



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2016 – 01:17 PM EDT

PDB ID : 5IZV
Title : Crystal structure of the legionella pneumophila effector protein RavZ - F222
Authors : Kwon, D.H.; Kim, L.-H.; Kim, B.-W.; Hong, S.B.; Song, H.K.
Deposited on : 2016-03-26
Resolution : 2.81 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
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) : rb-20028320

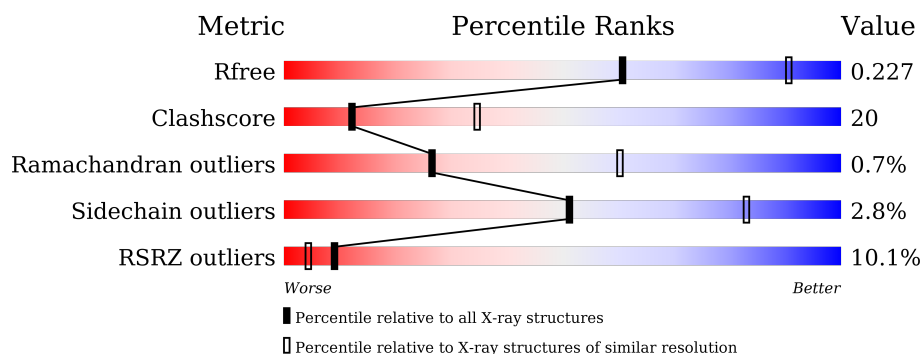
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 ≥ 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	502	<div> <div>9%</div> <div>48%</div> <div>25%</div> <div>•</div> <div>25%</div> </div>
1	B	502	<div> <div>6%</div> <div>45%</div> <div>27%</div> <div>•</div> <div>26%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5873 atoms, of which 0 are hydrogens and 0 are deuteriums.

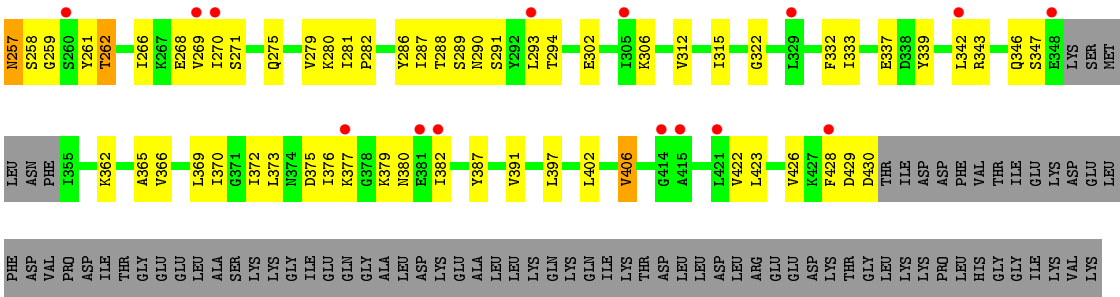
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Uncharacterized protein RavZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2965	1880	485	592	8			
1	B	369	Total	C	N	O	S	0	0	0
			2908	1847	475	578	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	SER	CYS	engineered mutation	UNP Q5ZUV9
B	258	SER	CYS	engineered mutation	UNP Q5ZUV9



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	72.25Å 313.00Å 314.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.55 – 2.81 46.90 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.55-2.81) 96.6 (46.90-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.188 , 0.227 0.186 , 0.227	Depositor DCC
R_{free} test set	2012 reflections (4.73%)	DCC
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.449 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5873	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, 0.333 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	0.58	3/3020 (0.1%)	0.81	5/4079 (0.1%)
1	B	0.49	0/2961	0.79	1/3998 (0.0%)
All	All	0.54	3/5981 (0.1%)	0.80	6/8077 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	GLU	CD-OE1	-7.61	1.17	1.25
1	A	172	LYS	CD-CE	-7.52	1.32	1.51
1	A	255	GLU	CD-OE2	-6.19	1.18	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	LEU	CA-CB-CG	8.42	134.67	115.30
