



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:32 PM GMT

PDB ID : 3U07
Title : Crystal Structure of the VPA0106 protein from *Vibrio parahaemolyticus*.
Northeast Structural Genomics Consortium Target VpR106.
Authors : Vorobiev, S.; Neely, H.; Seetharaman, J.; Patel, P.; Xiao, R.; Ciccocanti, C.;
Wang, H.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.;
Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-09-28
Resolution : 2.08 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

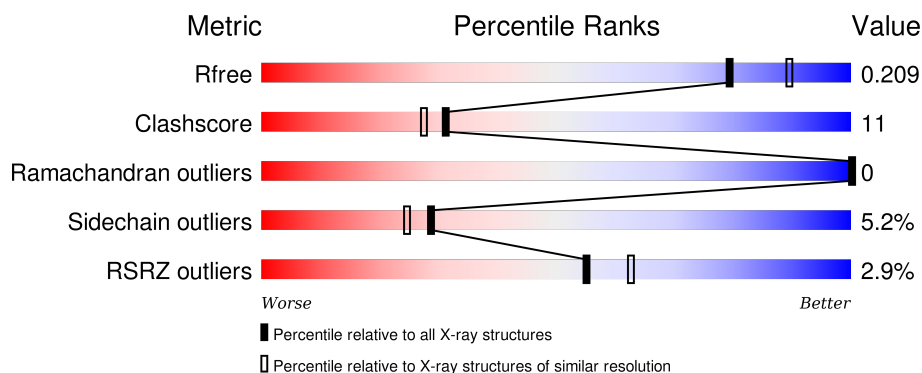
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	4546 (2.10-2.06)
Clashscore	102246	5101 (2.10-2.06)
Ramachandran outliers	100387	5048 (2.10-2.06)
Sidechain outliers	100360	5049 (2.10-2.06)
RSRZ outliers	91569	4556 (2.10-2.06)

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	443	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	443	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	443	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10329 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 uncharacterized protein VPA0106.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	Se	0	0	0
			3180	2013	537	611	2	17			
1	B	398	Total	C	N	O	S	Se	0	0	0
			3182	2014	537	612	2	17			
1	C	399	Total	C	N	O	S	Se	0	0	0
			3187	2017	538	613	2	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLU	ARG	engineered mutation	UNP Q87JZ2
A	64	ARG	ILE	engineered mutation	UNP Q87JZ2
A	436	LEU	-	EXPRESSION TAG	UNP Q87JZ2
A	437	GLU	-	EXPRESSION TAG	UNP Q87JZ2
A	438	HIS	-	EXPRESSION TAG	UNP Q87JZ2
A	439	HIS	-	EXPRESSION TAG	UNP Q87JZ2
A	440	HIS	-	EXPRESSION TAG	UNP Q87JZ2
A	441	HIS	-	EXPRESSION TAG	UNP Q87JZ2
A	442	HIS	-	EXPRESSION TAG	UNP Q87JZ2
A	443	HIS	-	EXPRESSION TAG	UNP Q87JZ2
B	60	GLU	ARG	engineered mutation	UNP Q87JZ2
B	64	ARG	ILE	engineered mutation	UNP Q87JZ2
B	436	LEU	-	EXPRESSION TAG	UNP Q87JZ2
B	437	GLU	-	EXPRESSION TAG	UNP Q87JZ2
B	438	HIS	-	EXPRESSION TAG	UNP Q87JZ2
B	439	HIS	-	EXPRESSION TAG	UNP Q87JZ2
B	440	HIS	-	EXPRESSION TAG	UNP Q87JZ2
B	441	HIS	-	EXPRESSION TAG	UNP Q87JZ2
B	442	HIS	-	EXPRESSION TAG	UNP Q87JZ2
B	443	HIS	-	EXPRESSION TAG	UNP Q87JZ2
C	60	GLU	ARG	engineered mutation	UNP Q87JZ2
C	64	ARG	ILE	engineered mutation	UNP Q87JZ2
C	436	LEU	-	EXPRESSION TAG	UNP Q87JZ2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	437	GLU	-	EXPRESSION TAG	UNP Q87JZ2
C	438	HIS	-	EXPRESSION TAG	UNP Q87JZ2
C	439	HIS	-	EXPRESSION TAG	UNP Q87JZ2
C	440	HIS	-	EXPRESSION TAG	UNP Q87JZ2
C	441	HIS	-	EXPRESSION TAG	UNP Q87JZ2
C	442	HIS	-	EXPRESSION TAG	UNP Q87JZ2
C	443	HIS	-	EXPRESSION TAG	UNP Q87JZ2

