

Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 12:19 PM JST

PDB ID	:	8K2Y
Title	:	Crystal structure of MucD
Authors	:	Kim, J.H.; Park, H.H.
Deposited on	:	2023-07-14
Resolution	:	2.70 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	:	2.36
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)	:	2.36

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 2.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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						
			16%						
1	A	386		49%		23%	••	26%	
			15%						
1	В	386		49%		24%	·	25%	
			11%						
1	С	386		47%	22	%	•	29%	



8K2Y

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6193 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	286	Total	С	Ν	0	\mathbf{S}	0	0	0
	А	280	2076	1302	360	411	3	0	0	0
1	р	200	Total	С	Ν	0	S	0	0	0
	D	200	2108	1327	365	413	3	0	0	0
1	С	275	Total	С	Ν	0	S	0	0	0
	U	210	2009	1263	350	393	3	U	0	U

• Molecule 1 is a protein called serine endoprotease DegP-like protein MucD.



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: serine endoprotease DegP-like protein MucD





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	133.70Å 91.46Å 81.03Å	Deneiten
a, b, c, α , β , γ	90.00° 116.06° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	29.56 - 2.70	Depositor
Resolution (A)	29.56 - 2.70	EDS
% Data completeness	99.2 (29.56-2.70)	Depositor
(in resolution range)	99.0 (29.56-2.70)	EDS
R _{merge}	0.86	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.29 (at 2.68 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.205 , 0.269	Depositor
n, n_{free}	0.205 , 0.267	DCC
R_{free} test set	1998 reflections (8.31%)	wwPDB-VP
Wilson B-factor $(Å^2)$	62.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33 , 53.8	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
	0.457 for -1/2 *h+1/2 *k+l, 1/2 *h-1/2 *k+l, 1	
Estimated twinning fraction	/2*h+1/2*k	Xtriage
	0.467 for -1/2 * h - 1/2 * k + 1, -1/2 * h - 1/2 * k - 1, 1/2	Intilage
	*h-1/2*k	DDC
$\mathbf{F}_{o}, \mathbf{F}_{c}$ correlation	0.95	EDS
Total number of atoms	6193	wwPDB-VP
Average B, all atoms $(Å^2)$	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.97% 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	0.53	3/2101~(0.1%)	0.83	5/2852~(0.2%)	
1	В	0.46	0/2135	0.74	1/2896~(0.0%)	
1	С	0.45	0/2034	0.75	3/2759~(0.1%)	
All	All	0.48	3/6270~(0.0%)	0.77	9/8507~(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	А	0	2
1	В	0	1
All	All	0	3

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	274	ARG	CG-CD	-5.78	1.37	1.51
1	А	324	SER	CB-OG	5.45	1.49	1.42
1	А	324	SER	CA-CB	5.04	1.60	1.52

All (3) bond length outliers are listed below:

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	344	LYS	CD-CE-NZ	8.97	132.34	111.70
1	А	274	ARG	CG-CD-NE	8.68	130.04	111.80
1	А	271	LYS	CA-CB-CG	8.34	131.75	113.40
1	В	200	ARG	CG-CD-NE	7.46	127.48	111.80
1	А	200	ARG	CD-NE-CZ	7.44	134.02	123.60
1	С	344	LYS	CG-CD-CE	-6.98	90.97	111.90
1	С	344	LYS	CB-CG-CD	6.41	128.27	111.60
1	А	200	ARG	NE-CZ-NH1	5.60	123.10	120.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	200	ARG	NE-CZ-NH2	-5.29	117.66	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	200	ARG	Sidechain
1	А	274	ARG	Sidechain
1	В	200	ARG	Sidechain

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	2076	0	2108	69	0
1	В	2108	0	2152	72	0
1	С	2009	0	2052	66	0
All	All	6193	0	6312	203	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 16.

