

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8RLL
Title	:	Structure of the apo form of PIB-1 in an Orthorombic space group
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Deposited on	:	2024-01-03
Resolution	:	2.72 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.72 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	Similar resolution $(//Fntrieg, resolution, renge(\&))$
	(#Entries)	(#Entries, resolution range(A))
R_{free}	130704	3359(2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622(2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 >=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 <=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	А	391	% 7 6%	21%	•••
1	В	391	78%	20%	•••
1	С	391	75%	21%	•••
1	D	391	66%	31%	••



 $\mathbf{2}$

Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12203 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	295	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	309	3041	1927	536	571	$\overline{7}$	0		0
1	р	295	Total	С	Ν	0	S	0	0	0
	D	300	3041	1927	536	571	7	0	0	U
1	C	n 90r	Total	С	Ν	0	S	0	0	0
	380	3041	1927	536	571	7	0	0	0	
1	П	385	Total	С	Ν	0	S	0	0	0
	I D	385	3041	1927	536	571	7		0	0

• Molecule 1 is a protein called Class C beta-lactamase-related serine hydrolase.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	25	PRO	ALA	cloning artifact	UNP A0A1J0J3U4
В	25	PRO	ALA	cloning artifact	UNP A0A1J0J3U4
С	25	PRO	ALA	cloning artifact	UNP A0A1J0J3U4
D	25	PRO	ALA	cloning artifact	UNP A0A1J0J3U4

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	14	Total O 14 14	0	0
2	В	16	Total O 16 16	0	0
2	С	6	Total O 6 6	0	0
2	D	3	$\begin{array}{cc} \text{Total} & \text{O} \\ 3 & 3 \end{array}$	0	0





3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Class C beta-lactamase-related serine hydrolase



• Molecule 1: Class C beta-lactamase-related serine hydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	149.49Å 149.49Å 247.01Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	48.00 - 2.72	Depositor
Resolution (A)	48.00 - 2.72	EDS
% Data completeness	99.7 (48.00-2.72)	Depositor
(in resolution range)	91.8 (48.00-2.72)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.56 (at 2.73 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_4746, PHENIX dev_4746	Depositor
D D.	0.183 , 0.227	Depositor
Π, Π_{free}	0.183 , 0.229	DCC
R_{free} test set	2006 reflections $(3.62%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	57.9	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 44.3	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12203	wwPDB-VP
Average B, all atoms $(Å^2)$	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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		Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/3117	0.65	0/4225	
1	В	0.44	0/3117	0.70	0/4225	
1	С	0.43	0/3117	0.65	1/4225~(0.0%)	
1	D	0.41	1/3117~(0.0%)	0.64	0/4225	
All	All	0.43	1/12468~(0.0%)	0.66	1/16900~(0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	30	GLU	C-N	5.01	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	С	310	ILE	C-N-CA	5.04	134.31	121.70

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	А	3041	0	2964	55	0
1	В	3041	0	2964	50	0
1	С	3041	0	2964	58	0
1	D	3041	0	2964	86	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	14	0	0	0	0
2	В	16	0	0	1	0
2	С	6	0	0	0	0
2	D	3	0	0	0	0
All	All	12203	0	11856	247	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 10.