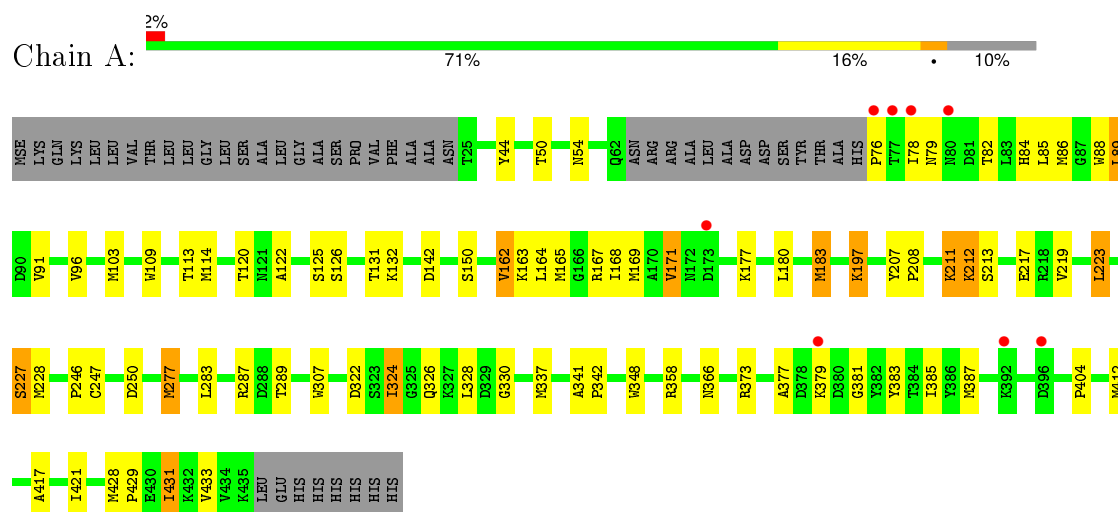
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	245	Total 245	O 245	0	0
2	B	265	Total 265	O 265	0	0
2	C	270	Total 270	O 270	0	0

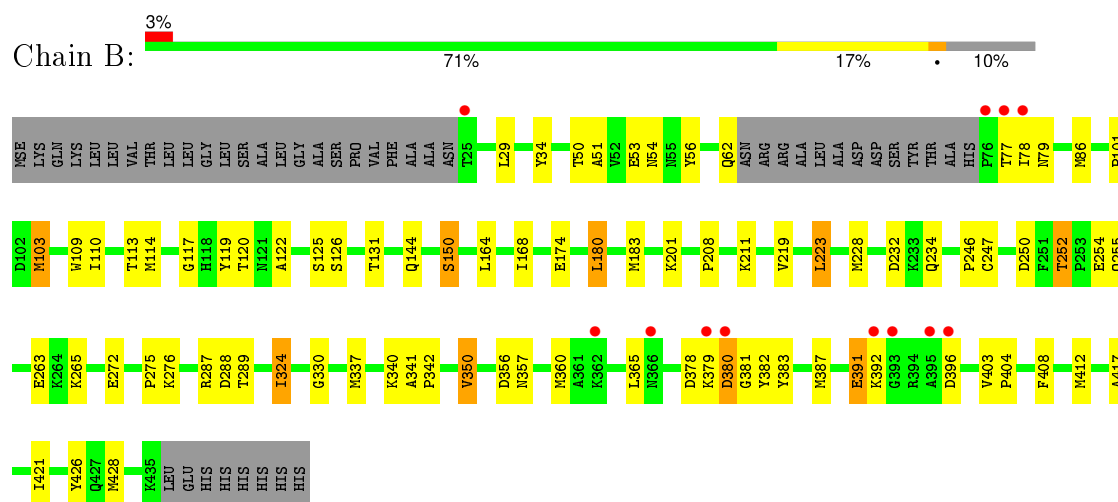
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: uncharacterized protein VPA0106