All (203) 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:324:SER:HB2	1:A:352:GLU:HB3	1.36	1.05
1:B:200:ARG:HA	1:B:209:PRO:HA	1.43	0.95
1:A:200:ARG:HA	1:A:209:PRO:HA	1.47	0.94
1:A:49:THR:HB	1:A:102:LEU:HD11	1.56	0.87
1:B:302:VAL:HG22	1:B:320:ASP:H	1.40	0.85
1:C:305:VAL:HB	1:C:317:GLN:HG3	1.59	0.83
1:C:222:SER:HB2	1:C:239:GLN:HG2	1.67	0.76
1:C:200:ARG:HA	1:C:209:PRO:HA	1.68	0.76
1:C:218:ASN:HD22	1:C:219:PRO:HD2	1.51	0.74
1:B:209:PRO:HG2	1:B:258:VAL:HG21	1.72	0.71



Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:28:GLU:HB2	1:C:229:MET:HB3	1.73	0.71		
1:B:109:SER:OG	1:B:111:ASP:OD1	2.08	0.70		
1:C:108:ILE:HD13	1:C:115:LEU:HG	1.73	0.70		
1:B:332:MET:HE1	1:B:334:ALA:HB3	1.75	0.69		
1:C:134:ARG:NH1	1:C:186:PHE:HB2	2.08	0.68		
1:A:48:SER:OG	1:A:130:ARG:NE	2.26	0.67		
1:A:249:GLY:N	1:B:217:ILE:O	2.28	0.66		
1:C:277:LEU:HD22	1:C:311:ALA:HB2	1.78	0.66		
1:A:302:VAL:HG22	1:A:320:ASP:H	1.61	0.66		
1:B:108:ILE:HD13	1:B:115:LEU:HG	1.77	0.66		
1:B:280:VAL:HG13	1:B:304:GLN:HB2	1.78	0.65		
1:C:209:PRO:HG2	1:C:258:VAL:HG21	1.79	0.64		
1:C:352:GLU:HB3	1:C:361:LYS:HE3	1.80	0.64		
1:B:200:ARG:HB3	1:B:209:PRO:HB3	1.80	0.64		
1:C:41:SER:HB3	1:C:188:HIS:CD2	2.32	0.64		
1:B:322:ILE:HD13	1:B:351:LEU:HD22	1.79	0.63		
1:C:239:GLN:HA	1:C:239:GLN:OE1	1.97	0.63		
1:B:279:VAL:HG21	1:B:302:VAL:HB	1.81	0.63		
1:A:328:GLN:HB2	1:A:339:LEU:HD21	1.80	0.63		
1:B:294:LEU:HD22	1:B:321:VAL:HG21	1.80	0.63		
1:A:141:LEU:HD11	1:A:144:THR:HG22	1.81	0.62		
1:B:27:ALA:O	1:B:28:GLU:HG2	2.00	0.62		
1:C:218:ASN:O	1:C:239:GLN:NE2	2.25	0.61		
1:B:322:ILE:HG12	1:B:353:VAL:HG12	1.81	0.61		
1:A:50:ARG:HA	1:A:50:ARG:NH1	2.15	0.61		
1:A:340:ILE:HA	1:A:343:LEU:HD22	1.83	0.61		
1:C:49:THR:HB	1:C:102:LEU:HD11	1.82	0.61		
1:C:145:ASP:OD2	1:C:274:ARG:NH2	2.33	0.61		
1:C:207:TYR:OH	1:C:274:ARG:HD3	2.02	0.60		
1:A:209:PRO:HG2	1:A:258:VAL:HG21	1.82	0.60		
1:A:180:ILE:HG12	1:A:190:VAL:HG22	1.84	0.59		
1:C:347:SER:O	1:C:366:VAL:HG12	2.02	0.59		
1:A:238:SER:O	1:A:239:GLN:HG3	2.02	0.58		
1:A:322:ILE:HG12	1:A:353:VAL:HG12	1.84	0.58		
1:B:117:ASN:HD21	1:B:238:SER:HB2	1.69	0.58		
1:A:28:GLU:HG3	1:A:30:LEU:H	1.68	0.58		
1:C:356:ASP:HB2	1:C:358:LYS:HE2	1.86	0.57		
1:A:37:VAL:O	1:A:41:SER:OG	2.19	0.57		
1:A:108:ILE:HD13	1:A:115:LEU:HG	1.86	0.57		
1:A:280:VAL:CG1	1:A:304:GLN:HB2	2.35	0.57		
1:B:141:LEU:HD11	1:B:144:THR:CG2	2.35	0.56		