All (247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:185:TRP:HE1	1:A:187:GLU:HG2	1.39	0.87
1:D:62:ARG:NH2	1:D:277:GLY:O	2.11	0.84
1:D:34:ILE:HA	1:D:51:THR:HG22	1.64	0.78
1:D:191:ASP:HB3	1:D:194:SER:HB3	1.65	0.78
1:B:358:GLU:OE1	1:B:414:ARG:NH2	2.17	0.78
1:C:62:ARG:NH2	1:C:277:GLY:O	2.18	0.77
1:B:146:GLN:NE2	1:B:309:ARG:HG2	2.00	0.77
1:D:329:ALA:HB3	1:D:332:LYS:HD2	1.67	0.76
1:A:396:ASP:O	1:A:400:GLU:HG3	1.85	0.76
1:D:235:SER:HB2	1:D:282:SER:HB3	1.70	0.73
1:C:94:ASP:O	1:C:98:ARG:HG3	1.89	0.72
1:C:265:GLU:HG3	1:C:294:ARG:NH1	2.04	0.71
1:D:369:ILE:H	1:D:369:ILE:HD12	1.56	0.71
1:C:184:ARG:HB2	1:C:221:GLN:HB2	1.71	0.70
1:D:71:ARG:O	1:D:294:ARG:NH1	2.24	0.70
1:D:99:ASN:HD21	1:D:401:GLU:HG2	1.56	0.70
1:C:152:LEU:HD13	1:C:174:GLU:HG3	1.73	0.70
1:D:94:ASP:O	1:D:98:ARG:HG3	1.91	0.70
1:C:358:GLU:OE1	1:C:414:ARG:NH2	2.24	0.70
1:B:306:ASP:OD1	1:B:307:GLY:N	2.25	0.69
1:A:62:ARG:NH2	1:A:277:GLY:O	2.26	0.68
1:A:235:SER:OG	1:A:345:GLN:NE2	2.23	0.68
1:B:217:SER:OG	2:B:501:HOH:O	2.12	0.67
1:A:151:ALA:HB3	1:A:154:GLN:HG2	1.76	0.66
1:D:79:ILE:HG21	1:D:413:LEU:HD21	1.76	0.66
1:B:146:GLN:HE22	1:B:309:ARG:HG2	1.59	0.66
1:D:83:TYR:HB3	1:D:408:ALA:HB2	1.77	0.66
1:D:303:GLY:HA3	1:D:311:LEU:HD12	1.79	0.65
1:B:317:ASP:OD1	1:B:378:ARG:NH1	2.27	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:185:TRP:NE1	1:A:187:GLU:HG2	2.11	0.65
1:D:395:MET:HE2	1:D:398:ARG:HG3	1.79	0.64
1:B:198:GLN:HB3	1:B:214:LEU:HD21	1.79	0.64
1:C:234:GLU:O	1:C:237:LEU:HB2	1.98	0.63
1:A:134:LYS:HZ1	1:A:232:THR:HG22	1.63	0.63
1:A:131:SER:HB3	1:A:134:LYS:HD2	1.79	0.63
1:D:262:MET:HE1	1:D:298:PHE:HB2	1.80	0.62
1:C:303:GLY:HA3	1:C:311:LEU:HB2	1.81	0.62
1:A:58:VAL:HG23	1:A:59:TYR:CD2	2.34	0.61
1:C:371:GLY:HA3	1:C:388:SER:HB2	1.83	0.61
1:C:134:LYS:HD3	1:C:345:GLN:HE22	1.66	0.61
1:D:221:GLN:HG2	1:D:222:TYR:CE2	2.35	0.60
1:B:186:ASN:OD1	1:B:188:THR:HG22	2.01	0.60
1:C:265:GLU:HG3	1:C:294:ARG:HH12	1.67	0.60
1:A:134:LYS:NZ	1:A:232:THR:HG22	2.17	0.59
1:B:222:TYR:HD2	1:D:337:GLU:HG3	1.68	0.59
1:C:239:SER:OG	1:C:278:GLN:NE2	2.32	0.58
1:B:84:ARG:HE	1:B:89:GLU:HG3	1.69	0.58
1:C:140:LEU:HD11	1:C:254:LEU:HB2	1.84	0.58
1:D:395:MET:CE	1:D:398:ARG:HE	2.17	0.58
1:A:371:GLY:HA3	1:A:388:SER:HB2	1.86	0.58
1:D:373:TYR:HB2	1:D:386:VAL:HB	1.86	0.58
1:A:134:LYS:HG2	1:A:235:SER:OG	2.03	0.58
1:B:199:MET:SD	1:B:232:THR:HG22	2.44	0.58
1:A:189:TYR:O	1:A:197:ARG:NH1	2.37	0.57
1:A:96:MET:HG3	1:A:97:ARG:N	2.20	0.57
1:D:206:GLU:HG2	1:D:275:PRO:HD3	1.85	0.57
1:C:102:GLY:N	1:C:387:TRP:O	2.32	0.57
1:D:33:ARG:HB3	1:D:47:TYR:CE1	2.39	0.57
1:D:259:TRP:CG	1:D:264:MET:HG3	2.39	0.57
1:D:79:ILE:HD12	1:D:80:ALA:H	1.69	0.57
1:A:152:LEU:HB3	1:A:174:GLU:HB2	1.88	0.56
1:C:134:LYS:HD3	1:C:345:GLN:NE2	2.21	0.56
1:A:187:GLU:OE2	1:A:196:ARG:HD2	2.05	0.56
1:C:305:ILE:HD12	1:C:310:ILE:HG13	1.86	0.56
1:D:236:HIS:HA	1:D:281:GLY:HA3	1.88	0.55
1:D:140:LEU:HD11	1:D:254:LEU:HB2	1.87	0.55
1:B:84:ARG:NE	1:B:89:GLU:HG3	2.21	0.55
1:C:374:LEU:HD13	1:C:385:VAL:HG22	1.90	0.54
1:A:251:SER:OG	1:A:279:GLU:OE2	2.20	0.54
1:D:107:LEU:HB2	1:D:383:VAL:HG13	1.90	0.54