• Molecule 1: uncharacterized protein VPA0106



• Molecule 1: uncharacterized protein VPA0106





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.45Å 96.32Å 100.54Å 60.61° 80.87° 86.55°	Depositor
Resolution (Å)	46.96 – 2.08 46.96 – 2.08	Depositor EDS
% Data completeness (in resolution range)	94.8 (46.96-2.08) 80.3 (46.96-2.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.194 , 0.216 0.185 , 0.209	Depositor DCC
R_{free} test set	4763 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
Estimated twinning fraction	0.007 for -h,k-l,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 95382 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10329	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	0.35	0/3242	0.64	0/4363
1	B	0.33	0/3244	0.63	0/4366
1	C	0.34	0/3249	0.64	0/4373
All	All	0.34	0/9735	0.64	0/13102

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	3180	0	3044	76	0
1	B	3182	0	3049	69	0
1	C	3187	0	3051	61	0
2	A	245	0	0	10	0
2	B	265	0	0	10	0
2	C	270	0	0	16	0
All	All	10329	0	9144	202	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 11.

All (202) 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:168:ILE:CD1	1:B:183:MSE:HE3	1.75	1.14
1:B:228:MSE:HE2	1:B:287:ARG:HH12	1.21	1.04
1:B:168:ILE:HD13	1:B:183:MSE:HE3	1.36	1.02
1:A:324:ILE:HG13	1:C:289:THR:O	1.60	1.01
1:A:289:THR:O	1:B:324:ILE:HG13	1.62	0.98
1:A:328:LEU:HD11	1:A:431:ILE:HD11	1.47	0.96
1:B:289:THR:O	1:C:324:ILE:HG13	1.66	0.94
1:A:277:MSE:HG2	1:A:283:LEU:HD21	1.50	0.93
1:B:252:THR:HG22	1:B:255:GLN:H	1.35	0.91
1:B:168:ILE:HD12	1:B:183:MSE:HE3	1.59	0.84
1:C:168:ILE:HG13	1:C:183:MSE:HG2	1.58	0.83
1:B:228:MSE:HE2	1:B:287:ARG:NH1	1.95	0.81
1:A:142:ASP:HB3	2:A:797:HOH:O	1.79	0.80
1:A:89:LEU:HB2	1:A:162:VAL:HG22	1.62	0.80
1:C:25:THR:HG22	1:C:28:ASP:H	1.47	0.79
1:A:114:MSE:SE	2:A:663:HOH:O	2.51	0.78
1:B:168:ILE:HD13	1:B:183:MSE:CE	2.13	0.78
1:C:373:ARG:HD3	2:C:765:HOH:O	1.84	0.77
1:C:103:MSE:HE1	1:C:168:ILE:HD12	1.67	0.76
1:C:113:THR:OG1	1:C:122:ALA:HB3	1.86	0.75
1:A:337:MSE:HG3	1:A:431:ILE:HG22	1.71	0.73
1:C:287:ARG:HH11	1:C:287:ARG:HG3	1.53	0.71
1:C:114:MSE:HE1	1:C:307:TRP:CA	2.20	0.71
1:C:114:MSE:HE1	1:C:307:TRP:HA	1.73	0.71
1:A:337:MSE:HE2	1:A:387:MSE:CE	2.21	0.70
1:A:114:MSE:HE1	1:A:307:TRP:CA	2.22	0.69
1:B:101:PRO:HG2	1:B:103:MSE:HE1	1.74	0.69
1:C:364:ASP:HB2	2:C:1051:HOH:O	1.93	0.69
1:A:373:ARG:HD3	2:A:1111:HOH:O	1.92	0.68
1:A:171:VAL:HB	2:A:1117:HOH:O	1.93	0.68
1:B:101:PRO:HG2	1:B:103:MSE:CE	2.24	0.68
1:C:168:ILE:HD11	1:C:186:TRP:CZ2	2.30	0.67
1:A:84:HIS:HD2	1:A:86:MSE:HG3	1.58	0.66
