

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 01:33 am BST

PDB ID	:	2R7D
Title	:	Crystal structure of ribonuclease II family protein from Deinococcus radiodu-
		rans, triclinic crystal form. NorthEast Structural Genomics target DrR63
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		lione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium
		(NESG)
Deposited on	:	2007-09-07
$\operatorname{Resolution}$:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11
EDS Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:::::::::::::::::::::::::::::::::::::::	2.11 20191225.v01 (using entries in the PDB archive December 25th 2015 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	$5950 \ (1.80-1.80)$		
Clashscore	141614	6793 (1.80-1.80)		
Ramachandran outliers	138981	6697 (1.80-1.80)		
Sidechain outliers	138945	6696 (1.80-1.80)		
RSRZ outliers	127900	5850(1.80-1.80)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	469	^{2%} 71%	26%	
1	В	469	64%	32%	
1	С	469	7%	26%	•••



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11897 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	1 1	461	Total	С	Ν	0	S	Se	0	0	0
	Л		3562	2228	652	671	2	9	0		
1	1 B	459	Total	С	Ν	0	S	\mathbf{Se}	0	0	0
			3545	2217	650	667	2	9			
1	1 C	450	Total	С	Ν	0	S	Se	0	0	0
	439	3545	2217	650	667	2	9	0	U	U	

• Molecule 1 is a protein called Ribonuclease II family protein.

Chain	Residue	Modelled	Actual	Comment	Reference
А	462	LEU	-	EXPRESSION TAG	UNP Q9RYD0
A	463	GLU	-	EXPRESSION TAG	UNP Q9RYD0
A	464	HIS	-	EXPRESSION TAG	UNP Q9RYD0
A	465	HIS	-	EXPRESSION TAG	UNP Q9RYD0
A	466	HIS	-	EXPRESSION TAG	UNP Q9RYD0
A	467	HIS	-	EXPRESSION TAG	UNP Q9RYD0
A	468	HIS	_	EXPRESSION TAG	UNP Q9RYD0
А	469	HIS	-	EXPRESSION TAG	UNP Q9RYD0
В	462	LEU	_	EXPRESSION TAG	UNP Q9RYD0
В	463	GLU	-	EXPRESSION TAG	UNP Q9RYD0
В	464	HIS	-	EXPRESSION TAG	UNP Q9RYD0
В	465	HIS	_	EXPRESSION TAG	UNP Q9RYD0
В	466	HIS	-	EXPRESSION TAG	UNP Q9RYD0
В	467	HIS	-	EXPRESSION TAG	UNP Q9RYD0
В	468	HIS	-	EXPRESSION TAG	UNP Q9RYD0
В	469	HIS	-	EXPRESSION TAG	UNP Q9RYD0
С	462	LEU	-	EXPRESSION TAG	UNP Q9RYD0
С	463	GLU	-	EXPRESSION TAG	UNP Q9RYD0
С	464	HIS	-	EXPRESSION TAG	UNP Q9RYD0
С	465	HIS	-	EXPRESSION TAG	UNP Q9RYD0
С	466	HIS	-	EXPRESSION TAG	UNP Q9RYD0
С	467	HIS	-	EXPRESSION TAG	UNP Q9RYD0
С	468	HIS	-	EXPRESSION TAG	UNP Q9RYD0

There are 24 discrepancies between the modelled and reference sequences:



Chain	Residue Modelled		Actual	Comment	Reference	
С	469	HIS	-	EXPRESSION TAG	UNP Q9RYD0	

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Mg 1 1	0	0
2	А	1	Total Mg 1 1	0	0
2	С	1	Total Mg 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	536	Total O 536 536	0	0
3	В	303	Total O 303 303	0	0
3	С	403	Total O 403 403	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Ribonuclease II family protein

26%

• •



Molecule 1: Ribonuclease II family protein
 7%
Chain C: 70%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	65.76\AA 92.20 Å 92.34 Å	Deneiter
a, b, c, α , β , γ	60.08° 89.57° 71.11°	Depositor
\mathbf{D} and \mathbf{D}	36.68 - 1.80	Depositor
Resolution (A)	36.68 - 1.80	EDS
% Data completeness	80.7 (36.68 - 1.80)	Depositor
(in resolution range)	94.5(36.68-1.80)	EDS
R _{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	$1.74 (at 1.81 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.221 , 0.243	Depositor
n, n_{free}	0.227 , 0.246	DCC
R_{free} test set	5136 reflections (1.67%)	wwPDB-VP
Wilson B-factor $(Å^2)$	23.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.40 , 56.6	EDS
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
	0.014 for h,h-k,-l	
Estimated twinning fraction	$0.016 { m for -h,-k+l,l}$	Xtriage
	0.008 for -h,-h+k-l,-l	
F_o, F_c correlation	0.94	EDS
Total number of atoms	11897	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.47% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.33	0/3624	0.62	3/4927~(0.1%)	
1	В	0.27	0/3607	0.58	6/4904~(0.1%)	
1	С	0.30	0/3607	0.59	2/4904~(0.0%)	
All	All	0.30	0/10838	0.60	11/14735~(0.1%)	

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	239	ASP	CB-CG-OD2	5.27	123.04	118.30
1	В	130	ASP	CB-CG-OD2	5.27	123.04	118.30
1	В	180	ASP	CB-CG-OD2	5.27	123.04	118.30
1	В	362	ASP	CB-CG-OD2	5.25	123.02	118.30
1	В	182	ASP	CB-CG-OD2	5.24	123.01	118.30
1	С	239	ASP	CB-CG-OD2	5.23	123.01	118.30
1	С	248	ASP	CB-CG-OD2	5.23	123.01	118.30
1	В	239	ASP	CB-CG-OD2	5.22	123.00	118.30
1	А	248	ASP	CB-CG-OD2	5.21	122.99	118.30
1	В	248	ASP	CB-CG-OD2	5.21	122.99	118.30
1	А	173	LEU	N-CA-C	-5.05	97.35	111.00

All (11) bond angle outliers are listed below:

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3562	0	3564	134	0
1	В	3545	0	3547	159	0
1	С	3545	0	3547	127	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
3	А	536	0	0	34	0
3	В	303	0	0	24	0
3	C	403	0	0	26	0
All	All	11897	0	10658	420	0

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.