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:324:SER:OG	1:C:352:GLU:HG2	2.06	0.56
1:A:348:LYS:HB3	1:A:363:THR:HG22	1.88	0.56
1:C:133:ASP:OD1	1:C:135:SER:OG	2.22	0.56
1:A:33:PHE:O	1:A:37:VAL:HG23	2.06	0.55
1:B:202:LEU:HD23	1:B:203:PRO:HG2	1.89	0.55
1:B:277:LEU:HD13	1:B:279:VAL:O	2.07	0.55
1:B:180:ILE:O	1:B:225:PRO:HD2	2.07	0.55
1:C:283:GLU:OE2	1:C:333:SER:N	2.29	0.55
1:A:352:GLU:HB2	1:A:361:LYS:HE2	1.89	0.54
1:B:352:GLU:HB2	1:B:361:LYS:HE3	1.88	0.54
1:C:277:LEU:HG	1:C:340:ILE:HD12	1.90	0.54
1:B:31:PRO:HB3	1:C:26:GLN:HB3	1.90	0.54
1:A:265:GLN:OE1	1:A:272:VAL:HG13	2.09	0.53
1:A:322:ILE:HG22	1:A:330:ILE:HD12	1.90	0.53
1:A:317:GLN:N	1:A:317:GLN:OE1	2.38	0.53
1:B:141:LEU:HD11	1:B:144:THR:HG22	1.90	0.53
1:B:355:ARG:HH22	1:B:362:LEU:HD21	1.73	0.53
1:B:33:PHE:O	1:B:37:VAL:HG23	2.08	0.53
1:A:46:ASN:OD1	1:A:130:ARG:NE	2.42	0.53
1:B:212:GLN:OE1	1:B:250:LEU:HD13	2.09	0.53
1:B:49:THR:HB	1:B:102:LEU:HD11	1.91	0.52
1:B:283:GLU:OE2	1:B:332:MET:HG2	2.09	0.52
1:A:180:ILE:O	1:A:225:PRO:HD2	2.10	0.52
1:C:46:ASN:OD1	1:C:130:ARG:HG3	2.08	0.52
1:B:337:PRO:O	1:B:341:GLY:N	2.39	0.52
1:A:239:GLN:HA	1:A:252:PHE:H	1.76	0.51
1:C:218:ASN:H	1:C:239:GLN:NE2	2.08	0.51
1:B:302:VAL:HG23	1:B:318:VAL:HA	1.93	0.51
1:B:277:LEU:HD12	1:B:278:GLY:H	1.75	0.51
1:B:355:ARG:O	1:B:358:LYS:HG2	2.11	0.51
1:B:182:SER:HB2	1:B:188:HIS:HD2	1.76	0.51
1:A:202:LEU:HD12	1:A:204:ASN:OD1	2.11	0.51
1:A:202:LEU:HD13	1:A:203:PRO:HD2	1.93	0.51
1:B:49:THR:HA	1:B:126:GLU:O	2.11	0.51
1:C:355:ARG:HB3	1:C:358:LYS:HE3	1.92	0.50
1:C:110:PRO:N	1:C:162:THR:HG21	2.26	0.50
1:A:324:SER:CB	1:A:352:GLU:HB3	2.24	0.50
1:B:305:VAL:HG11	1:B:316:VAL:O	2.12	0.50
1:A:273:SER:O	1:A:274:ARG:HG2	2.12	0.50
1:C:279:VAL:HG12	1:C:305:VAL:HG22	1.94	0.49
1:A:348:LYS:HA	1:A:364:VAL:O	2.11	0.49