1:A:109:TRP:O	1:A:125:SER:HB2	1.96	0.66
1:B:252:THR:HG21	2:B:1130:HOH:O	1.95	0.66
1:B:412:MSE:HE3	1:B:428:MSE:HE3	1.77	0.66
1:B:276:LYS:HG3	2:B:1008:HOH:O	1.95	0.66
1:B:340:LYS:HE2	1:B:382:TYR:CE1	2.31	0.65
1:A:91:VAL:HG12	1:A:96:VAL:HG12	1.78	0.65
1:B:337:MSE:HE1	1:B:350:VAL:HG21	1.78	0.65
1:A:85:LEU:HG	1:A:183:MSE:HE3	1.78	0.64
1:C:107:ARG:NH1	2:C:621:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PRO:HG3	2:B:1030:HOH:O	1.97	0.63
1:A:328:LEU:CD1	1:A:431:ILE:HD11	2.25	0.63
1:A:212:LYS:HG3	2:A:826:HOH:O	1.98	0.62
1:B:392:LYS:O	1:B:392:LYS:HG3	2.00	0.62
1:A:113:THR:OG1	1:A:122:ALA:HB3	2.00	0.62
1:B:117:GLY:HA3	1:B:228:MSE:HE1	1.82	0.62
1:C:289:THR:HA	2:C:1176:HOH:O	1.99	0.62
1:A:114:MSE:HG2	1:A:120:THR:HA	1.82	0.62
1:C:103:MSE:CE	1:C:168:ILE:HD12	2.30	0.61
1:B:340:LYS:HD3	1:B:381:GLY:O	2.00	0.61
1:A:114:MSE:HE1	1:A:307:TRP:HA	1.81	0.61
1:A:412:MSE:HE3	1:A:428:MSE:HE3	1.83	0.61
1:C:114:MSE:HG2	1:C:120:THR:HA	1.82	0.60
1:B:113:THR:OG1	1:B:122:ALA:HB3	2.00	0.60
1:B:109:TRP:O	1:B:125:SER:HB2	2.02	0.59
1:A:180:LEU:HA	1:A:183:MSE:HG3	1.85	0.59
1:C:179:ALA:O	1:C:183:MSE:HG3	2.04	0.57
1:B:252:THR:HG22	1:B:255:GLN:N	2.15	0.57
1:C:77:THR:O	1:C:77:THR:HG22	2.04	0.57
1:C:168:ILE:HG13	1:C:183:MSE:CG	2.31	0.57
1:C:365:LEU:N	2:C:1051:HOH:O	2.36	0.57
1:C:219:VAL:HG12	1:C:223:LEU:HD22	1.87	0.57
1:A:50:THR:O	1:A:54:ASN:HB2	2.05	0.57
1:B:50:THR:O	1:B:54:ASN:HB2	2.05	0.56
1:A:103:MSE:HE3	1:A:109:TRP:CG	2.40	0.56
1:C:109:TRP:CD1	1:C:126:SER:HB3	2.40	0.56
1:C:164:LEU:C	1:C:164:LEU:HD23	2.25	0.56
1:C:214:THR:OG1	1:C:217:GLU:HG2	2.05	0.56
1:A:328:LEU:HD11	1:A:431:ILE:CD1	2.29	0.56
1:B:168:ILE:HD13	1:B:183:MSE:HG2	1.88	0.56
1:A:227:SER:HB2	2:A:672:HOH:O	2.06	0.56
1:A:114:MSE:HE1	1:A:307:TRP:HB3	1.88	0.55
1:A:277:MSE:CG	1:A:283:LEU:HD21	2.30	0.55
1:C:28:ASP:HA	2:C:1140:HOH:O	2.05	0.55
1:B:275:PRO:HG2	2:B:1008:HOH:O	2.06	0.55
1:A:164:LEU:HD23	1:A:164:LEU:C	2.27	0.55
1:C:83:LEU:HB2	1:C:183:MSE:SE	2.58	0.54
1:B:378:ASP:OD1	1:B:382:TYR:N	2.31	0.54
1:A:82:THR:HG22	1:A:169:MSE:HA	1.90	0.54
1:A:337:MSE:HE2	1:A:387:MSE:HE2	1.90	0.54
1:B:101:PRO:O	1:B:103:MSE:HE3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:SER:HB2	2:B:1243:HOH:O	2.07	0.54
1:A:228:MSE:HE2	1:A:287:ARG:NH2	2.23	0.54
1:C:143:TRP:CZ2	1:C:145:GLY:HA3	2.44	0.53
1:C:417:ALA:HB1	1:C:421:ILE:HB	1.89	0.53
1:B:117:GLY:N	1:B:228:MSE:HE1	2.23	0.53
1:A:322:ASP:OD1	1:A:324:ILE:HG12	2.07	0.53
1:A:412:MSE:HE1	1:A:429:PRO:HD2	1.90	0.53
1:B:110:ILE:HG13	1:B:125:SER:HB3	1.90	0.53
1:B:117:GLY:CA	1:B:228:MSE:HE1	2.38	0.53
