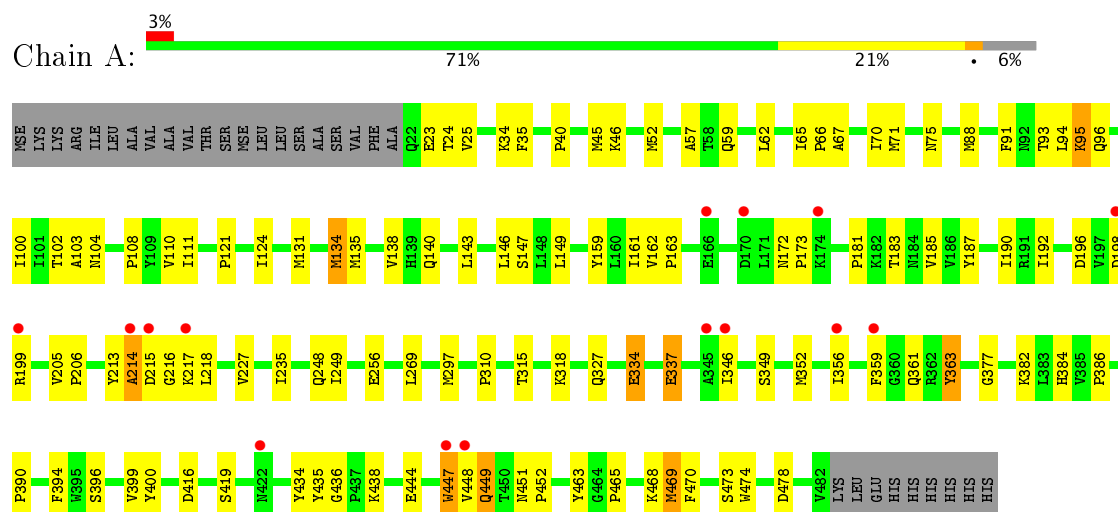
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	326	Total O 326 326	0	0
2	B	364	Total O 364 364	0	0

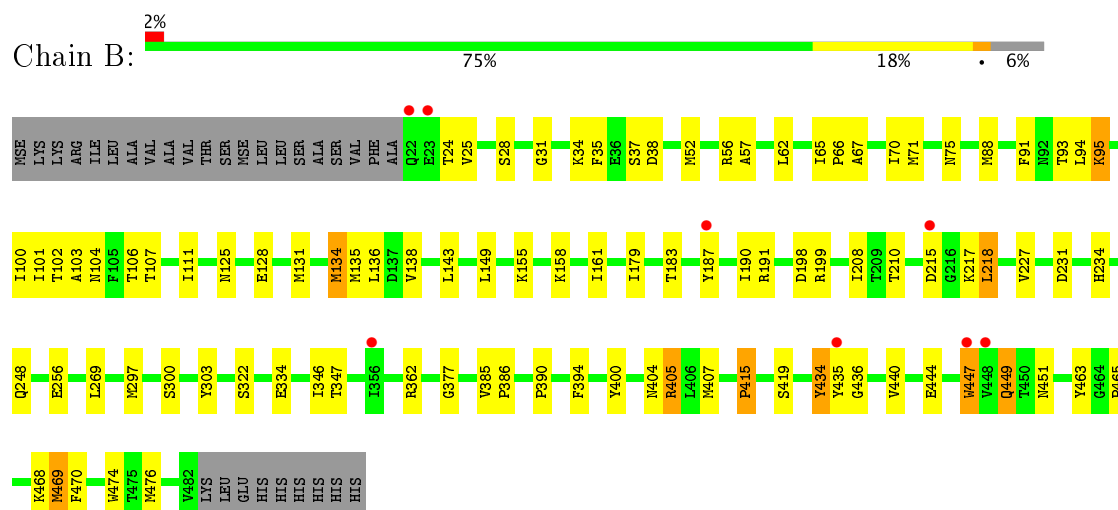
### 3 Residue-property plots [i](#)