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

Atom 1	Atom 0	Interatomic	Clash
Atom-1	Atom-2	$distance (m \AA)$	overlap (Å)
1:C:328:HIS:HB3	3:C:3394:HOH:O	1.60	1.01
1:B:180:ASP:HB2	1:B:181:PRO:HD2	1.41	0.98
1:A:353:GLN:HE22	1:A:364:LEU:H	1.00	0.96
1:B:239:ASP:O	1:B:308:MSE:SE	2.39	0.91
1:A:375:GLU:HA	1:A:378:MSE:HE2	1.53	0.90
1:A:463:GLU:HG2	3:A:1122:HOH:O	1.70	0.90
1:B:321:GLN:HA	3:B:2261:HOH:O	1.72	0.89
1:A:83:ASP:OD2	1:A:85:THR:HG22	1.73	0.89
1:C:52:GLU:HG2	1:C:451:LEU:HD12	1.56	0.88
1:A:370:ALA:HA	3:A:1315:HOH:O	1.74	0.88
1:A:370:ALA:HB3	3:A:1531:HOH:O	1.76	0.85
1:A:26:ARG:HH11	1:A:29:ARG:HH11	1.24	0.85
1:A:176:CYS:SG	1:A:189:ASP:HB2	2.16	0.85
1:C:12:THR:O	1:C:16:LEU:HD23	1.77	0.82
1:B:375:GLU:HA	1:B:378:MSE:HE3	1.61	0.82
1:C:83:ASP:OD2	1:C:85:THR:HG22	1.80	0.82
1:B:124:ALA:HB3	1:B:355:ARG:HD3	1.61	0.81
1:A:159:VAL:HA	1:A:342:MSE:HE1	1.61	0.81
1:C:176:CYS:SG	1:C:189:ASP:HB2	2.22	0.79
1:B:69:GLU:C	1:B:70:LEU:HD12	2.04	0.78
1:A:380:ALA:HB1	1:A:384:ARG:HH12	1.47	0.78
1:B:373:ILE:HB	3:B:2244:HOH:O	1.84	0.78



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1:C:414:ARG:HB3	1:C:414:ABG:NH1	1.99	0.77
1:B:238:ILE:HG21	1:B:315:LEU:HD11	1.66	0.77
1:B:133:LEU:H	1:B:133:LEU:HD12	1.49	0.76
1:A:380:ALA:HB1	1:A:384:ABG:NH1	2.01	0.76
1:B:353:GLN:HE22	1:B:364:LEU:H	1.31	0.76
1:A:420:THR:HG22	1:A:431:GLN:OE1	1.85	0.76
1:A:162:ALA:HB3	1:A:342:MSE:HE3	1.68	0.76
1:C:279:ILE:HD13	1:C:334:LEU:HD11	1.66	0.76
1:B:70:LEU:CD1	1:B:70:LEU:N	2.50	0.75
1:B:418:GLN:HA	1:B:433:ASN:HA	1.68	0.75
1:B:12:THR:O	1:B:16:LEU:HD23	1.87	0.75
1:A:373:ILE:HB	3:A:1315:HOH:O	1.85	0.75
1:A:367:LYS:HA	3:A:1531:HOH:O	1.85	0.74
1:B:370:ALA:HA	3:B:2244:HOH:O	1.87	0.74
1:A:196:LYS:HG3	1:A:196:LYS:O	1.86	0.74
1:C:414:ARG:HB3	1:C:414:ARG:HH11	1.51	0.74
1:C:196:LYS:HE2	3:C:3032:HOH:O	1.87	0.73
1:C:125:ALA:HB2	1:C:355:ARG:HH12	1.53	0.72
1:C:228:ARG:NH1	1:C:228:ARG:HB2	2.04	0.72
1:C:354:LEU:O	1:C:358:LEU:HD23	1.89	0.72
1:B:176:CYS:SG	1:B:189:ASP:HB2	2.29	0.72
1:A:159:VAL:HA	1:A:342:MSE:CE	2.19	0.72
1:C:196:LYS:O	1:C:196:LYS:HG3	1.89	0.71
1:C:133:LEU:HD12	1:C:133:LEU:H	1.54	0.71
1:A:24:LYS:HB2	1:A:24:LYS:NZ	2.06	0.70
1:B:70:LEU:N	1:B:70:LEU:HD12	2.07	0.70
1:A:118:VAL:CG1	1:A:175:ILE:HB	2.21	0.69
1:A:162:ALA:HB3	1:A:342:MSE:CE	2.22	0.69
1:C:353:GLN:HE22	1:C:364:LEU:H	1.41	0.69
1:C:443:GLN:HA	1:C:443:GLN:HE21	1.58	0.69
1:B:220:ALA:O	1:B:224:ARG:HG3	1.94	0.68
1:A:12:THR:O	1:A:16:LEU:HD23	1.94	0.67
1:A:223:ALA:HB1	1:A:227:ARG:HH12	1.60	0.67
1:B:455:ARG:HD2	3:B:2253:HOH:O	1.95	0.67
1:C:69:GLU:C	1:C:70:LEU:HD12	2.15	0.67
1:A:26:ARG:HH11	1:A:29:ARG:NH1	1.94	0.66
1:B:129:PRO:HG2	3:B:2119:HOH:O	1.96	0.66
1:C:70:LEU:N	1:C:70:LEU:CD1	2.59	0.66
1:B:414:ARG:NH2	1:B:435:PRO:HA	2.11	0.66
1:A:184:ASN:HD22	1:A:185:ALA:N	1.93	0.65
1:B:305:LEU:HB2	1:B:306:PRO:HD3	1.78	0.65