1	A	413	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	A	256	GLY	N-CA-C	-5.45	99.47	113.10
1	A	376	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	A	413	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	253	LEU	CB-CG-CD2	-5.20	102.16	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	THR	Peptide

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	2965	0	2941	109	0
1	B	2908	0	2893	123	0
All	All	5873	0	5834	232	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 (232) 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:A:200:GLY:O	1:A:201:ARG:HD3	1.47	1.13
1:A:201:ARG:NH2	1:A:249:HIS:HA	1.66	1.09
1:A:201:ARG:HH22	1:A:249:HIS:HA	0.92	1.05
1:A:201:ARG:HH22	1:A:249:HIS:CA	1.71	1.03
1:A:409:HIS:O	1:A:413:LEU:HD23	1.59	1.03
1:B:252:ARG:NH1	1:B:256:GLY:CA	2.25	0.99
1:B:56:SER:O	1:B:61:LYS:NZ	1.96	0.98
1:A:362:LYS:HE3	1:A:396:CYS:SG	2.04	0.97
1:B:252:ARG:HH11	1:B:256:GLY:H	1.06	0.96
1:B:376:ILE:HD11	1:B:422:VAL:HG23	1.56	0.87
1:B:58:GLU:HG2	1:B:61:LYS:HE2	1.55	0.86
1:A:219:THR:HG22	1:A:221:ASP:H	1.40	0.85
1:B:252:ARG:HH12	1:B:256:GLY:C	1.80	0.84
1:B:252:ARG:NH1	1:B:256:GLY:C	2.32	0.83
1:B:252:ARG:NH1	1:B:256:GLY:H	1.76	0.82
1:B:252:ARG:HH11	1:B:256:GLY:N	1.79	0.81
1:B:252:ARG:NH1	1:B:256:GLY:N	2.29	0.80
1:B:258:SER:O	1:B:262:THR:HG23	1.83	0.79
1:B:250:GLN:HE22	1:B:261:TYR:HE1	1.32	0.77
1:A:194:THR:HG23	1:A:243:THR:HG23	1.67	0.77
1:B:252:ARG:NH1	1:B:257:ASN:N	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ASP:O	1:B:380:ASN:HB2	1.86	0.75
1:A:217:ARG:NH2	1:A:222:GLU:OE1	2.19	0.74
1:B:217:ARG:NH2	1:B:222:GLU:OE1	2.20	0.74
1:B:252:ARG:HH12	1:B:257:ASN:N	1.86	0.74
1:A:258:SER:O	1:A:262:THR:HG23	1.88	0.73
1:B:219:THR:HG22	1:B:221:ASP:H	1.52	0.72
1:B:232:ILE:O	1:B:235:THR:HG22	1.87	0.72
1:A:381:GLU:HG3	1:A:425:CYS:O	1.88	0.72
1:A:287:ILE:H	1:A:287:ILE:HD12	1.55	0.72
1:B:252:ARG:NH1	1:B:256:GLY:HA3	2.03	0.70
1:B:85:GLY:O	1:B:105:LYS:NZ	2.23	0.70
1:B:114:PHE:CG	1:B:161:LEU:HD13	2.26	0.70
1:B:109:GLN:NE2	1:B:158:THR:HG23	2.07	0.69
1:B:287:ILE:H	1:B:287:ILE:HD12	1.56	0.68
1:A:362:LYS:NZ	1:A:396:CYS:O	2.19	0.68