1:B:341:ALA:HB2	1:B:383:TYR:HE1	1.74	0.53
1:B:232:ASP:OD1	1:B:287:ARG:NH2	2.42	0.52
1:A:250:ASP:HB3	2:A:849:HOH:O	2.09	0.52
1:B:378:ASP:OD1	1:B:381:GLY:N	2.42	0.52
1:B:228:MSE:CE	1:B:287:ARG:HH12	2.08	0.52
1:A:114:MSE:HE1	1:A:307:TRP:CB	2.39	0.52
1:B:356:ASP:OD2	1:B:357:ASN:N	2.42	0.52
1:A:328:LEU:HD21	1:A:431:ILE:HG13	1.90	0.52
1:C:318:LYS:HB2	1:C:411:ILE:HD13	1.92	0.52
1:C:27:VAL:HG12	2:C:1140:HOH:O	2.09	0.51
1:C:338:ARG:NH1	2:C:727:HOH:O	2.39	0.51
1:B:119:TYR:CG	1:B:287:ARG:HG2	2.45	0.51
1:C:378:ASP:HB3	2:C:574:HOH:O	2.09	0.51
1:B:164:LEU:C	1:B:164:LEU:HD23	2.31	0.51
1:A:219:VAL:HG12	1:A:223:LEU:HD22	1.91	0.51
1:A:322:ASP:OD2	1:A:326:GLN:HB2	2.11	0.51
1:C:114:MSE:CE	1:C:307:TRP:HA	2.41	0.51
1:A:76:PRO:HB2	1:A:358:ARG:O	2.11	0.51
1:B:365:LEU:HD13	1:B:391:GLU:OE2	2.12	0.51
1:B:337:MSE:HG3	1:B:387:MSE:HE1	1.92	0.50
1:A:44:TYR:OH	1:A:208:PRO:HD2	2.12	0.50
1:B:101:PRO:O	1:B:103:MSE:CE	2.59	0.50
1:A:168:ILE:HD12	1:A:183:MSE:CG	2.41	0.50
1:B:250:ASP:HB3	2:B:768:HOH:O	2.11	0.50
1:B:330:GLY:HA3	1:B:404:PRO:O	2.12	0.50
1:A:150:SER:HB2	2:A:877:HOH:O	2.11	0.49
1:C:287:ARG:HG3	1:C:287:ARG:NH1	2.24	0.49
1:A:168:ILE:HD12	1:A:183:MSE:HG2	1.94	0.49
1:B:53:GLU:HB3	2:B:1220:HOH:O	2.11	0.49
1:A:168:ILE:HD12	1:A:183:MSE:SE	2.63	0.48
1:C:78:ILE:HG13	1:C:79:ASN:H	1.78	0.48
1:A:89:LEU:HG	1:A:96:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ASN:HB2	1:C:360:MSE:SE	2.64	0.48
1:B:219:VAL:HG12	1:B:223:LEU:HD22	1.96	0.48
1:B:417:ALA:HB1	1:B:421:ILE:HB	1.96	0.48
1:A:433:VAL:HG21	2:C:1176:HOH:O	2.13	0.48
1:C:142:ASP:HB3	2:C:1096:HOH:O	2.13	0.47
1:C:234:GLN:HG2	1:C:235:TRP:N	2.29	0.47
1:A:114:MSE:CE	1:A:307:TRP:HA	2.45	0.47
1:C:379:LYS:HB3	2:C:923:HOH:O	2.15	0.47
1:C:294:PRO:HB2	1:C:297:ILE:HD12	1.96	0.47
1:C:40:ILE:HG13	2:C:1066:HOH:O	2.13	0.47
1:A:337:MSE:CG	1:A:431:ILE:HG22	2.42	0.47
1:C:31:GLU:OE1	1:C:265:LYS:HE3	2.15	0.47
1:A:84:HIS:CD2	1:A:86:MSE:HG3	2.46	0.46
1:B:379:LYS:HG2	1:B:380:ASP:N	2.29	0.46
1:A:213:SER:HB2	1:A:217:GLU:HG3	1.96	0.46
1:A:211:LYS:HB2	1:A:211:LYS:HE2	1.46	0.46
1:B:77:THR:HG22	1:B:77:THR:O	2.14	0.46
1:A:328:LEU:HD21	1:A:431:ILE:CD1	2.46	0.46
1:A:207:TYR:HA	1:A:208:PRO:HD3	1.90	0.45
1:A:417:ALA:HB1	1:A:421:ILE:HB	1.98	0.45
1:A:88:TRP:CZ3	1:A:163:LYS:HB2	2.51	0.45
1:B:287:ARG:HG3	2:B:507:HOH:O	2.15	0.45
1:A:324:ILE:HG21	1:C:289:THR:HB	1.99	0.45
1:C:114:MSE:HE1	1:C:307:TRP:CB	2.47	0.45
1:A:330:GLY:HA3	1:A:404:PRO:O	2.16	0.45
1:B:78:ILE:O	1:B:360:MSE:HE2	2.17	0.45
1:A:132:LYS:HE3	2:A:755:HOH:O	2.17	0.45
1:C:208:PRO:HG3	2:C:1257:HOH:O	2.16	0.45