Continued from previous page					
Atom-1	Atom-2	distance $(\hat{\Delta})$	overlap(Å)		
1·A·449·ILE·HG13	1.A.456.VAL.HG12	1 77	0.65		
1:B:404:GLU:H	1:B:404:GLU:CD	$\frac{1.00}{2.00}$	0.65		
1·A·24·LYS·HD3	3·A·1151·HOH·O	1.96	0.65		
1:A:203:GLN:HG3	3:A:1466:HOH:O	1.96	0.65		
1:C:369:MSE:O	1:C:373:ILE:HD13	1.96	0.65		
1:B:165:GLY:HA2	1:B:197:VAL:HG13	1.79	0.65		
1:B:95:GLU:HG2	1:B:201:ALA:HB1	1.78	0.65		
1:A:364:LEU:HB3	1:A:368:VAL:CG2	2.26	0.65		
1:B:244:ARG:HH21	1:B:246:LYS:HZ3	1.44	0.65		
1:B:133:LEU:HD12	1:B:133:LEU:N	2.11	0.64		
1:A:125:ALA:HB2	1:A:355:ARG:HH12	1.61	0.64		
1:A:66:ASN:H	1:A:66:ASN:HD22	1.44	0.64		
1:A:353:GLN:HE22	1:A:364:LEU:N	1.83	0.64		
1:B:227:ARG:HH22	1:B:268:GLU:HB2	1.63	0.64		
1:A:457:ARG:HG3	3:A:1445:HOH:O	1.98	0.64		
1:B:364:LEU:HB3	1:B:368:VAL:CG2	2.28	0.64		
1:B:124:ALA:CB	1:B:355:ARG:HD3	2.28	0.64		
1:B:191:LEU:HD23	1:B:191:LEU:N	2.13	0.63		
1:C:322:PRO:HD3	3:C:3163:HOH:O	1.96	0.63		
1:C:444:VAL:HG11	1:C:458:ALA:HB1	1.81	0.63		
1:C:441:ALA:C	1:C:442:LEU:HD12	2.18	0.63		
1:C:449:ILE:HG13	1:C:456:VAL:HG12	1.79	0.63		
1:A:180:ASP:OD2	1:A:184:ASN:HB3	1.97	0.63		
1:B:240:LEU:HB3	1:B:241:PRO:HD2	1.80	0.62		
1:A:69:GLU:C	1:A:70:LEU:HD12	2.19	0.62		
1:A:165:GLY:HA2	1:A:197:VAL:HG13	1.82	0.62		
1:C:133:LEU:HD12	1:C:133:LEU:N	2.15	0.62		
1:A:364:LEU:HB3	1:A:368:VAL:HG21	1.82	0.61		
1:A:129:PRO:HG3	3:A:1342:HOH:O	2.01	0.61		
1:A:11:ARG:NH2	3:A:1408:HOH:O	2.33	0.61		
1:B:129:PRO:O	1:B:130:ASP:HB3	2.01	0.61		
1:B:364:LEU:HB3	1:B:368:VAL:HG21	1.81	0.61		
1:C:87:LEU:HB3	3:C:3349:HOH:O	1.99	0.61		
1:B:85:THR:O	1:B:196:LYS:HE3	2.01	0.61		
1:B:30:ASP:HB2	3:B:2088:HOH:O	2.00	0.61		
1:B:422:LEU:O	1:B:424:PRO:HD3	2.01	0.61		
1:B:66:ASN:H	1:B:66:ASN:HD22	1.47	0.61		
1:A:118:VAL:HG11	1:A:273:ALA:CB	2.30	0.61		
1:B:4:PRO:HG2	1:B:47:LEU:HD21	1.83	0.61		
1:A:54:ARG:HG2	3:A:1341:HOH:O	2.01	0.60		
1:B:244:ARG:HH21	1:B:246:LYS:NZ	1.97	0.60		