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:141:VAL:HG11	1:C:177:LEU:HD11	1.90	0.54	
1:D:92:VAL:HG21	1:D:114:LEU:HD21	1.90	0.53	
1:A:48:GLN:HB2	1:A:49:PRO:HD3	1.90	0.53	
1:D:151:ALA:HB3	1:D:154:GLN:HG2	1.91	0.53	
1:B:66:LYS:NZ	1:B:67:GLY:O	2.41	0.53	
1:A:133:VAL:HA	1:A:136:ILE:HD12	1.91	0.53	
1:B:366:ALA:HB3	1:B:374:LEU:HB3	1.91	0.53	
1:D:90:TYR:HB3	1:D:94:ASP:HB2	1.90	0.52	
1:A:140:LEU:HD11	1:A:254:LEU:HD13	1.91	0.52	
1:B:331:GLY:O	1:B:336:GLY:HA2	2.09	0.52	
1:D:157:ASP:OD1	1:D:157:ASP:N	2.35	0.52	
1:B:397:ASP:N	1:B:397:ASP:OD1	2.42	0.52	
1:D:101:VAL:HA	1:D:388:SER:HA	1.91	0.52	
1:C:140:LEU:HB3	1:C:242:LEU:HD21	1.92	0.52	
1:D:122:ASP:H	1:D:125:THR:HG23	1.75	0.52	
1:D:259:TRP:CD2	1:D:264:MET:HG3	2.44	0.52	
1:C:317:ASP:OD1	1:C:378:ARG:NH1	2.33	0.52	
1:C:174:GLU:OE1	1:C:344:TYR:OH	2.23	0.51	
1:C:65:HIS:O	1:C:255:SER:OG	2.24	0.51	
1:C:199:MET:HG3	1:C:211:ILE:HG23	1.92	0.51	
1:D:363:ALA:HB2	1:D:377:ASN:HD22	1.75	0.51	
1:A:108:LYS:HD3	1:A:413:LEU:HB3	1.93	0.51	
1:C:79:ILE:HG13	1:C:81:PRO:HD3	1.93	0.51	
1:C:131:SER:OG	1:C:134:LYS:NZ	2.44	0.51	
1:D:64:ILE:HD13	1:D:254:LEU:HD23	1.93	0.50	
1:D:141:VAL:O	1:D:145:VAL:HG23	2.11	0.50	
1:D:378:ARG:HG2	1:D:378:ARG:HH11	1.77	0.50	
1:C:71:ARG:NH2	1:C:301:GLU:OE1	2.45	0.50	
1:D:33:ARG:HB3	1:D:47:TYR:CZ	2.47	0.50	
1:C:61:THR:HG22	1:C:271:GLN:HA	1.93	0.50	
1:D:99:ASN:HA	1:D:398:ARG:HD3	1.93	0.50	
1:C:238:GLN:O	1:C:242:LEU:HD12	2.12	0.49	
1:B:64:ILE:HD13	1:B:254:LEU:HD23	1.93	0.49	
1:C:309:ARG:CZ	1:C:313:GLU:HG3	2.43	0.49	
1:D:301:GLU:O	1:D:304:VAL:HG22	2.13	0.49	
1:D:98:ARG:O	1:D:398:ARG:NH1	2.46	0.49	
1:D:49:PRO:O	1:D:53:ARG:HG2	2.14	0.48	
1:D:406:LEU:O	1:D:410:VAL:HG23	2.13	0.48	
1:B:342:TYR:OH	1:B:345:GLN:HA	2.13	0.48	
1:D:156:VAL:HG13	1:D:171:VAL:O	2.14	0.48	
1:D:296:GLY:O	1:D:299:VAL:HG12	2.13	0.48	