1:B:250:ASP:HB3	2:B:845:HOH:O	2.17	0.45
1:A:377:ALA:HB1	1:A:381:GLY:C	2.36	0.45
1:A:213:SER:HB2	1:A:217:GLU:CG	2.47	0.45
1:A:165:MSE:HE3	1:A:167:ARG:HG2	2.00	0.44
1:C:357:ASN:O	1:C:358:ARG:HB2	2.16	0.44
1:B:234:GLN:NE2	2:B:1144:HOH:O	2.49	0.44
1:A:328:LEU:HD21	1:A:431:ILE:CG1	2.48	0.44
1:C:229:GLY:HA2	1:C:236:LEU:CD1	2.47	0.44
1:A:328:LEU:HD21	1:A:431:ILE:HD11	1.99	0.44
1:B:117:GLY:H	1:B:228:MSE:HE1	1.81	0.44
1:A:342:PRO:HD2	1:A:348:TRP:NE1	2.33	0.44
1:A:197:LYS:NZ	2:A:883:HOH:O	2.48	0.44
1:C:330:GLY:HA3	1:C:404:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:HG23	1:B:254:GLU:H	1.83	0.43
1:C:114:MSE:HE1	1:C:307:TRP:HB3	1.99	0.43
1:B:403:VAL:HG11	1:B:408:PHE:CE2	2.53	0.43
1:C:82:THR:HG22	1:C:169:MSE:HA	2.00	0.43
1:A:337:MSE:HE3	1:A:385:ILE:HB	2.01	0.43
1:B:341:ALA:HA	1:B:342:PRO:HD3	1.89	0.43
1:B:34:TYR:CE1	1:B:263:GLU:HG3	2.53	0.43
1:B:109:TRP:CD1	1:B:126:SER:HB3	2.54	0.43
1:C:164:LEU:HD23	1:C:165:MSE:N	2.34	0.43
1:C:103:MSE:HE2	1:C:109:TRP:HB3	1.99	0.43
1:C:356:ASP:OD2	1:C:357:ASN:N	2.45	0.42
1:B:114:MSE:HG2	1:B:120:THR:HA	2.00	0.42
1:B:51:ALA:HA	1:B:56:TYR:CD2	2.54	0.42
1:A:183:MSE:HE3	1:A:183:MSE:HB3	1.89	0.42
1:C:114:MSE:SE	2:C:1138:HOH:O	2.87	0.42
1:A:103:MSE:O	1:A:131:THR:HB	2.20	0.42
1:C:376:LYS:HE2	2:C:1169:HOH:O	2.20	0.42
1:B:101:PRO:HG2	1:B:103:MSE:HE2	1.99	0.41
1:B:421:ILE:HA	1:B:426:TYR:HB3	2.02	0.41
1:B:246:PRO:O	1:B:247:CYS:CB	2.67	0.41
1:B:228:MSE:CE	1:B:287:ARG:NH1	2.73	0.41
1:B:337:MSE:HE2	1:B:387:MSE:CE	2.51	0.41
1:C:379:LYS:NZ	1:C:380:ASP:OD2	2.42	0.41
1:B:86:MSE:HB2	1:B:86:MSE:HE3	1.93	0.41
1:A:164:LEU:HD23	1:A:165:MSE:N	2.36	0.41
1:A:78:ILE:HG12	1:A:79:ASN:N	2.35	0.41
1:A:341:ALA:HB2	1:A:383:TYR:HE1	1.85	0.41
1:C:401:LEU:HD12	1:C:402:PRO:HD2	2.01	0.41
1:C:114:MSE:HE3	1:C:307:TRP:HE3	1.86	0.41
1:A:342:PRO:HD2	1:A:348:TRP:CD1	2.55	0.41
1:A:246:PRO:O	1:A:247:CYS:CB	2.69	0.41
1:B:103:MSE:O	1:B:131:THR:HB	2.21	0.40
1:C:337:MSE:HG3	1:C:387:MSE:HE1	2.03	0.40
1:C:379:LYS:O	1:C:379:LYS:HG2	2.20	0.40
1:C:287:ARG:CG	1:C:287:ARG:NH1	2.83	0.40
1:B:180:LEU:HA	1:B:180:LEU:HD23	1.80	0.40
1:A:109:TRP:CD1	1:A:126:SER:HB3	2.56	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	394/443 (89%)	384 (98%)	10 (2%)	0	100	100
1	B	394/443 (89%)	382 (97%)	12 (3%)	0	100	100
1	C	395/443 (89%)	386 (98%)	9 (2%)	0	100	100
All	All	1183/1329 (89%)	1152 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	338/358 (94%)	323 (96%)	15 (4%)	35	32
1	B	339/358 (95%)	319 (94%)	20 (6%)	24	20
1	C	339/358 (95%)	321 (95%)	18 (5%)	28	24
All	All	1016/1074 (95%)	963 (95%)	53 (5%)	29	25