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: Hypothetical protein VPA0735



#### • Molecule 1: Hypothetical protein VPA0735



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.76Å 64.25Å 78.52Å 84.81° 89.14° 76.47°	Depositor
Resolution (Å)	35.70 – 1.80 35.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	80.7 (35.70-1.80) 85.2 (35.70-1.80)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.02	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.39 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.204 , 0.234 0.219 , 0.214	Depositor DCC
$R_{free}$ test set	4409 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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	0.43	0/3812	0.60	0/5149
1	B	0.46	1/3812 (0.0%)	0.66	3/5149 (0.1%)
All	All	0.45	1/7624 (0.0%)	0.63	3/10298 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	GLU	CD-OE1	-5.46	1.19	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	TYR	N-CA-CB	-13.17	86.89	110.60
1	B	435	TYR	N-CA-C	-8.07	89.21	111.00
1	B	434	TYR	N-CA-C	-5.14	97.11	111.00

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	3726	0	3651	102	0
1	B	3726	0	3651	88	0
2	A	326	0	0	7	0
2	B	364	0	0	4	0
All	All	8142	0	7302	180	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 12.

All (180) 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:B:134:MSE:O	1:B:134:MSE:HE2	1.52	1.07
1:A:45:MSE:HE1	1:B:303:TYR:HB2	1.37	1.04
1:A:45:MSE:HE2	1:B:300:SER:HA	1.40	1.00
1:B:407:MSE:HE3	1:B:415:PRO:HG3	1.42	0.97
1:A:124:ILE:HD12	1:A:135:MSE:HE2	1.49	0.95
1:B:474:TRP:HH2	1:B:476:MSE:HE3	1.30	0.94
1:A:91:PHE:CD2	1:A:227:VAL:HG21	2.03	0.94
1:B:91:PHE:CE2	1:B:227:VAL:HG21	2.04	0.92
1:B:88:MSE:HE2	1:B:210:THR:HG23	1.52	0.90
1:A:62:LEU:HD11	1:A:297:MSE:HE2	1.55	0.88
1:B:91:PHE:CD2	1:B:227:VAL:HG21	2.09	0.87
1:B:75:ASN:HD21	1:B:248:GLN:HE22	1.22	0.86
1:A:75:ASN:HD21	1:A:248:GLN:HE22	1.24	0.85
1:B:474:TRP:CH2	1:B:476:MSE:HE3	2.14	0.83
1:A:91:PHE:CE2	1:A:227:VAL:HG21	2.13	0.82
1:A:108:PRO:HG2	1:A:192:ILE:HB	1.59	0.81
1:A:465:PRO:HB2	1:A:469:MSE:HG2	1.65	0.79
1:A:297:MSE:HE3	1:B:52:MSE:HB2	1.64	0.79
1:A:52:MSE:HB2	1:B:297:MSE:HE3	1.66	0.77
1:B:62:LEU:HD11	1:B:297:MSE:HE2	1.66	0.76
1:B:436:GLY:O	1:B:449:GLN:HA	1.86	0.75
1:A:134:MSE:O	1:A:134:MSE:HE2	1.86	0.75