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:301:ALA:HB1	3:C:3350:HOH:O	2.01	0.60
1:B:375:GLU:HA	1:B:378:MSE:CE	2.30	0.60
1:A:26:ARG:NH1	1:A:29:ARG:HH11	1.95	0.60
1:B:430:VAL:HG21	1:B:458:ALA:HB2	1.84	0.60
1:C:3:GLN:HB2	1:C:4:PRO:HD3	1.84	0.60
1:B:151:ILE:N	1:B:151:ILE:HD12	2.17	0.59
1:A:305:LEU:HB2	1:A:306:PRO:HD3	1.84	0.59
1:B:227:ARG:NH1	3:B:2072:HOH:O	2.36	0.59
1:A:102:ASP:HB2	3:A:1211:HOH:O	2.02	0.59
1:C:396:LEU:HD22	1:C:456:VAL:CG1	2.33	0.59
1:A:118:VAL:HG11	1:A:273:ALA:HB2	1.85	0.58
1:A:396:LEU:HD22	1:A:456:VAL:CG1	2.33	0.58
1:B:330:MSE:HB3	1:B:332:LEU:HD23	1.83	0.58
1:C:369:MSE:HG3	3:C:3163:HOH:O	2.02	0.58
1:B:319:ARG:HB3	1:B:319:ARG:NH1	2.18	0.58
1:A:318:THR:HG23	3:A:1087:HOH:O	2.02	0.58
1:C:220:ALA:O	1:C:224:ARG:HG3	2.03	0.58
1:B:354:LEU:O	1:B:358:LEU:HD13	2.03	0.58
1:A:24:LYS:HB2	1:A:24:LYS:HZ2	1.68	0.57
1:A:354:LEU:O	1:A:358:LEU:HD13	2.03	0.57
1:B:227:ARG:NH2	1:B:264:THR:HG22	2.18	0.57
1:B:8:PRO:HG2	3:B:2047:HOH:O	2.04	0.57
1:A:420:THR:HG23	3:A:1182:HOH:O	2.02	0.57
1:B:449:ILE:HG13	1:B:456:VAL:HG12	1.84	0.57
1:B:418:GLN:HG3	1:B:431:GLN:HG3	1.87	0.57
1:B:380:ALA:HB1	1:B:384:ARG:NH1	2.19	0.57
1:A:165:GLY:CA	1:A:197:VAL:HG13	2.35	0.57
1:A:319:ARG:HD2	3:A:1232:HOH:O	2.04	0.57
1:A:453:GLN:HB2	1:A:455:ARG:HH11	1.70	0.57
1:C:24:LYS:HD2	3:C:3329:HOH:O	2.04	0.57
1:A:184:ASN:HD22	1:A:185:ALA:H	1.52	0.56
1:B:180:ASP:HB2	1:B:181:PRO:CD	2.27	0.56
1:A:30:ASP:HB2	3:A:1154:HOH:O	2.05	0.56
1:B:227:ARG:O	1:B:231:GLU:HG3	2.05	0.56
1:C:244:ARG:HG3	1:C:257:LEU:HD21	1.86	0.56
1:A:361:ARG:HD3	3:A:1424:HOH:O	2.05	0.56
1:B:402:GLN:OE1	1:B:405:ARG:HD2	2.05	0.56
1:C:26:ARG:HH11	1:C:26:ARG:HG2	1.71	0.56
1:C:443:GLN:HA	1:C:443:GLN:NE2	2.21	0.56
1:A:375:GLU:HA	1:A:378:MSE:CE	2.29	0.56
1:C:396:LEU:HD22	1:C:456:VAL:HG13	1.87	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:463:GLU:HB2	3:A:1184:HOH:O	2.05	0.56
1:A:66:ASN:H	1:A:66:ASN:ND2	2.04	0.56
1:A:70:LEU:N	1:A:70:LEU:CD1	2.68	0.56
1:C:275:TRP:O	1:C:279:ILE:HG12	2.06	0.56
1:A:24:LYS:HG2	1:A:35:GLU:OE1	2.07	0.55
1:B:374:ALA:O	1:B:378:MSE:HG3	2.06	0.55
1:A:196:LYS:HE2	3:A:1007:HOH:O	2.06	0.55
1:A:444:VAL:HG23	1:A:459:ARG:O	2.06	0.55
1:C:98:GLN:HA	1:C:199:ARG:HH22	1.71	0.55
1:B:373:ILE:HD12	3:B:2261:HOH:O	2.07	0.55
1:C:54:ARG:HD2	3:C:3145:HOH:O	2.06	0.55
1:A:227:ARG:O	1:A:231:GLU:HG3	2.07	0.55
1:A:43:LEU:HD22	1:A:47:LEU:HG	1.89	0.55
1:B:16:LEU:HD22	1:B:19:ARG:HH21	1.69	0.55
1:C:3:GLN:HB2	1:C:4:PRO:CD	2.35	0.55
1:B:227:ARG:NH1	1:B:268:GLU:OE1	2.40	0.55
1:B:34:PRO:HG2	1:B:39:ALA:HB2	1.88	0.55
1:C:52:GLU:HG2	1:C:451:LEU:CD1	2.35	0.55
1:B:317:ARG:HG2	1:B:317:ARG:HH11	1.71	0.55
1:C:353:GLN:NE2	1:C:364:LEU:HD23	2.21	0.55
1:A:413:ASP:HB3	1:A:420:THR:OG1	2.06	0.55
1:C:70:LEU:HD12	1:C:70:LEU:N	2.22	0.55
1:A:275:TRP:O	1:A:279:ILE:HG12	2.06	0.55
1:C:444:VAL:CG1	1:C:458:ALA:HB1	2.37	0.55
1:B:338:ALA:HB2	1:B:350:VAL:HG11	1.88	0.54
1:C:165:GLY:HA2	1:C:197:VAL:HG13	1.89	0.54
1:C:59:ASP:OD1	1:C:65:LEU:HD11	2.06	0.54
1:A:340:SER:HB3	1:A:343:ARG:HG2	1.90	0.54
1:A:3:GLN:N	1:A:4:PRO:HD2	2.23	0.54
1:B:348:LEU:O	1:B:352:GLN:HG3	2.07	0.54
1:B:432:VAL:HG22	1:B:458:ALA:HB3	1.90	0.54
1:C:228:ARG:HH11	1:C:228:ARG:HB2	1.71	0.54
1:B:11:ARG:NH2	3:B:2226:HOH:O	2.40	0.54
1:B:279:ILE:HD13	1:B:334:LEU:HD11	1.89	0.54
1:B:7:THR:HB	1:B:8:PRO:HD2	1.89	0.54
1:C:327:HIS:CE1	1:C:330:MSE:HG3	2.44	0.53
1:A:19:ARG:NH2	1:A:54:ARG:HH22	2.06	0.53
1:B:449:ILE:HD12	1:B:449:ILE:N	2.23	0.53
1:C:420:THR:HB	3:C:3247:HOH:O	2.09	0.53
1:A:118:VAL:HG13	1:A:118:VAL:O	2.08	0.53
1:C:191:LEU:HD23	1:C:191:LEU:N	2.22	0.53