1:B:221:ASP:OD2	1:B:244:ARG:NH1	2.28	0.67
1:B:114:PHE:CD2	1:B:161:LEU:HD13	2.30	0.67
1:B:199:ILE:HB	1:B:248:ASN:OD1	1.96	0.66
1:A:188:SER:OG	1:A:190:GLN:N	2.28	0.66
1:A:362:LYS:HE2	1:A:402:LEU:HD23	1.78	0.65
1:B:302:GLU:O	1:B:306:LYS:HG3	1.96	0.65
1:A:369:LEU:HD22	1:A:397:LEU:HD13	1.78	0.65
1:A:346:GLN:HB2	1:A:347:SER:HA	1.78	0.65
1:B:208:LEU:O	1:B:213:LYS:NZ	2.25	0.64
1:B:387:TYR:O	1:B:391:VAL:HG23	1.98	0.63
1:A:355:ILE:HG13	1:A:356:GLY:H	1.64	0.62
1:B:289:SER:O	1:B:293:LEU:N	2.32	0.62
1:B:333:ILE:HG23	1:B:370:ILE:HG23	1.81	0.62
1:A:109:GLN:HG3	1:A:110:GLN:N	2.14	0.61
1:A:311:GLY:O	1:A:315:ILE:HD12	2.00	0.61
1:A:51:TYR:CZ	1:A:312:VAL:HG12	2.35	0.61
1:B:288:THR:O	1:B:291:SER:OG	2.16	0.61
1:A:235:THR:OG1	1:A:236:ASP:N	2.34	0.61
1:B:252:ARG:CZ	1:B:256:GLY:HA3	2.29	0.61
1:B:235:THR:OG1	1:B:236:ASP:N	2.34	0.61
1:B:372:ILE:HG23	1:B:382:ILE:HD12	1.82	0.60
1:A:133:GLY:C	1:A:223:ILE:HD13	2.21	0.60
1:A:255:GLU:HG2	1:A:256:GLY:C	2.22	0.60
1:A:55:THR:O	1:A:306:LYS:HE3	2.01	0.60
1:A:201:ARG:NH2	1:A:249:HIS:O	2.34	0.60
1:B:247:TYR:HB3	1:B:281:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:O	1:A:337:GLU:HG3	2.02	0.59
1:B:190:GLN:HG3	1:B:238:THR:HB	1.84	0.59
1:B:194:THR:HG22	1:B:243:THR:HB	1.83	0.59
1:A:333:ILE:HG23	1:A:370:ILE:HG23	1.84	0.59
1:A:422:VAL:O	1:A:425:CYS:HB2	2.03	0.59
1:B:114:PHE:CG	1:B:161:LEU:CD1	2.86	0.59
1:B:199:ILE:HD12	1:B:248:ASN:ND2	2.18	0.58
1:A:373:LEU:O	1:A:376:ILE:HG22	2.04	0.58
1:A:201:ARG:CZ	1:A:249:HIS:HA	2.31	0.58
1:A:397:LEU:HD12	1:A:418:LEU:HD13	1.85	0.58
1:A:91:LEU:HD23	1:A:92:GLU:N	2.19	0.58
1:A:142:ARG:NH2	1:A:145:GLU:OE1	2.36	0.58
1:B:332:PHE:HZ	1:B:406:VAL:HG13	1.68	0.58
1:A:235:THR:HG21	1:A:237:PHE:CD2	2.39	0.57
1:A:288:THR:O	1:A:291:SER:OG	2.22	0.56
1:B:249:HIS:CG	1:B:289:SER:OG	2.58	0.56
1:A:91:LEU:HD22	1:A:94:LYS:N	2.20	0.56
1:B:402:LEU:O	1:B:406:VAL:HG23	2.06	0.56
1:B:51:TYR:CZ	1:B:312:VAL:HG12	2.40	0.55
1:B:379:LYS:HB2	1:B:380:ASN:HA	1.88	0.55
1:A:204:TYR:C	1:A:206:GLU:H	2.09	0.55
1:B:51:TYR:HE2	1:B:315:ILE:HD12	1.72	0.55
1:B:343:ARG:O	1:B:343:ARG:HG2	2.07	0.55
1:B:379:LYS:N	1:B:380:ASN:OD1	2.38	0.55
1:A:201:ARG:HH22	1:A:249:HIS:C	2.10	0.55
1:A:400:SER:O	1:A:402:LEU:N	2.38	0.54