1:B:135:MSE:HE2	1:B:179:ILE:HG21	1.69	0.74
1:B:465:PRO:HB2	1:B:469:MSE:HG2	1.69	0.74
1:A:71:MSE:HE3	1:A:249:ILE:HG12	1.70	0.73
1:A:135:MSE:HE3	1:A:146:LEU:HD21	1.71	0.72
1:A:468:LYS:HG2	1:A:474:TRP:HB2	1.70	0.72
1:B:107:THR:HG21	1:B:191:ARG:NH1	2.08	0.69
1:A:23:GLU:HB2	2:A:565:HOH:O	1.93	0.69
1:A:88:MSE:HE2	1:A:110:VAL:HG12	1.73	0.69
1:B:386:PRO:HD3	1:B:476:MSE:HG3	1.76	0.68
1:B:88:MSE:HE1	1:B:208:ILE:HG22	1.74	0.67
1:A:40:PRO:CG	1:A:45:MSE:HE3	2.25	0.67
1:A:416:ASP:HB2	2:A:643:HOH:O	1.96	0.66
1:B:106:THR:HG21	2:B:771:HOH:O	1.97	0.65
1:B:385:VAL:HG13	1:B:476:MSE:CE	2.26	0.65
1:A:40:PRO:HG2	1:A:45:MSE:HE3	1.79	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LYS:O	1:B:218:LEU:HB2	1.95	0.65
1:A:24:THR:CG2	1:A:35:PHE:HB2	2.27	0.64
1:A:124:ILE:HD12	1:A:135:MSE:CE	2.27	0.64
1:B:385:VAL:HG13	1:B:476:MSE:HE2	1.80	0.63
1:A:297:MSE:HE3	1:B:52:MSE:CB	2.29	0.62
1:B:434:TYR:O	1:B:447:TRP:HA	1.99	0.62
1:A:396:SER:HB2	2:A:643:HOH:O	2.00	0.61
1:A:71:MSE:HE1	1:A:185:VAL:HG21	1.82	0.61
1:A:436:GLY:O	1:A:449:GLN:HA	2.00	0.61
1:B:135:MSE:HE1	1:B:161:ILE:HG13	1.83	0.61
1:B:161:ILE:N	1:B:161:ILE:HD12	2.16	0.61
1:B:465:PRO:CB	1:B:469:MSE:HG2	2.32	0.60
1:A:45:MSE:HE1	1:B:303:TYR:CB	2.23	0.59
1:A:334:GLU:HB3	1:A:337:GLU:CG	2.33	0.59
1:B:24:THR:CG2	1:B:35:PHE:HB2	2.33	0.59
1:B:322:SER:HB3	2:B:621:HOH:O	2.03	0.59
1:A:349:SER:CB	1:A:352:MSE:HE3	2.34	0.58
1:A:377:GLY:HA3	1:A:451:ASN:O	2.03	0.58
1:A:45:MSE:HE2	1:B:300:SER:CA	2.25	0.58
1:A:465:PRO:CB	1:A:469:MSE:HG2	2.33	0.58
1:A:52:MSE:CB	1:B:297:MSE:HE3	2.33	0.57
1:B:149:LEU:HB2	2:B:814:HOH:O	2.03	0.57
1:B:101:ILE:HD11	1:B:405:ARG:HG3	1.85	0.57
1:B:385:VAL:HA	1:B:476:MSE:HE2	1.87	0.57
2:A:597:HOH:O	1:B:52:MSE:HG3	2.04	0.57
1:B:104:ASN:ND2	1:B:463:TYR:OH	2.39	0.56
1:A:435:TYR:HD1	1:A:448:VAL:HG11	1.70	0.56
1:A:135:MSE:HE1	1:A:159:TYR:HB3	1.85	0.56
1:A:349:SER:OG	1:A:352:MSE:HE3	2.07	0.55
1:B:404:ASN:O	1:B:405:ARG:HG2	2.05	0.55
1:A:469:MSE:HG3	1:A:470:PHE:N	2.22	0.55
1:B:131:MSE:HB3	1:B:190:ILE:CG2	2.38	0.54
1:A:45:MSE:CE	1:B:300:SER:HA	2.27	0.54
1:A:131:MSE:O	1:A:147:SER:HB3	2.08	0.54
1:A:91:PHE:CE2	1:A:227:VAL:CG2	2.89	0.54
1:B:161:ILE:H	1:B:161:ILE:HD12	1.72	0.53
1:B:91:PHE:CE2	1:B:227:VAL:CG2	2.86	0.53
1:A:75:ASN:ND2	1:A:248:GLN:HE22	2.03	0.52