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:165:GLY:CA	1:B:197:VAL:HG13	2.39	0.53
1:B:174:SER:C	1:B:175:ILE:HD12	2.29	0.53
1:A:69:GLU:O	1:A:70:LEU:HD12	2.09	0.53
1:B:396:LEU:HD22	1:B:456:VAL:CG1	2.39	0.53
1:C:69:GLU:O	1:C:70:LEU:HD12	2.09	0.53
1:A:346:LEU:HB2	3:A:1356:HOH:O	2.09	0.52
1:C:364:LEU:HD22	1:C:364:LEU:H	1.74	0.52
1:A:158:LEU:HD23	1:A:342:MSE:CE	2.38	0.52
1:A:396:LEU:HD22	1:A:456:VAL:HG11	1.91	0.52
1:B:227:ARG:NH1	3:B:2138:HOH:O	2.42	0.52
1:B:334:LEU:N	1:B:334:LEU:HD23	2.25	0.52
1:C:133:LEU:H	1:C:133:LEU:CD1	2.20	0.52
1:C:449:ILE:HG13	1:C:456:VAL:CG1	2.39	0.52
1:C:184:ASN:ND2	3:C:3378:HOH:O	2.40	0.52
1:B:418:GLN:N	1:B:418:GLN:HE21	2.07	0.52
1:B:180:ASP:C	1:B:182:ASP:H	2.12	0.52
1:B:180:ASP:OD2	1:B:184:ASN:HB2	2.08	0.52
1:A:453:GLN:HG3	1:A:455:ARG:NH1	2.25	0.51
1:A:118:VAL:HG13	1:A:175:ILE:HB	1.93	0.51
1:A:151:ILE:HD12	1:A:151:ILE:N	2.25	0.51
1:C:140:ARG:NH1	3:C:3325:HOH:O	2.43	0.51
1:C:95:GLU:HG3	3:C:3025:HOH:O	2.09	0.51
1:A:361:ARG:HH11	1:A:361:ARG:HG3	1.76	0.51
1:B:300:VAL:HG23	1:B:311:ARG:HE	1.76	0.51
1:B:133:LEU:CD1	1:B:133:LEU:H	2.18	0.51
1:B:85:THR:C	3:B:2300:HOH:O	2.48	0.51
1:C:194:ARG:HG3	1:C:194:ARG:HH11	1.76	0.51
1:B:89:THR:HG22	1:B:103:ALA:HB1	1.93	0.51
1:B:453:GLN:NE2	3:B:2263:HOH:O	2.43	0.51
1:B:406:VAL:HG12	1:B:443:GLN:HG3	1.93	0.50
1:B:180:ASP:OD1	1:B:182:ASP:HB2	2.11	0.50
1:B:327:HIS:CE1	1:B:330:MSE:HG3	2.46	0.50
1:C:338:ALA:HB2	1:C:350:VAL:HG11	1.92	0.50
1:C:133:LEU:HD11	3:C:3119:HOH:O	2.11	0.50
1:A:147:PRO:O	1:A:246:LYS:HD3	2.10	0.50
1:A:117:TRP:HZ3	1:A:191:LEU:HD11	1.77	0.50
1:A:355:ARG:NH2	3:A:1020:HOH:O	2.45	0.50
1:B:129:PRO:O	1:B:130:ASP:CB	2.59	0.50
1:B:149:ARG:HD2	1:B:151:ILE:HD11	1.94	0.50
1:B:405:ARG:HD3	1:B:407:TRP:CZ2	2.46	0.50
1:B:95:GLU:HG3	3:B:2101:HOH:O	2.12	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:412:VAL:HG22	1:B:420:THR:O	2.12	0.50
1:B:3:GLN:N	1:B:4:PRO:HD2	2.27	0.50
1:A:191:LEU:HD13	1:A:193:THR:CG2	2.42	0.50
1:A:52:GLU:O	1:A:393:HIS:HE1	1.95	0.50
1:B:392:ARG:NH1	1:B:454:MSE:HB3	2.27	0.50
1:C:85:THR:O	1:C:196:LYS:HD2	2.11	0.50
1:A:449:ILE:HG13	1:A:456:VAL:CG1	2.42	0.49
1:C:145:TYR:HE1	3:C:3360:HOH:O	1.95	0.49
1:B:109:LEU:HB2	1:B:113:LEU:HB3	1.94	0.49
1:C:238:ILE:HD13	1:C:315:LEU:HD11	1.94	0.49
1:A:133:LEU:HD13	3:A:1019:HOH:O	2.12	0.49
1:A:158:LEU:HD23	1:A:342:MSE:HE2	1.94	0.49
1:C:85:THR:O	1:C:196:LYS:CD	2.61	0.49
1:A:460:SER:HB3	3:A:1184:HOH:O	2.12	0.49
1:B:82:LEU:HB2	3:B:2063:HOH:O	2.11	0.49
1:C:113:LEU:HD11	1:C:186:GLU:OE1	2.13	0.49
1:C:364:LEU:HD22	1:C:364:LEU:N	2.28	0.49
1:A:453:GLN:HG3	1:A:455:ARG:HH12	1.78	0.48
1:B:69:GLU:O	1:B:70:LEU:HD12	2.12	0.48
1:B:8:PRO:HD3	3:B:2226:HOH:O	2.12	0.48
1:C:359:ALA:HB3	1:C:361:ARG:HG3	1.95	0.48
1:A:191:LEU:HD13	1:A:193:THR:HG23	1.95	0.48
1:A:240:LEU:HB3	1:A:241:PRO:HD2	1.96	0.48
1:B:229:LEU:O	1:B:233:GLU:HG2	2.14	0.48
1:B:124:ALA:HB3	1:B:355:ARG:CD	2.38	0.48
1:B:311:ARG:O	1:B:315:LEU:HG	2.12	0.48
1:B:414:ARG:HG2	1:B:416:GLY:H	1.77	0.48