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:48:SER:OG	1:B:130:ARG:HD2	2.12	0.49
1:B:202:LEU:HD22	1:B:204:ASN:CG	2.33	0.49
1:A:50:ARG:HA	1:A:50:ARG:HH11	1.76	0.49
1:C:306:LEU:O	1:C:312:ALA:HB2	2.13	0.49
1:C:322:ILE:HG12	1:C:353:VAL:HG12	1.95	0.49
1:A:330:ILE:HG23	1:A:332:MET:O	2.12	0.49
1:B:328:GLN:HG3	1:B:339:LEU:HD11	1.95	0.49
1:C:171:LEU:HG	1:C:195:VAL:HG21	1.94	0.49
1:B:317:GLN:NE2	1:B:320:ASP:OD1	2.45	0.48
1:B:134:ARG:HA	1:B:186:PHE:CD2	2.47	0.48
1:B:205:ASP:OD1	1:B:206:THR:N	2.46	0.48
1:B:332:MET:CE	1:B:334:ALA:HB3	2.42	0.48
1:A:115:LEU:HD13	1:A:236:ILE:HD11	1.96	0.48
1:C:316:VAL:HG13	1:C:317:GLN:N	2.28	0.48
1:B:277:LEU:HD12	1:B:278:GLY:N	2.28	0.48
1:A:339:LEU:O	1:A:343:LEU:HD13	2.14	0.48
1:A:345:ASP:OD1	1:A:367:GLY:HA2	2.14	0.48
1:C:121:ILE:HG21	1:C:153:LEU:HD21	1.94	0.48
1:C:300:ALA:HB2	1:C:333:SER:HA	1.96	0.48
1:A:310:PRO:HB2	1:A:364:VAL:HG13	1.96	0.47
1:C:178:LEU:HD11	1:C:190:VAL:HG13	1.96	0.47
1:C:271:LYS:HB3	1:C:271:LYS:HE2	1.72	0.47
1:C:317:GLN:H	1:C:317:GLN:CD	2.16	0.47
1:A:40:ALA:HB1	1:A:227:PHE:CZ	2.49	0.47
1:A:115:LEU:HD11	1:A:260:MET:CE	2.44	0.47
1:A:192:LYS:O	1:A:192:LYS:HD3	2.15	0.47
1:A:202:LEU:HD22	1:A:203:PRO:HD2	1.97	0.47
1:C:50:ARG:HD2	1:C:50:ARG:HA	1.69	0.47
1:A:196:SER:N	1:A:212:GLN:O	2.43	0.47
1:C:238:SER:O	1:C:252:PHE:O	2.33	0.47
1:B:289:ALA:HA	1:B:294:LEU:HB3	1.96	0.47
1:B:212:GLN:HG3	1:B:252:PHE:CE1	2.49	0.46
1:B:349:ALA:HB3	1:B:364:VAL:HB	1.97	0.46
1:C:137:LEU:HD12	1:C:155:ILE:HD12	1.97	0.46
1:A:106:PHE:HB3	1:A:225:PRO:HG3	1.97	0.46
1:C:191:THR:HG23	1:C:215:VAL:HG13	1.96	0.46
1:A:290:GLU:OE1	1:A:291:SER:N	2.49	0.46
1:A:202:LEU:HD13	1:A:203:PRO:CD	2.45	0.46
1:C:136:GLU:O	1:C:137:LEU:HD23	2.15	0.46
1:A:273:SER:C	1:A:274:ARG:HG2	2.37	0.45
1:B:150:VAL:HB	1:B:262:VAL:HG11	1.99	0.45



Interatomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:316:VAL:HG12	1:C:355:ARG:NH2	2.31	0.45	
1:B:280:VAL:CG1	1:B:304:GLN:HB2	2.46	0.45	
1:B:171:LEU:HG	1:B:195:VAL:HG21	1.98	0.45	
1:C:316:VAL:HG22	1:C:317:GLN:OE1	2.17	0.45	
1:B:354:ILE:HD13	1:B:359:ARG:HG3	1.99	0.45	
1:B:116:THR:CG2	1:B:151:ALA:HB3	2.47	0.44	
1:B:209:PRO:CG	1:B:258:VAL:HG21	2.45	0.44	
1:C:345:ASP:OD1	1:C:367:GLY:HA2	2.18	0.44	
1:B:344:LYS:HD2	1:B:344:LYS:HA	1.68	0.44	
1:A:336:LEU:HB3	1:A:337:PRO:HD3	1.98	0.44	
1:B:46:ASN:HB2	1:B:182:SER:OG	2.18	0.44	
1:B:119:HIS:ND1	1:B:149:ASP:OD2	2.43	0.44	
1:C:105:GLY:HA2	1:C:223:GLY:O	2.17	0.44	
1:B:300:ALA:HB2	1:B:333:SER:HA	2.00	0.44	
1:C:350:GLU:HG3	1:C:363:THR:OG1	2.18	0.44	
1:B:354:ILE:CD1	1:B:359:ARG:HG3	2.48	0.44	
1:C:283:GLU:OE2	1:C:332:MET:HG3	2.18	0.43	
1:A:332:MET:O	1:A:335:ASP:HB2	2.18	0.43	
1:B:302:VAL:HG13	1:B:320:ASP:O	2.18	0.43	
1:C:171:LEU:HD22	1:C:234:VAL:HB	1.99	0.43	
1:A:36:LEU:HD23	1:A:178:LEU:HD22	1.99	0.43	
1:B:279:VAL:HB	1:B:305:VAL:HA	2.01	0.43	
1:B:334:ALA:O	1:B:338:HIS:HB2	2.19	0.43	
1:B:355:ARG:HD2	1:B:358:LYS:HE3	2.01	0.43	
1:A:141:LEU:HD11	1:A:144:THR:CG2	2.49	0.43	
1:B:40:ALA:HB1	1:B:227:PHE:CZ	2.54	0.43	
1:C:352:GLU:O	1:C:352:GLU:HG3	2.19	0.43	
1:A:171:LEU:HG	1:A:195:VAL:HG21	2.00	0.42	
1:B:176:TRP:NE1	1:C:31:PRO:O	2.40	0.42	
1:B:183:PRO:HB3	1:B:220:GLY:HA3	2.01	0.42	
1:C:160:LEU:O	1:C:162:THR:HG23	2.19	0.42	
1:C:134:ARG:CZ	1:C:186:PHE:HB2	2.49	0.42	
1:A:333:SER:O	1:A:337:PRO:HD3	2.19	0.42	
1:B:126:GLU:OE2	1:B:127:ILE:N	2.53	0.42	
1:B:296:LYS:O	1:B:296:LYS:NZ	2.50	0.42	
1:C:164:LYS:HB2	1:C:164:LYS:HE3	1.71	0.42	
1:C:212:GLN:OE1	1:C:250:LEU:HD13	2.19	0.42	
1:A:334:ALA:O	1:A:337:PRO:HD2	2.20	0.42	
1:A:266:LEU:CD1	1:A:272:VAL:HG23	2.50	0.42	
1:C:302:VAL:HG11	1:C:305:VAL:HG23	2.02	0.41	
1:A:278:GLY:O	1:A:306:LEU:HG	2.19	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:317:GLN:HE22	1:A:355:ARG:HB2	1.86	0.41
1:A:348:LYS:HE3	1:A:365:THR:OG1	2.20	0.41
1:C:134:ARG:NH2	1:C:187:ASP:OD1	2.53	0.41
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.88	0.41
1:C:212:GLN:HG3	1:C:252:PHE:CE2	2.56	0.41
1:A:28:GLU:HG3	1:A:30:LEU:HB2	2.02	0.41
1:A:321:VAL:HB	1:A:354:ILE:HG22	2.02	0.41
1:A:104:SER:OG	1:A:220:GLY:O	2.28	0.41
1:C:204:ASN:OD1	1:C:204:ASN:N	2.48	0.41
1:A:130:ARG:HB3	1:A:186:PHE:CD2	2.56	0.41
1:A:130:ARG:HB3	1:A:186:PHE:CE2	2.55	0.41
1:A:192:LYS:HD3	1:A:192:LYS:C	2.41	0.41
1:C:277:LEU:HD23	1:C:277:LEU:HA	1.78	0.41
1:C:302:VAL:HG11	1:C:317:GLN:HA	2.03	0.41
1:A:41:SER:HB3	1:A:188:HIS:ND1	2.36	0.41
1:A:302:VAL:HG13	1:A:320:ASP:O	2.20	0.41
1:B:136:GLU:O	1:B:137:LEU:HD23	2.21	0.41
1:B:307:GLU:C	1:B:309:GLY:H	2.23	0.41
1:B:283:GLU:CD	1:B:332:MET:HG2	2.42	0.40
1:C:322:ILE:HG22	1:C:330:ILE:HD12	2.03	0.40
1:B:142:VAL:HB	1:B:152:VAL:HG12	2.04	0.40
1:B:279:VAL:HG23	1:B:304:GLN:O	2.22	0.40
1:C:202:LEU:HB3	1:C:204:ASN:OD1	2.21	0.40
1:C:191:THR:CG2	1:C:215:VAL:HG13	2.51	0.40
1:C:330:ILE:HG23	1:C:332:MET:O	2.21	0.40
1:A:347:SER:O	1:A:366:VAL:HG22	2.22	0.40
1:B:137:LEU:HD12	1:B:155:ILE:HD12	2.04	0.40
1:B:217:ILE:HD12	1:B:217:ILE:H	1.87	0.40
1:C:310:PRO:O	1:C:313:LYS:HB3	2.22	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	А	278/386~(72%)	265~(95%)	13~(5%)	0	100 100
1	В	280/386~(72%)	263~(94%)	17 (6%)	0	100 100
1	С	267/386~(69%)	255~(96%)	12 (4%)	0	100 100
All	All	825/1158 (71%)	783~(95%)	42 (5%)	0	100 100