1:B:271:SER:O	1:B:275:GLN:HG3	2.08	0.54
1:B:210:SER:HA	1:B:213:LYS:HE2	1.90	0.54
1:B:252:ARG:NE	1:B:254:THR:OG1	2.40	0.54
1:B:250:GLN:NE2	1:B:261:TYR:HE1	2.02	0.54
1:A:89:SER:HB3	1:A:105:LYS:HE3	1.88	0.54
1:A:381:GLU:OE1	1:A:425:CYS:SG	2.66	0.54
1:B:142:ARG:NH2	1:B:145:GLU:OE1	2.41	0.54
1:B:235:THR:HG23	1:B:237:PHE:H	1.73	0.54
1:B:177:GLN:HG2	1:B:259:GLY:HA2	1.90	0.54
1:A:346:GLN:HA	1:A:348:GLU:N	2.23	0.53
1:B:54:GLU:OE1	1:B:67:ARG:NH1	2.41	0.53
1:A:355:ILE:HG13	1:A:356:GLY:N	2.24	0.53
1:B:109:GLN:HE21	1:B:158:THR:HG23	1.72	0.53
1:A:373:LEU:HA	1:A:376:ILE:HG22	1.90	0.53
1:B:236:ASP:OD1	1:B:236:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ILE:HD11	1:A:386:GLN:HB3	1.92	0.52
1:A:362:LYS:CE	1:A:396:CYS:SG	2.91	0.52
1:B:55:THR:O	1:B:306:LYS:HE3	2.09	0.52
1:A:277:THR:HG22	1:A:278:GLU:O	2.09	0.52
1:B:114:PHE:HB2	1:B:161:LEU:HD12	1.91	0.52
1:A:141:ARG:O	1:A:145:GLU:HG3	2.09	0.51
1:B:382:ILE:HG23	1:B:426:VAL:HA	1.92	0.51
1:A:328:GLN:HG3	1:A:330:SER:OG	2.11	0.51
1:A:255:GLU:HB2	1:A:258:SER:OG	2.11	0.51
1:A:85:GLY:O	1:A:105:LYS:NZ	2.32	0.51
1:A:255:GLU:HG2	1:A:256:GLY:CA	2.41	0.50
1:B:262:THR:O	1:B:266:ILE:HG13	2.11	0.50
1:B:333:ILE:O	1:B:337:GLU:HG3	2.11	0.50
1:B:247:TYR:HD1	1:B:282:PRO:HG2	1.76	0.50
1:B:70:LYS:O	1:B:73:SER:OG	2.30	0.50
1:B:51:TYR:CE2	1:B:315:ILE:HD12	2.47	0.50
1:B:154:THR:OG1	1:B:155:GLN:OE1	2.25	0.49
1:B:342:LEU:O	1:B:342:LEU:HD23	2.11	0.49
1:B:114:PHE:CB	1:B:161:LEU:HD12	2.42	0.49
1:B:232:ILE:HB	1:B:235:THR:HG21	1.95	0.48
1:A:378:GLY:C	1:A:380:ASN:HB2	2.33	0.48
1:B:339:TYR:CZ	1:B:402:LEU:HB2	2.48	0.48
1:B:428:PHE:O	1:B:430:ASP:HA	2.13	0.48
1:B:268:GLU:HG3	1:B:268:GLU:O	2.14	0.48
1:A:236:ASP:OD2	1:A:236:ASP:N	2.40	0.48
1:B:114:PHE:CB	1:B:161:LEU:CD1	2.90	0.48
1:A:269:VAL:HG22	1:A:279:VAL:HG21	1.95	0.48
1:A:176:HIS:NE2	1:A:199:ILE:HG12	2.29	0.48
1:B:369:LEU:HD22	1:B:397:LEU:HD13	1.95	0.48
1:A:201:ARG:NH2	1:A:249:HIS:CA	2.48	0.47
1:A:409:HIS:C	1:A:413:LEU:HD23	2.32	0.47
1:B:266:ILE:O	1:B:270:ILE:HG13	2.14	0.47
1:A:247:TYR:HB3	1:A:281:ILE:HD12	1.95	0.47
1:B:91:LEU:O	1:B:92:GLU:HG3	2.15	0.47
1:A:176:HIS:CE1	1:A:199:ILE:HG12	2.49	0.47
1:B:155:GLN:HB3	1:B:156:PRO:HD2	1.97	0.47