		Interatomic Clash			
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1.D.131.SER.O	1.D.134.LYS.HB2	2.14	0.48		
1:B:382:ILE:HD12	1:B:410:VAL:HG22	1.96	0.47		
1.C·265·GLU·HG3	$1 \cdot C \cdot 294 \cdot ABG \cdot CZ$	$\frac{2.33}{2.45}$	0.47		
1:B:187:GLU:O	1:B:187:GLU:HG3	2.14	0.47		
1:C:134:LYS:HB3	1:C:345:GLN:HE21	1.79	0.47		
1.D.319.ALA.HB1	1·D·344·TYR·HB2	1.96	0.47		
1·B·71·ABG·HH12	1:B:301:GLU:CD	2.17	0.47		
$1 \cdot D \cdot 100 \cdot ABG \cdot HG2$	1.D.119.LEU.HD21	1.95	0.47		
1:D:212:LEU:HD23	1:D:212:LEU:HA	1.78	0.47		
1.D.79.ILE.HD11	1.D.412.ALA.HB1	1.96	0.47		
1.D.168.TYB.HE2	$1 \cdot D \cdot 215 \cdot L EU \cdot HD 22$	1.80	0.47		
1:A:116:ARG:HD3	1:B:147:GLN:HA	1.90	0.47		
1.C.129.SEB.HB3	1.C.292.TYB.OH	2.14	0.47		
1:A:129:SEB:HB2	1:A:132:VAL:HB	1.96	0.46		
1.D.99.ASN.HA	1.D.398.ABG.HH11	1.80	0.46		
1·B·373·TYB·OH	1.B.399.GLU.HG3	2.15	0.46		
1:C:354·LYS·HE3	1.C.354.LVS.HB3	1.80	0.46		
1.B.305.ILE.O	1.B.306.ASP.HB3	2.16	0.46		
$1 \cdot D \cdot 168 \cdot TYB \cdot CE2$	1.D.215.LEU.HD22	2.50	0.46		
1.D.121.ASN.HA	1.D.125.THB.HG21	1.96	0.46		
1:A:55:MET:HG3	1:A·128·THB·HB	1.98	0.46		
1.D.323.GLU.OE1	1.D.326.SEB.N	2 49	0.46		
1.A.49.PRO.O	1.A.53.ABG.HG2	2.15	0.46		
1:A:322:VAL:HG13	1:A:330:PRO:HD2	1.98	0.46		
1:C:40:LEU:HB2	1.C:59.TYB.OH	2.16	0.46		
1:D:53:ARG:HA	1:D:126:ABG:O	2.16	0.46		
1.C.322.VAL:HG23	1.C.330.PRO.HD2	1.97	0.46		
1.D.47.TYR.O	1.D.51.THR.HG23	2.16	0.46		
1:A:255:SER:HA	1:A:259:TRP:HB3	1.98	0.46		
1:B:140:LEU:HD11	1:B:254:LEU:HB2	1.97	0.46		
1:A:206:GLU:HA	1:A:273:GLU:O	2.16	0.45		
1:A:314:GLY:O	1:A:318:ABG:HG2	2.16	0.45		
1:D:347:TRP:CD1	1:D:367:GLN:HB3	2.51	0.45		
1:A:342:TYR:CZ	1:A:345:GLN:HA	2.51	0.45		
1:A:331:GLY:O	1:A:336:GLY:HA2	2.16	0.45		
1:A:131:SER:O	1:A:134:LYS:HB2	2.17	0.45		
1:B:98:ARG:NE	1:B:401:GLU:OE2	2.40	0.45		
1:B:306:ASP:CG	1:B:307:GLY:H	2.20	0.45		
1:B:212:LEU:HD23	1:B:215:LEU:HD12	1.98	0.45		
1:D:329:ALA:O	1:D:332:LYS:HB2	2.17	0.45		
1:D:369:ILE:H	1:D:369:ILE:CD1	2.20	0.45		