1:A:435:TYR:CD1	1:A:448:VAL:HG11	2.45	0.52
1:A:70:ILE:CD1	1:A:346:ILE:HD11	2.39	0.52
1:A:70:ILE:HD11	1:A:346:ILE:HD11	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLN:HG2	2:A:699:HOH:O	2.09	0.51
1:A:444:GLU:O	1:A:447:TRP:CD1	2.63	0.51
1:A:46:LYS:NZ	1:A:46:LYS:HB3	2.26	0.51
1:A:135:MSE:CE	1:A:161:ILE:HD11	2.41	0.51
1:A:468:LYS:HG3	1:A:473:SER:OG	2.09	0.51
1:B:444:GLU:O	1:B:447:TRP:CD1	2.64	0.51
1:B:70:ILE:CD1	1:B:346:ILE:HD11	2.40	0.51
1:A:217:LYS:O	1:A:218:LEU:HB2	2.11	0.51
1:A:135:MSE:SE	1:A:146:LEU:HD21	2.61	0.50
1:B:102:THR:HA	1:B:400:TYR:CE1	2.47	0.50
1:B:94:LEU:HD23	1:B:94:LEU:O	2.10	0.50
1:A:93:THR:OG1	1:A:95:LYS:HD3	2.12	0.50
1:A:196:ASP:O	1:A:199:ARG:HB3	2.11	0.49
1:A:172:ASN:N	1:A:173:PRO:HD3	2.27	0.49
1:A:135:MSE:CE	1:A:146:LEU:HD21	2.42	0.49
1:B:128:GLU:HG3	1:B:155:LYS:HA	1.93	0.49
1:B:469:MSE:SE	1:B:469:MSE:C	3.01	0.49
1:A:143:LEU:HD11	1:A:181:PRO:HB3	1.95	0.48
1:B:25:VAL:HG22	1:B:34:LYS:HG2	1.94	0.48
1:B:57:ALA:HB2	1:B:269:LEU:HD11	1.95	0.48
1:A:111:ILE:HD13	1:A:187:TYR:OH	2.14	0.48
1:A:434:TYR:O	1:A:447:TRP:HA	2.14	0.48
1:B:447:TRP:CH2	1:B:449:GLN:HB2	2.48	0.48
1:A:143:LEU:CD1	1:A:181:PRO:HB3	2.45	0.47
1:A:149:LEU:HD12	1:A:149:LEU:N	2.30	0.47
1:A:214:ALA:C	1:A:216:GLY:H	2.17	0.47
1:A:121:PRO:HB2	1:A:213:TYR:HB3	1.96	0.47
1:B:101:ILE:H	1:B:234:HIS:HE2	1.62	0.47
1:A:100:ILE:HB	1:A:103:ALA:HB2	1.97	0.47
1:B:377:GLY:HA3	1:B:451:ASN:O	2.14	0.47
1:B:131:MSE:SE	1:B:190:ILE:HG21	2.64	0.47
1:B:385:VAL:HG13	1:B:476:MSE:HE1	1.96	0.47
1:A:131:MSE:HB3	1:A:190:ILE:CG2	2.44	0.46
1:A:102:THR:HA	1:A:400:TYR:CE1	2.50	0.46
1:A:438:LYS:NZ	1:A:438:LYS:HB2	2.29	0.46
1:A:448:VAL:O	1:A:448:VAL:HG22	2.14	0.46
1:A:390:PRO:HD3	1:A:474:TRP:CD2	2.51	0.46
1:A:45:MSE:HE1	1:B:303:TYR:CD2	2.50	0.46
1:A:447:TRP:CH2	1:A:449:GLN:HB2	2.50	0.46
1:A:327:GLN:O	1:A:334:GLU:HG2	2.16	0.46
1:B:390:PRO:HD3	1:B:474:TRP:CD2	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:HH11	1:B:199:ARG:HG3	1.80	0.46
1:B:70:ILE:HD11	1:B:346:ILE:HD11	1.98	0.46
1:B:93:THR:OG1	1:B:95:LYS:HD3	2.16	0.46
1:A:65:ILE:HB	1:A:66:PRO:HD3	1.97	0.45
1:B:71:MSE:HE3	1:B:71:MSE:HA	1.99	0.45
1:A:183:THR:HG22	1:A:256:GLU:OE2	2.15	0.45
1:B:75:ASN:ND2	1:B:248:GLN:HE22	2.03	0.45
1:A:356:ILE:HB	1:A:359:PHE:HB3	1.98	0.45