1:C:364:LEU:CD2	1:C:364:LEU:H	2.26	0.48
1:C:165:GLY:CA	1:C:197:VAL:HG13	2.43	0.48
1:C:361:ARG:HG2	1:C:361:ARG:HH11	1.78	0.48
1:A:26:ARG:NH1	3:A:1382:HOH:O	2.43	0.48
1:A:393:HIS:HD2	3:A:1061:HOH:O	1.97	0.48
1:A:58:ALA:CB	1:A:65:LEU:HD21	2.43	0.48
1:B:175:ILE:HD12	1:B:175:ILE:N	2.29	0.48
1:B:180:ASP:O	1:B:182:ASP:N	2.46	0.48
1:C:151:ILE:HD12	1:C:151:ILE:N	2.28	0.48
1:B:317:ARG:NH1	1:B:317:ARG:HG2	2.28	0.48
1:B:418:GLN:HB3	1:B:433:ASN:CG	2.33	0.48
1:A:355:ARG:CZ	3:A:1020:HOH:O	2.60	0.48
1:B:112:GLY:O	1:B:181:PRO:HD3	2.13	0.48
1:B:194:ARG:HH11	1:B:194:ARG:HG3	1.78	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:C:330:MSE:O	1:C:332:LEU:HD13	2.14	0.47
1:C:374:ALA:O	1:C:378:MSE:HG2	2.15	0.47
1:A:364:LEU:HB3	1:A:368:VAL:HG23	1.96	0.47
1:C:414:ARG:HH11	1:C:414:ARG:CB	2.25	0.47
1:B:396:LEU:HD22	1:B:456:VAL:HG11	1.96	0.47
1:B:367:LYS:HD2	1:B:367:LYS:C	2.34	0.47
1:B:75:PHE:O	1:B:77:PRO:HD3	2.14	0.47
1:C:422:LEU:O	1:C:424:PRO:HD3	2.15	0.47
1:A:7:THR:O	1:A:11:ARG:HG3	2.14	0.47
1:A:461:VAL:HG22	1:A:462:LEU:HG	1.97	0.47
1:B:418:GLN:N	1:B:418:GLN:NE2	2.63	0.47
1:A:70:LEU:N	1:A:70:LEU:HD12	2.28	0.47
1:C:125:ALA:CB	1:C:355:ARG:HH12	2.24	0.47
1:C:421:LEU:HD13	1:C:432:VAL:HB	1.97	0.47
1:A:158:LEU:HD23	1:A:158:LEU:C	2.34	0.47
1:C:305:LEU:N	1:C:306:PRO:HD2	2.30	0.47
1:C:58:ALA:CB	1:C:65:LEU:HD21	2.45	0.47
1:C:94:ASP:OD2	1:C:263:ARG:NH2	2.46	0.47
1:B:227:ARG:HG3	1:B:227:ARG:HH11	1.80	0.47
1:B:240:LEU:HB3	1:B:241:PRO:CD	2.45	0.47
1:B:83:ASP:OD2	1:B:85:THR:HG22	2.15	0.47
1:C:415:ARG:O	1:C:418:GLN:HB2	2.15	0.47
1:A:158:LEU:CD2	1:A:342:MSE:HE2	2.45	0.46
1:C:43:LEU:HD22	1:C:47:LEU:HG	1.97	0.46
1:C:271:THR:HG23	1:C:330:MSE:HE2	1.97	0.46
1:B:411:VAL:CG1	1:B:438:PRO:HA	2.46	0.46
1:B:66:ASN:ND2	1:B:66:ASN:H	2.11	0.46
1:C:181:PRO:HD2	3:C:3339:HOH:O	2.14	0.46
1:C:423:ILE:N	1:C:423:ILE:HD12	2.30	0.46
1:A:38:GLU:HG2	3:A:1332:HOH:O	2.14	0.46
1:B:373:ILE:CD1	3:B:2261:HOH:O	2.63	0.46
1:C:318:THR:HG23	3:C:3115:HOH:O	2.14	0.46
1:C:393:HIS:HD2	3:C:3125:HOH:O	1.97	0.46
1:B:17:LEU:HD23	1:B:28:LEU:HD12	1.97	0.46
1:B:292:THR:HG22	1:B:325:GLY:O	2.16	0.46
1:C:34:PRO:HG2	1:C:39:ALA:HB2	1.97	0.46
1:B:271:THR:HG23	1:B:330:MSE:HE2	1.97	0.46
1:B:380:ALA:HB1	1:B:384:ARG:HH12	1.80	0.46
1:C:228:ARG:HH11	1:C:228:ARG:CB	2.29	0.46
1:B:275:TRP:O	1:B:279:ILE:HG12	2.15	0.46
1:B:87:LEU:HB3	3:B:2303:HOH:O	2.14	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:98:GLN:O	1:A:98:GLN:HG2	2.16	0.45
1:C:25:SER:OG	1:C:28:LEU:HD13	2.15	0.45
1:C:196:LYS:HE3	3:C:3327:HOH:O	2.15	0.45
1:B:418:GLN:CA	1:B:433:ASN:HA	2.43	0.45
1:B:70:LEU:N	1:B:70:LEU:HD13	2.32	0.45
1:C:248:ASP:C	1:C:248:ASP:OD1	2.55	0.45
1:B:192:LEU:HD22	1:B:355:ARG:NH1	2.31	0.45
1:B:61:LEU:HD12	1:B:386:ALA:HB2	1.98	0.45
1:C:449:ILE:HA	1:C:456:VAL:HG12	1.98	0.45
1:B:158:LEU:HD23	1:B:158:LEU:C	2.36	0.45
1:B:343:ARG:NH2	3:B:2287:HOH:O	2.49	0.45
1:A:165:GLY:N	1:A:197:VAL:HG13	2.32	0.45
1:B:238:ILE:HD13	1:B:315:LEU:CD1	2.47	0.45