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

Mol	Chain	Res	Type
1	A	89	LEU
1	A	162	VAL
1	A	171	VAL
1	A	177	LYS
1	A	183	MSE

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Mol	Chain	Res	Type
1	A	197	LYS
1	A	211	LYS
1	A	212	LYS
1	A	223	LEU
1	A	227	SER
1	A	277	MSE
1	A	324	ILE
1	A	366	ASN
1	A	379	LYS
1	A	431	ILE
1	B	29	LEU
1	B	62	GLN
1	B	79	ASN
1	B	103	MSE
1	B	144	GLN
1	B	150	SER
1	B	174	GLU
1	B	180	LEU
1	B	201	LYS
1	B	211	LYS
1	B	223	LEU
1	B	252	THR
1	B	265	LYS
1	B	272	GLU
1	B	288	ASP
1	B	324	ILE
1	B	350	VAL
1	B	380	ASP
1	B	391	GLU
1	B	396	ASP
1	C	29	LEU
1	C	78	ILE
1	C	89	LEU
1	C	180	LEU
1	C	211	LYS
1	C	223	LEU
1	C	234	GLN
1	C	272	GLU
1	C	287	ARG
1	C	288	ASP
1	C	324	ILE
1	C	340	LYS

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Mol	Chain	Res	Type
1	C	350	VAL
1	C	362	LYS
1	C	365	LEU
1	C	376	LYS
1	C	379	LYS
1	C	392	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	84	HIS
1	A	144	GLN
1	B	49	HIS
1	C	368	HIS

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, 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	381/443 (86%)	-0.28	8 (2%) 67 71	14, 28, 62, 86	0
1	B	381/443 (86%)	-0.22	12 (3%) 52 60	15, 27, 67, 97	0
1	C	382/443 (86%)	-0.26	13 (3%) 49 57	12, 25, 61, 100	0
All	All	1144/1329 (86%)	-0.25	33 (2%) 55 63	12, 27, 63, 100	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	76	PRO	10.8
1	B	78	ILE	7.7
1	A	76	PRO	5.9
1	A	78	ILE	5.8
1	B	76	PRO	5.6
1	C	78	ILE	5.3
1	B	77	THR	4.1
1	A	80	ASN	4.0
1	C	77	THR	3.5
1	B	395	ALA	3.4
1	C	393	GLY	3.4
1	B	392	LYS	3.3
1	B	379	LYS	3.1
1	C	396	ASP	3.0
1	A	77	THR	3.0
1	C	392	LYS	2.9
1	C	366	ASN	2.8
1	B	396	ASP	2.7
1	B	362	LYS	2.7
1	C	362	LYS	2.6
1	C	25	THR	2.5
1	C	364	ASP	2.4
1	B	366	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	79	ASN	2.3
1	A	392	LYS	2.3
1	A	396	ASP	2.3
1	B	25	THR	2.3
1	C	395	ALA	2.3
1	B	380	ASP	2.2
1	C	376	LYS	2.1
1	A	379	LYS	2.1
1	B	393	GLY	2.0
1	A	173	ASP	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.