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:342:TYR:OH	1:A:345:GLN:HA	2.17	0.45	
1:C:83:TYR:HB3	1:C:408:ALA:HB2	1.98	0.45	
1:D:79:ILE:HG13	1:D:81:PRO:HD3	1.98	0.45	
1:A:127:TRP:O	1:A:286:SER:HA	2.17	0.45	
1:B:342:TYR:CZ	1:B:345:GLN:HA	2.52	0.45	
1:D:328:LEU:HD22	1:D:342:TYR:HB3	1.98	0.45	
1:B:290:ARG:O	1:B:294:ARG:HG3	2.16	0.45	
1:C:305:ILE:HG22	1:C:306:ASP:OD2	2.17	0.44	
1:D:107:LEU:O	1:D:382:ILE:HD13	2.16	0.44	
1:D:209:GLY:O	1:D:213:ARG:HG3	2.17	0.44	
1:D:46:GLU:OE1	1:D:46:GLU:N	2.47	0.44	
1:D:66:LYS:NZ	1:D:67:GLY:O	2.50	0.44	
1:A:206:GLU:HB3	1:A:275:PRO:HD3	2.00	0.44	
1:D:152:LEU:HD11	1:D:315:TRP:HZ3	1.82	0.44	
1:B:56:ASP:N	1:B:56:ASP:OD1	2.51	0.44	
1:D:105:LEU:HA	1:D:114:LEU:O	2.18	0.44	
1:D:361:GLY:HA2	1:D:379:LYS:HE2	2.00	0.44	
1:A:156:VAL:HG23	1:A:241:LEU:HD11	1.99	0.44	
1:A:317:ASP:OD1	1:A:378:ARG:NH1	2.48	0.43	
1:B:58:VAL:HB	1:B:59:TYR:CD2	2.53	0.43	
1:C:55:MET:HG3	1:C:128:THR:HB	2.00	0.43	
1:D:35:GLY:H	1:D:51:THR:CG2	2.31	0.43	
1:A:82:ARG:NH1	1:A:89:GLU:OE2	2.51	0.43	
1:D:98:ARG:HD3	1:D:401:GLU:OE2	2.19	0.43	
1:A:238:GLN:NE2	1:A:345:GLN:HE21	2.16	0.43	
1:C:82:ARG:HA	1:C:90:TYR:O	2.19	0.43	
1:D:237:LEU:HD12	1:D:237:LEU:HA	1.78	0.43	
1:D:377:ASN:OD1	1:D:380:GLU:HB2	2.19	0.43	
1:B:354:LYS:HA	1:B:354:LYS:HD3	1.81	0.43	
1:D:395:MET:HE1	1:D:398:ARG:HE	1.84	0.43	
1:D:35:GLY:H	1:D:51:THR:HG21	1.83	0.43	
1:D:134:LYS:HZ1	1:D:232:THR:HG22	1.84	0.43	
1:B:373:TYR:HH	1:B:390:TRP:HH2	1.65	0.43	
1:C:33:ARG:O	1:C:50:ASP:HB2	2.19	0.43	
1:A:382:ILE:HD12	1:A:410:VAL:HG22	2.01	0.42	
1:D:105:LEU:O	1:D:384:ALA:HA	2.19	0.42	
1:D:261:ARG:HG2	1:D:305:ILE:HG21	2.01	0.42	
1:B:54:ASN:HB3	1:B:57:LYS:HD2	2.00	0.42	
1:B:189:TYR:CE1	1:B:197:ARG:HD3	2.54	0.42	
1:B:199:MET:O	1:B:203:GLN:HG3	2.18	0.42	
1:B:338:TYR:CE2	1:B:340:LEU:HB2	2.53	0.42	