1:B:330:MSE:O	1:B:332:LEU:HD22	2.16	0.45
1:B:281:ALA:HB2	1:B:288:LEU:HD11	1.99	0.45
1:B:423:ILE:HD12	1:B:423:ILE:N	2.32	0.45
1:A:113:LEU:HD11	1:A:186:GLU:OE2	2.17	0.45
1:A:279:ILE:CD1	1:A:334:LEU:HD21	2.47	0.45
1:B:443:GLN:HB3	1:B:461:VAL:HG12	1.98	0.45
1:A:52:GLU:HG3	3:A:1200:HOH:O	2.17	0.44
1:B:406:VAL:CG1	1:B:443:GLN:HG3	2.46	0.44
1:C:353:GLN:NE2	1:C:353:GLN:HA	2.32	0.44
1:B:128:ALA:HB1	1:B:129:PRO:HD2	1.99	0.44
1:C:455:ARG:NE	3:C:3317:HOH:O	2.50	0.44
1:B:188:VAL:HG11	1:B:276:GLY:CA	2.48	0.44
1:C:346:LEU:HB2	3:C:3101:HOH:O	2.16	0.44
1:B:353:GLN:NE2	1:B:364:LEU:H	2.06	0.44
1:A:7:THR:OG1	1:A:10:GLN:HG3	2.18	0.44
1:A:62:ARG:HH11	1:A:62:ARG:HG3	1.82	0.44
1:A:95:GLU:HG3	3:A:1105:HOH:O	2.17	0.44
1:B:180:ASP:CB	1:B:181:PRO:HD2	2.25	0.44
1:C:165:GLY:N	1:C:197:VAL:HG13	2.33	0.44
1:A:228:ARG:HD3	3:A:1421:HOH:O	2.17	0.44
1:B:180:ASP:C	1:B:182:ASP:N	2.70	0.44
1:C:150:THR:HG21	3:C:3360:HOH:O	2.18	0.44
1:A:453:GLN:HB2	1:A:455:ARG:NH1	2.33	0.43
1:C:64:ALA:HB3	3:C:3325:HOH:O	2.18	0.43
1:B:157:GLU:HG3	3:B:2202:HOH:O	2.18	0.43
1:B:418:GLN:NE2	1:B:418:GLN:H	2.15	0.43
1:C:367:LYS:HD2	1:C:367:LYS:O	2.18	0.43
1:B:300:VAL:CG2	1:B:311:ARG:HE	2.31	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:298:ARG:HG3	1:C:298:ARG:HH11	1.83	0.43
1:A:72:VAL:HA	1:A:73:PRO:HD3	1.86	0.43
1:C:322:PRO:HB2	1:C:366:SER:HB2	2.00	0.43
1:B:430:VAL:HG21	1:B:458:ALA:CB	2.49	0.43
1:B:421:LEU:HD12	1:B:421:LEU:N	2.34	0.43
1:B:87:LEU:N	3:B:2300:HOH:O	2.52	0.43
1:C:223:ALA:HB1	1:C:227:ARG:HH12	1.84	0.43
1:C:334:LEU:N	1:C:334:LEU:HD23	2.34	0.43
1:B:177:LEU:HD12	1:B:177:LEU:N	2.34	0.43
1:B:81:ARG:HD3	1:B:193:THR:O	2.19	0.43
1:C:173:LEU:HD23	1:C:173:LEU:C	2.39	0.43
1:C:26:ARG:NH1	1:C:26:ARG:HG2	2.32	0.43
1:C:429:ASP:HB2	3:C:3247:HOH:O	2.19	0.43
1:A:455:ARG:HG2	1:A:455:ARG:HH11	1.83	0.42
1:C:52:GLU:O	1:C:393:HIS:HE1	2.02	0.42
1:C:69:GLU:C	1:C:70:LEU:CD1	2.85	0.42
1:B:79:GLU:OE2	1:B:192:LEU:HD13	2.19	0.42
1:A:118:VAL:HG23	3:A:1211:HOH:O	2.17	0.42
1:A:373:ILE:HD12	3:A:1315:HOH:O	2.18	0.42
1:C:146:LEU:HD12	1:C:149:ARG:NH1	2.35	0.42
1:A:294:ASP:CG	1:A:295:TYR:H	2.23	0.42
1:A:451:LEU:HB2	1:A:452:PRO:HD3	2.01	0.42
1:A:165:GLY:N	1:A:197:VAL:CG1	2.83	0.42
1:B:231:GLU:HA	1:B:235:ALA:HB3	2.01	0.42
1:B:346:LEU:HD13	3:B:2010:HOH:O	2.18	0.42
1:C:94:ASP:O	1:C:97:ASN:OD1	2.37	0.42
1:A:180:ASP:HB2	1:A:181:PRO:CD	2.49	0.42
1:C:293:GLN:CG	3:C:3394:HOH:O	2.67	0.42
1:C:443:GLN:O	1:C:460:SER:HA	2.19	0.42
1:A:422:LEU:O	1:A:424:PRO:HD3	2.20	0.42
1:C:286:ILE:HD11	1:C:357:PHE:CG	2.55	0.42
1:B:319:ARG:HH11	1:B:319:ARG:CB	2.32	0.42
1:C:31:LEU:O	1:C:32:LYS:HB2	2.19	0.42
1:B:322:PRO:HD3	3:B:2261:HOH:O	2.20	0.41
1:B:81:ARG:NH2	1:B:122:ASP:OD2	2.53	0.41
1:B:68:VAL:HG12	1:B:155:PRO:HG3	2.01	0.41
1:C:161:LYS:CB	1:C:161:LYS:NZ	2.82	0.41
1:A:423:ILE:N	1:A:423:ILE:HD12	2.35	0.41
1:B:414:ARG:NH1	1:B:414:ARG:HG3	2.34	0.41
1:C:19:ARG:NH1	3:C:3030:HOH:O	2.52	0.41
1:A:396:LEU:HD22	1:A:456:VAL:HG13	2.02	0.41