1:B:249:HIS:NE2	1:B:288:THR:HG23	2.30	0.47
1:B:247:TYR:CD1	1:B:282:PRO:HG2	2.49	0.47
1:A:92:GLU:HA	1:A:93:ASP:HA	1.56	0.47
1:A:201:ARG:NH2	1:A:249:HIS:C	2.67	0.47
1:A:93:ASP:HB3	1:A:95:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:HG22	1:A:221:ASP:N	2.20	0.46
1:A:271:SER:O	1:A:275:GLN:HG3	2.13	0.46
1:A:339:TYR:CZ	1:A:402:LEU:HB2	2.49	0.46
1:A:365:ALA:HB1	1:A:397:LEU:CD2	2.46	0.46
1:A:93:ASP:N	1:A:94:LYS:HA	2.31	0.46
1:B:423:LEU:HA	1:B:426:VAL:HG23	1.96	0.46
1:B:93:ASP:HB3	1:B:95:PRO:CD	2.46	0.46
1:B:96:LEU:HB3	1:B:99:ALA:HB3	1.96	0.46
1:A:130:SER:O	1:A:217:ARG:NH1	2.49	0.46
1:B:94:LYS:NZ	1:B:110:GLN:HE22	2.13	0.46
1:A:328:GLN:CD	1:A:329:LEU:H	2.19	0.46
1:A:176:HIS:HE1	1:A:197:ASP:OD2	1.98	0.45
1:B:379:LYS:CB	1:B:380:ASN:HA	2.46	0.45
1:A:108:ASP:OD1	1:A:108:ASP:N	2.48	0.45
1:A:184:TYR:HB2	1:A:191:LEU:HD22	1.98	0.45
1:A:387:TYR:O	1:A:391:VAL:HG23	2.17	0.45
1:B:209:SER:O	1:B:212:PHE:N	2.49	0.45
1:A:268:GLU:HG3	1:A:268:GLU:O	2.16	0.45
1:A:170:ILE:HG21	1:A:170:ILE:HD13	1.53	0.45
1:B:175:GLN:O	1:B:255:GLU:HA	2.17	0.44
1:B:269:VAL:HG22	1:B:279:VAL:HG21	2.00	0.44
1:A:248:ASN:ND2	1:A:261:TYR:CZ	2.85	0.44
1:A:109:GLN:NE2	1:A:158:THR:OG1	2.51	0.44
1:B:109:GLN:HG3	1:B:110:GLN:N	2.32	0.44
1:A:262:THR:O	1:A:266:ILE:HG13	2.18	0.44
1:A:190:GLN:HA	1:A:238:THR:O	2.17	0.44
1:B:75:PHE:HB3	1:B:84:LEU:HD12	2.00	0.44
1:B:288:THR:HG22	1:B:289:SER:N	2.33	0.44
1:B:332:PHE:CD2	1:B:373:LEU:HD21	2.52	0.44
1:B:362:LYS:HE2	1:B:402:LEU:HD23	2.00	0.44
1:A:423:LEU:HA	1:A:426:VAL:HG23	1.99	0.43
1:B:141:ARG:O	1:B:145:GLU:HG3	2.18	0.43
1:A:190:GLN:HG3	1:A:238:THR:HG23	2.00	0.43
1:A:72:TYR:CZ	1:A:116:PRO:HD3	2.53	0.43
1:B:253:LEU:H	1:B:253:LEU:HD23	1.83	0.43
1:A:346:GLN:HA	1:A:348:GLU:H	1.81	0.43
1:B:362:LYS:O	1:B:366:VAL:HG13	2.17	0.43
1:B:235:THR:CG2	1:B:237:PHE:H	2.31	0.43
1:A:286:TYR:CE1	1:A:292:TYR:HD2	2.37	0.43
1:A:429:ASP:HA	1:A:430:ASP:HA	1.69	0.43
1:B:429:ASP:HA	1:B:430:ASP:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:TYR:CZ	1:A:186:PRO:HA	2.54	0.43
1:B:184:TYR:HB2	1:B:191:LEU:HD22	2.00	0.43
1:A:76:PHE:CD1	1:A:322:GLY:HA2	2.54	0.43
1:B:184:TYR:CZ	1:B:186:PRO:HA	2.53	0.43