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:342:TYR:CZ	1:C:345:GLN:HA	2.54	0.42	
1:C:366:ALA:HB3	1:C:374:LEU:HB3	2.01	0.42	
1:D:114:LEU:HD12	1:D:114:LEU:HA	1.84	0.42	
1:D:122:ASP:OD1	1:D:125:THR:HG23	2.19	0.42	
1:A:53:ARG:HD3	1:A:121:ASN:OD1	2.19	0.42	
1:B:138:SER:HB2	1:B:345:GLN:HG3	2.01	0.42	
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.95	0.42	
1:D:264:MET:HB3	1:D:291:ASP:OD1	2.20	0.42	
1:A:79:ILE:HD12	1:A:81:PRO:HD3	2.02	0.42	
1:C:172:THR:OG1	1:C:175:GLN:HG3	2.19	0.42	
1:C:321:ARG:HH21	1:C:323:GLU:HG2	1.84	0.42	
1:A:137:SER:OG	1:A:238:GLN:NE2	2.53	0.42	
1:A:93:ASP:O	1:A:96:MET:HG2	2.20	0.42	
1:B:220:ARG:NH1	1:B:222:TYR:O	2.51	0.42	
1:D:215:LEU:HD11	1:D:233:GLY:O	2.20	0.42	
1:A:156:VAL:HG22	1:A:241:LEU:HD21	2.01	0.42	
1:B:140:LEU:HD23	1:B:140:LEU:HA	1.79	0.42	
1:A:369:ILE:HG13	1:A:370:PHE:CD2	2.55	0.41	
1:B:237:LEU:HD23	1:B:237:LEU:HA	1.71	0.41	
1:B:391:PRO:HD2	1:B:395:MET:SD	2.60	0.41	
1:C:95:PHE:O	1:C:99:ASN:ND2	2.51	0.41	
1:B:322:VAL:HG13	1:B:330:PRO:HD2	2.02	0.41	
1:C:105:LEU:HB2	1:C:289:LEU:HG	2.01	0.41	
1:D:109:ASP:OD1	1:D:381:LYS:HE2	2.20	0.41	
1:B:309:ARG:HG3	1:B:311:LEU:O	2.21	0.41	
1:A:96:MET:HA	1:A:101:VAL:HB	2.02	0.41	
1:C:262:MET:HA	1:C:305:ILE:HG21	2.02	0.41	
1:C:177:LEU:HD23	1:C:238:GLN:HE22	1.86	0.41	
1:C:187:GLU:HG3	1:C:187:GLU:O	2.21	0.41	
1:C:309:ARG:NE	1:C:313:GLU:HG3	2.35	0.41	
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.90	0.41	
1:A:312:PRO:HD2	1:A:315:TRP:HB2	2.01	0.41	
1:C:140:LEU:HD11	1:C:254:LEU:HD13	2.02	0.41	
1:C:177:LEU:HD23	1:C:238:GLN:NE2	2.36	0.41	
1:C:340:LEU:HD21	1:C:349:PHE:CD1	2.56	0.41	
1:D:73:LEU:HD23	1:D:73:LEU:HA	1.81	0.41	
1:D:102:GLY:N	1:D:387:TRP:O	2.52	0.41	
1:A:69:LYS:HE3	1:A:262:MET:O	2.22	0.40	
1:A:128:THR:HA	1:A:285:LEU:O	2.21	0.40	
1:A:318:ARG:HB3	1:A:321:ARG:NH1	2.36	0.40	
1:B:152:LEU:HB3	1:B:174:GLU:HB2	2.03	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:134:LYS:HB3	1:D:345:GLN:HE21	1.85	0.40
1:A:71:ARG:HA	1:A:72:PRO:HD3	1.92	0.40
1:B:55:MET:HG3	1:B:128:THR:HB	2.02	0.40
1:C:115:GLU:OE2	1:C:290:ARG:NH1	2.44	0.40
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.79	0.40
1:B:84:ARG:NH1	1:B:87:GLY:O	2.54	0.40
1:C:340:LEU:HD21	1:C:349:PHE:CE1	2.56	0.40
1:A:239:SER:OG	1:A:278:GLN:NE2	2.44	0.40
1:B:232:THR:HG23	1:B:282:SER:OG	2.21	0.40
1:C:237:LEU:HD23	1:C:237:LEU:HA	1.72	0.40
1:D:117:TYR:CZ	1:D:123:GLU:HA	2.56	0.40
1:C:191:ASP:OD1	1:C:193:LYS:N	2.55	0.40
1:C:322:VAL:HG21	1:C:351:VAL:HG22	2.04	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	Perce	entiles
1	А	383/391~(98%)	363~(95%)	20~(5%)	0	100	100
1	В	383/391~(98%)	370~(97%)	13 (3%)	0	100	100
1	С	383/391~(98%)	366~(96%)	17 (4%)	0	100	100
1	D	383/391~(98%)	356~(93%)	25~(6%)	2~(0%)	29	53
All	All	1532/1564~(98%)	1455 (95%)	75 (5%)	2(0%)	51	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	357	PRO
1	D	77	VAL