There are no Ramachandran outliers to report.

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	225/310~(73%)	213~(95%)	12~(5%)	22 48
1	В	229/310~(74%)	219~(96%)	10 (4%)	28 56
1	С	218/310 (70%)	202~(93%)	16 (7%)	14 33
All	All	672/930~(72%)	634 (94%)	38~(6%)	20 44

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	41	SER
1	А	48	SER
1	А	140	LYS
1	А	192	LYS
1	А	200	ARG
1	А	201	SER
1	А	215	VAL
1	А	269	ASN
1	А	276	TRP
1	А	318	VAL
1	А	328	GLN
1	А	362	LEU
1	В	41	SER
1	В	100	GLN
1	В	125	ASP



Mol	Chain	Res	Type
1	В	126	GLU
1	В	134	ARG
1	В	192	LYS
1	В	200	ARG
1	В	279	VAL
1	В	318	VAL
1	В	338	HIS
1	С	101	SER
1	С	130	ARG
1	С	135	SER
1	С	147	ARG
1	С	186	PHE
1	С	192	LYS
1	С	206	THR
1	С	218	ASN
1	С	251	SER
1	С	269	ASN
1	С	277	LEU
1	С	305	VAL
1	С	316	VAL
1	С	333	SER
1	С	338	HIS
1	С	362	LEU

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	328	GLN
1	С	39	GLN
1	С	218	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 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	$\langle RSRZ \rangle$	# RSRZ >	$\cdot 2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	286/386~(74%)	1.10	62~(21%) 0	0	39, 71, 131, 144	0
1	В	288/386~(74%)	1.02	56 (19%) 1	0	39, 72, 128, 146	0
1	С	275/386~(71%)	1.08	44 (16%) 1	1	41, 68, 123, 151	0
All	All	849/1158~(73%)	1.07	162 (19%) 1	0	39, 70, 129, 151	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	353	VAL	13.8
1	А	350	GLU	11.5
1	С	206	THR	10.9
1	В	284	VAL	9.9
1	С	330	ILE	8.3
1	С	324	SER	7.8
1	С	329	PRO	7.7
1	В	339	LEU	7.5
1	А	354	ILE	7.4
1	А	275	GLY	7.0
1	С	354	ILE	7.0
1	В	290	GLU	6.8
1	С	207	TYR	6.7
1	С	328	GLN	6.6
1	А	102	LEU	6.3
1	А	288	LEU	6.1
1	С	334	ALA	5.9
1	А	331	VAL	5.8
1	А	306	LEU	5.7
1	С	310	PRO	5.7
1	С	323	LEU	5.7
1	В	204	ASN	5.7
1	А	341	GLY	5.7



Mol	Chain	Res	Type	RSRZ
1	A	304	GLN	5.5
1	В	294	LEU	5.4
1	А	321	VAL	5.3
1	В	334	ALA	5.3
1	В	306	LEU	5.2
1	С	325	ALA	5.2
1	С	237	ASN	5.1
1	В	252	PHE	4.9
1	В	307	GLU	4.9
1	А	276	TRP	4.9
1	А	324	SER	4.9
1	А	301	LEU	4.8
1	С	309	GLY	4.8
1	С	201	SER	4.8
1	С	161	PRO	4.8
1	А	277	LEU	4.7
1	С	344	LYS	4.7
1	А	349	ALA	4.6
1	С	186	PHE	4.6
1	А	302	VAL	4.6
1	С	360	GLN	4.5
1	С	277	LEU	4.5
1	В	336	LEU	4.4
1	А	284	VAL	4.4
1	А	292	PHE	4.4
1	А	286	LYS	4.3
1	А	351	LEU	4.3
1	В	295	ASP	4.2
1	С	128	LEU	4.2
1	С	333	SER	4.2
1	В	207	TYR	4.1
1	С	321	VAL	4.1
1	А	326	ASN	4.1
1	А	128	LEU	4.1
1	А	305	VAL	4.1
1	В	348	LYS	4.1
1	А	203	PRO	4.0
1	В	316	VAL	4.0
1	А	280	VAL	4.0
1	С	355	ARG	3.9
1	А	332	MET	3.9
1	С	327	GLY	3.8