1:B:76:PHE:CE2	1:B:322:GLY:HA2	2.53	0.43
1:A:362:LYS:O	1:A:366:VAL:HG13	2.19	0.42
1:B:110:GLN:O	1:B:157:ALA:HA	2.19	0.42
1:A:167:PRO:HB2	1:A:170:ILE:HG22	2.02	0.42
1:A:366:VAL:O	1:A:370:ILE:HG13	2.19	0.42
1:B:198:SER:HA	1:B:247:TYR:O	2.20	0.42
1:B:58:GLU:OE2	1:B:60:ASN:HB2	2.20	0.42
1:A:382:ILE:HG23	1:A:426:VAL:HA	2.00	0.42
1:A:365:ALA:HB1	1:A:397:LEU:HD23	2.01	0.42
1:B:232:ILE:HB	1:B:235:THR:CG2	2.48	0.42
1:B:290:ASN:O	1:B:294:THR:HG22	2.19	0.42
1:B:365:ALA:HB1	1:B:397:LEU:CD2	2.49	0.42
1:A:224:LEU:O	1:A:228:ILE:HG13	2.19	0.42
1:A:376:ILE:HG21	1:A:376:ILE:HD13	1.76	0.42
1:B:126:VAL:O	1:B:216:TYR:HA	2.20	0.42
1:A:365:ALA:HA	1:A:393:GLU:HG2	2.01	0.42
1:A:346:GLN:CB	1:A:347:SER:HA	2.42	0.42
1:B:232:ILE:HD11	1:B:239:LEU:HB2	2.02	0.42
1:A:123:GLY:HA2	1:A:166:MET:O	2.20	0.41
1:A:241:LYS:HD2	1:A:241:LYS:HA	1.75	0.41
1:B:255:GLU:HB2	1:B:256:GLY:HA2	2.01	0.41
1:B:346:GLN:HA	1:B:347:SER:HA	1.79	0.41
1:B:93:ASP:HB3	1:B:95:PRO:N	2.35	0.41
1:A:287:ILE:H	1:A:287:ILE:CD1	2.28	0.41
1:B:333:ILE:HD12	1:B:377:LYS:HE2	2.02	0.41
1:A:355:ILE:CG1	1:A:356:GLY:H	2.32	0.41
1:A:84:LEU:HD21	1:A:267:LYS:HD2	2.03	0.41
1:A:126:VAL:O	1:A:216:TYR:HA	2.20	0.41
1:A:201:ARG:NH1	1:A:249:HIS:HA	2.36	0.41
1:B:123:GLY:HA2	1:B:166:MET:O	2.21	0.41
1:B:280:LYS:HB2	1:B:286:TYR:HE1	1.84	0.41
1:B:257:ASN:C	1:B:257:ASN:OD1	2.59	0.41
1:B:56:SER:O	1:B:56:SER:OG	2.38	0.41
1:B:63:MET:HG3	1:B:64:ASN:N	2.36	0.41
1:B:223:ILE:HD12	1:B:223:ILE:HA	1.88	0.41
1:B:93:ASP:OD1	1:B:95:PRO:HA	2.21	0.41
1:A:266:ILE:O	1:A:270:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:VAL:O	1:A:398:MET:HG2	2.21	0.40
1:A:188:SER:OG	1:A:190:GLN:HB2	2.21	0.40
1:B:190:GLN:HA	1:B:238:THR:O	2.21	0.40
1:B:241:LYS:NZ	1:B:242:PHE:H	2.19	0.40
1:A:93:ASP:HB3	1:A:95:PRO:N	2.37	0.40
1:B:110:GLN:C	1:B:111:ILE:HD13	2.42	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	372/502 (74%)	353 (95%)	15 (4%)	4 (1%)	17	48
1	B	363/502 (72%)	350 (96%)	12 (3%)	1 (0%)	46	78
All	All	735/1004 (73%)	703 (96%)	27 (4%)	5 (1%)	26	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	HIS
1	A	248	ASN
1	A	254	THR
1	B	257	ASN
1	A	201	ARG

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	337/449 (75%)	327 (97%)	10 (3%)	48	81