1:B:100:ILE:HB	1:B:103:ALA:HB2	1.99	0.45
1:B:183:THR:HG22	1:B:256:GLU:OE2	2.17	0.45
1:A:334:GLU:HB3	1:A:337:GLU:HG3	1.97	0.45
1:A:104:ASN:ND2	1:A:463:TYR:OH	2.50	0.44
1:A:59:GLN:HE22	1:A:297:MSE:HE1	1.82	0.44
1:A:93:THR:OG1	1:A:96:GLN:HG3	2.17	0.44
1:A:140:GLN:OE1	1:A:346:ILE:HD12	2.17	0.44
1:A:25:VAL:HG22	1:A:34:LYS:HG2	1.99	0.44
1:A:468:LYS:HG2	1:A:474:TRP:CB	2.44	0.44
1:A:135:MSE:HE1	1:A:159:TYR:CB	2.47	0.44
1:B:104:ASN:CG	1:B:107:THR:HG22	2.38	0.44
1:A:135:MSE:HE3	1:A:146:LEU:CD2	2.46	0.44
1:B:468:LYS:HD3	2:B:747:HOH:O	2.18	0.44
1:B:135:MSE:HG3	1:B:143:LEU:HB2	2.00	0.43
1:B:24:THR:HG22	1:B:35:PHE:HB2	2.00	0.43
1:B:215:ASP:OD1	1:B:215:ASP:O	2.37	0.43
1:B:125:ASN:HD22	1:B:158:LYS:HG2	1.84	0.43
1:B:136:LEU:HD11	1:B:347:THR:HA	2.01	0.43
1:A:394:PHE:HB2	1:A:419:SER:OG	2.19	0.43
1:B:386:PRO:CD	1:B:476:MSE:HG3	2.47	0.43
1:A:205:VAL:HB	1:A:206:PRO:HD3	2.00	0.43
1:A:363:TYR:N	1:A:363:TYR:CD2	2.87	0.43
1:B:434:TYR:CD1	1:B:440:VAL:HG21	2.54	0.43
1:A:94:LEU:HD23	1:A:94:LEU:O	2.19	0.42
1:B:111:ILE:HD13	1:B:187:TYR:OH	2.18	0.42
1:B:404:ASN:C	1:B:405:ARG:HG2	2.39	0.42
1:B:65:ILE:HB	1:B:66:PRO:HD3	2.01	0.42
1:A:310:PRO:HA	1:A:318:LYS:HG2	2.01	0.42
1:A:67:ALA:HA	1:A:138:VAL:O	2.20	0.42
1:A:235:ILE:HD13	2:A:705:HOH:O	2.19	0.42
1:A:399:VAL:HG21	1:A:448:VAL:HG11	2.02	0.42
1:A:214:ALA:O	1:A:216:GLY:N	2.53	0.42
1:A:162:VAL:HA	1:A:163:PRO:HD3	1.96	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:THR:HA	1:A:478:ASP:OD2	2.21	0.41
1:A:24:THR:HG23	1:A:35:PHE:HB2	1.99	0.41
1:A:57:ALA:HB2	1:A:269:LEU:CD1	2.50	0.41
1:B:469:MSE:HG3	1:B:470:PHE:N	2.35	0.41
1:A:382:LYS:HB3	1:A:382:LYS:NZ	2.35	0.41
1:B:394:PHE:HB2	1:B:419:SER:OG	2.21	0.41
1:A:349:SER:HB3	1:A:352:MSE:HE3	2.01	0.41
1:B:57:ALA:HB2	1:B:269:LEU:CD1	2.51	0.41
2:A:597:HOH:O	1:B:56:ARG:NH2	2.52	0.41
1:B:37:SER:O	1:B:38:ASP:HB2	2.21	0.41
1:A:451:ASN:HA	1:A:452:PRO:HD3	1.95	0.41
1:B:67:ALA:HA	1:B:138:VAL:O	2.21	0.41
1:B:104:ASN:HB3	1:B:107:THR:HG22	2.01	0.40
1:B:94:LEU:C	1:B:94:LEU:HD23	2.42	0.40
1:A:57:ALA:HB2	1:A:269:LEU:HD11	2.03	0.40
1:A:384:HIS:O	1:A:386:PRO:HD3	2.20	0.40
1:B:362:ARG:HD2	1:B:362:ARG:HA	1.89	0.40
1:B:75:ASN:HA	1:B:75:ASN:HD22	1.69	0.40
1:A:438:LYS:HZ2	1:A:438:LYS:HB2	1.86	0.40
1:B:28:SER:HB3	1:B:31:GLY:O	2.21	0.40