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Mol	Chain	Res	Type	RSRZ
1	А	206	THR	3.7
1	С	308	ASP	3.7
1	В	304	GLN	3.6
1	А	279	VAL	3.6
1	А	274	ARG	3.6
1	В	335	ASP	3.6
1	С	358	LYS	3.6
1	С	366	VAL	3.5
1	А	316	VAL	3.5
1	В	358	LYS	3.4
1	А	285	ASN	3.3
1	А	217	ILE	3.3
1	В	257	ASP	3.2
1	В	354	ILE	3.2
1	С	127	ILE	3.2
1	В	351	LEU	3.1
1	С	166	GLY	3.1
1	В	153	LEU	3.0
1	А	368	ALA	3.0
1	С	367	GLY	3.0
1	А	342	ASN	3.0
1	С	364	VAL	2.9
1	В	315	GLY	2.9
1	В	305	VAL	2.9
1	В	338	HIS	2.9
1	В	45	VAL	2.9
1	А	362	LEU	2.9
1	А	328	GLN	2.8
1	С	249	GLY	2.8
1	C	322	ILE	2.8
1	A	160	LEU	2.8
1	B	233	VAL	2.8
1	A	240	ILE	2.8
1	В	147	ARG	2.8
1	A	281	ILE	2.8
1	В	356	ASP	2.7
1	А	323	LEU	2.7
1	A	325	ALA	2.7
1	В	286	LYS	2.7
1	A	187	ASP	2.7
1	В	359	ARG	2.7
1	В	337	PRO	2.7



Mol	Chain	Res	Type	RSRZ
1	С	203	PRO	2.6
1	А	358	LYS	2.6
1	А	289	ALA	2.6
1	В	239	GLN	2.6
1	В	279	VAL	2.5
1	В	168	SER	2.5
1	В	302	VAL	2.5
1	В	364	VAL	2.5
1	А	313	LYS	2.5
1	В	310	PRO	2.5
1	С	283	GLU	2.4
1	В	343	LEU	2.4
1	А	152	VAL	2.4
1	В	262	VAL	2.4
1	В	292	PHE	2.4
1	В	349	ALA	2.4
1	С	99	ALA	2.4
1	С	205	ASP	2.4
1	А	117	ASN	2.4
1	В	357	GLY	2.4
1	А	200	ARG	2.4
1	А	208	VAL	2.4
1	В	283	GLU	2.3
1	С	279	VAL	2.3
1	В	333	SER	2.3
1	С	178	LEU	2.3
1	В	224	GLY	2.3
1	С	300	ALA	2.3
1	В	352	GLU	2.3
1	A	111	ASP	2.3
1	B	367	GLY	2.2
1	B	329	PRO	2.2
1	В	219	PRO	2.2
1	А	340	ILE	2.2
1	В	327	GLY	2.2
1	A	189	SER	2.2
1	A	357	GLY	2.2
1	A	140	LYS	2.2
1	A	30	LEU	2.1
1	A	318	VAL	2.1
1	С	107	ILE	2.1
1	С	363	THR	2.1



	5	1	1 5	
Mol	Chain	Res	Type	RSRZ
1	А	120	VAL	2.1
1	В	129	VAL	2.1
1	В	365	THR	2.1
1	А	218	ASN	2.1
1	А	355	ARG	2.1
1	С	276	TRP	2.1
1	А	210	PHE	2.1
1	В	274	ARG	2.1
1	В	322	ILE	2.1
1	А	99	ALA	2.1
1	А	181	GLY	2.1
1	В	121	ILE	2.0
1	В	114	VAL	2.0

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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.