1	B	331/449 (74%)	322 (97%)	9 (3%)	52	84
All	All	668/898 (74%)	649 (97%)	19 (3%)	51	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	109	GLN
1	A	140	ASP
1	A	181	THR
1	A	201	ARG
1	A	253	LEU
1	A	267	LYS
1	A	360	THR
1	A	368	LEU
1	A	413	LEU
1	B	49	SER
1	B	65	SER
1	B	73	SER
1	B	91	LEU
1	B	96	LEU
1	B	140	ASP
1	B	248	ASN
1	B	262	THR
1	B	406	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	226	GLN
1	B	110	GLN
1	B	226	GLN

5.3.3 RNA ⓘ

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 [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	376/502 (74%)	0.91	46 (12%) 5 3	49, 89, 162, 260	0
1	B	369/502 (73%)	0.85	29 (7%) 15 8	49, 89, 153, 235	0
All	All	745/1004 (74%)	0.88	75 (10%) 9 4	49, 89, 157, 260	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	GLU	11.3
1	A	348	GLU	9.1
1	B	250	GLN	7.2
1	B	249	HIS	6.6
1	A	205	SER	5.3
1	A	379	LYS	4.2
1	B	428	PHE	4.0
1	A	202	ASP	3.7
1	A	208	LEU	3.7
1	A	74	LEU	3.5
1	A	249	HIS	3.5
1	A	339	TYR	3.5
1	B	94	LYS	3.4
1	B	329	LEU	3.0
1	A	252	ARG	3.0
1	A	126	VAL	2.9
1	A	139	LEU	2.9
1	A	111	ILE	2.9
1	B	215	LYS	2.9
1	A	176	HIS	2.8
1	A	421	LEU	2.8
1	A	170	ILE	2.8
1	A	93	ASP	2.7
1	B	415	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	377	LYS	2.7
1	A	325	LEU	2.7
1	A	261	TYR	2.7
1	A	287	ILE	2.7
1	B	270	ILE	2.7
1	B	414	GLY	2.6
1	A	94	LYS	2.6
1	A	363	LEU	2.6
1	A	124	TYR	2.6
1	A	84	LEU	2.5
1	A	428	PHE	2.5
1	B	72	TYR	2.5
1	A	292	TYR	2.5
1	A	390	LEU	2.5
1	A	88	VAL	2.5
1	A	174	VAL	2.5
1	B	247	TYR	2.4
1	A	347	SER	2.4
1	A	430	ASP	2.4
1	B	111	ILE	2.4
1	A	180	LEU	2.4
1	A	260	SER	2.4
1	B	84	LEU	2.4
1	B	305	ILE	2.4
1	B	421	LEU	2.4
1	A	342	LEU	2.3
1	A	407	GLN	2.3
1	B	135	VAL	2.3
1	A	250	GLN	2.3
1	B	93	ASP	2.3
1	A	122	ALA	2.3
1	A	201	ARG	2.2
1	B	260	SER	2.2
1	A	378	GLY	2.2
1	A	167	PRO	2.2
1	B	269	VAL	2.1
1	A	82	PHE	2.1
1	B	57	TRP	2.1
1	B	293	LEU	2.1
1	B	382	ILE	2.1
1	B	199	ILE	2.1
1	B	342	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	THR	2.0
1	B	255	GLU	2.0
1	A	373	LEU	2.0
1	A	343	ARG	2.0
1	A	143	LEU	2.0
1	B	239	LEU	2.0
1	A	209	SER	2.0
1	A	319	LEU	2.0
1	B	381	GLU	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.