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	312/315~(99%)	301~(96%)	11 (4%)	36	63
1	В	312/315~(99%)	301 (96%)	11 (4%)	36	63
1	С	312/315~(99%)	302~(97%)	10 (3%)	39	67
1	D	312/315~(99%)	300 (96%)	12 (4%)	33	60
All	All	1248/1260~(99%)	1204 (96%)	44 (4%)	36	63

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	89	GLU
1	А	98	ARG
1	А	100	ARG
1	А	152	LEU
1	А	156	VAL
1	А	162	SER
1	А	196	ARG
1	А	235	SER
1	А	264	MET
1	А	326	SER
1	А	396	ASP
1	В	33	ARG
1	В	89	GLU
1	В	137	SER
1	В	138	SER
1	В	162	SER
1	В	235	SER
1	В	264	MET
1	В	286	SER
1	В	318	ARG
1	В	321	ARG
1	В	325	SER
1	С	68	THR
1	С	71	ARG



Mol	Chain	Res	Type
1	С	98	ARG
1	С	109	ASP
1	С	156	VAL
1	С	184	ARG
1	С	264	MET
1	С	309	ARG
1	С	322	VAL
1	С	335	ASP
1	D	30	GLU
1	D	31	ASN
1	D	70	VAL
1	D	82	ARG
1	D	94	ASP
1	D	98	ARG
1	D	157	ASP
1	D	180	SER
1	D	259	TRP
1	D	354	LYS
1	D	396	ASP
1	D	397	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	238	GLN
1	С	203	GLN
1	С	345	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^{th} 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 $>$	#RSR	Z>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	385/391~(98%)	0.02	2 (0%) 91	1 92	50, 66, 83, 104	0
1	В	385/391~(98%)	-0.11	2 (0%) 91	1 92	51, 64, 84, 110	0
1	С	385/391~(98%)	-0.11	4 (1%) 82	2 83	58, 71, 92, 114	0
1	D	385/391~(98%)	0.29	20 (5%) 2	27 26	55, 83, 106, 127	0
All	All	1540/1564~(98%)	0.02	28 (1%) 6	58 70	50, 70, 99, 127	0

All (28) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	D	77	VAL	5.9
1	D	85	ILE	4.7
1	D	76	GLY	4.1
1	D	113	ALA	3.8
1	D	414	ARG	3.5
1	D	75	ALA	3.5
1	D	351	VAL	3.3
1	С	88	GLU	2.9
1	D	84	ARG	2.9
1	D	79	ILE	2.8
1	В	96	MET	2.7
1	D	114	LEU	2.7
1	D	190	ARG	2.7
1	D	379	LYS	2.7
1	D	83	TYR	2.5
1	D	89	GLU	2.5
1	D	361	GLY	2.4
1	D	410	VAL	2.4
1	С	414	ARG	2.4
1	D	382	ILE	2.4
1	С	86	GLY	2.3



Continued	from	previous	page

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	D	362	GLY	2.3
1	В	77	VAL	2.3
1	D	413	LEU	2.3
1	С	87	GLY	2.1
1	А	207	ARG	2.1
1	А	96	MET	2.1
1	D	412	ALA	2.1

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.