There are no symmetry-related clashes.

## 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	459/491 (94%)	444 (97%)	11 (2%)	4 (1%)	20	6
1	B	459/491 (94%)	444 (97%)	13 (3%)	2 (0%)	38	23
All	All	918/982 (94%)	888 (97%)	24 (3%)	6 (1%)	25	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	334	GLU
1	A	449	GLN
1	B	449	GLN
1	A	215	ASP
1	B	218	LEU

### 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	406/416 (98%)	399 (98%)	7 (2%)	66	55
1	B	406/416 (98%)	398 (98%)	8 (2%)	60	48
All	All	812/832 (98%)	797 (98%)	15 (2%)	64	53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LYS
1	A	134	MSE
1	A	198	ASP
1	A	337	GLU
1	A	363	TYR
1	A	447	TRP
1	A	469	MSE
1	B	95	LYS
1	B	134	MSE
1	B	198	ASP
1	B	231	ASP
1	B	405	ARG
1	B	415	PRO
1	B	447	TRP
1	B	469	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	125	ASN
1	A	207	ASN
1	A	316	ASN
1	A	361	GLN
1	A	368	GLN
1	A	373	ASN
1	A	404	ASN
1	A	422	ASN
1	A	451	ASN
1	B	42	GLN
1	B	75	ASN
1	B	125	ASN
1	B	207	ASN
1	B	278	ASN
1	B	331	ASN
1	B	404	ASN
1	B	451	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](#)

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 ⓘ

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	447/491 (91%)	0.13	15 (3%) 46 41	11, 21, 32, 43	0
1	B	447/491 (91%)	0.05	8 (1%) 69 65	9, 18, 30, 49	0
All	All	894/982 (91%)	0.09	23 (2%) 56 52	9, 19, 31, 49	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	GLN	6.0
1	A	215	ASP	5.3
1	A	448	VAL	4.9
1	A	214	ALA	4.9
1	A	217	LYS	3.4
1	B	215	ASP	3.0
1	B	435	TYR	2.9
1	A	359	PHE	2.8
1	B	23	GLU	2.8
1	B	447	TRP	2.7
1	A	199	ARG	2.7
1	B	356	ILE	2.5
1	A	447	TRP	2.5
1	B	448	VAL	2.5
1	A	170	ASP	2.3
1	A	166	GLU	2.2
1	A	356	ILE	2.1
1	A	198	ASP	2.1
1	B	187	TYR	2.1
1	A	174	LYS	2.1
1	A	422	ASN	2.1
1	A	345	ALA	2.0
1	A	346	ILE	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 carbohydrates 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.