A 4 1	A 4 5 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:236:LEU:HD12	3:B:2234:HOH:O	2.20	0.41
1:B:330:MSE:CB	1:B:332:LEU:HD23	2.47	0.41
1:C:259:LYS:N	1:C:260:PRO:CD	2.83	0.41
1:A:294:ASP:CG	1:A:295:TYR:N	2.74	0.41
1:C:289:PRO:HB3	1:C:373:ILE:HD11	2.03	0.41
1:A:184:ASN:ND2	1:A:185:ALA:N	2.65	0.41
1:B:257:LEU:HA	1:B:258:PRO:HD3	1.95	0.41
1:C:158:LEU:C	1:C:158:LEU:HD23	2.41	0.41
1:A:202:TYR:CD1	1:A:263:ARG:HA	2.56	0.41
1:B:6:LEU:HD21	1:B:27:VAL:HG11	2.03	0.41
1:C:449:ILE:N	1:C:449:ILE:HD12	2.35	0.41
1:A:117:TRP:CZ3	1:A:191:LEU:HD11	2.56	0.41
1:C:161:LYS:NZ	3:C:3399:HOH:O	2.47	0.41
1:A:343:ARG:NH1	3:A:1284:HOH:O	2.54	0.41
1:C:206:GLN:O	1:C:210:GLU:HG3	2.21	0.41
1:A:220:ALA:O	1:A:224:ARG:HG3	2.20	0.41
1:A:24:LYS:HB2	1:A:24:LYS:HZ3	1.83	0.41
1:A:449:ILE:N	1:A:449:ILE:HD12	2.36	0.41
1:A:449:ILE:HA	1:A:456:VAL:HG12	2.03	0.41
1:B:191:LEU:CD2	1:B:191:LEU:N	2.81	0.40
1:C:355:ARG:HH11	1:C:355:ARG:HG3	1.87	0.40
1:A:143:THR:HG23	1:A:152:GLY:HA2	2.03	0.40
1:A:301:ALA:HB1	3:A:1411:HOH:O	2.19	0.40
1:C:6:LEU:HG	1:C:10:GLN:HB3	2.03	0.40
1:C:95:GLU:HG2	1:C:201:ALA:HB1	2.02	0.40
1:A:279:ILE:HD13	1:A:334:LEU:HD21	2.03	0.40
1:C:194:ARG:NH1	1:C:194:ARG:HG3	2.36	0.40
1:B:411:VAL:HG12	1:B:438:PRO:HA	2.03	0.40
1:C:117:TRP:CE3	1:C:176:CYS:HB3	2.57	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	459/469~(98%)	450 (98%)	9 (2%)	0	100	100
1	В	457/469~(97%)	441 (96%)	15 (3%)	1 (0%)	47	33
1	С	457/469~(97%)	450 (98%)	6 (1%)	1 (0%)	47	33
All	All	1373/1407~(98%)	1341 (98%)	30 (2%)	2(0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	239	ASP
1	В	181	PRO

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	Percent	tiles
1	А	371/369~(100%)	357~(96%)	14 (4%)	33	18
1	В	369/369~(100%)	359~(97%)	10 (3%)	44	31
1	С	369/369~(100%)	357~(97%)	12 (3%)	38	23
All	All	1109/1107~(100%)	1073~(97%)	36 (3%)	39	25

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	24	LYS
1	А	43	LEU
1	А	66	ASN
1	А	70	LEU
1	А	80	GLU
1	А	130	ASP
1	А	184	ASN
1	А	191	LEU
1	А	197	VAL
1	А	209	LEU
1	А	332	LEU



Mol	Chain	Res	Type
1	А	347	ASP
1	А	404	GLU
1	А	434	THR
1	В	56	PRO
1	В	66	ASN
1	В	70	LEU
1	В	101	ASP
1	В	168	GLU
1	В	197	VAL
1	В	367	LYS
1	В	404	GLU
1	В	418	GLN
1	В	443	GLN
1	С	6	LEU
1	С	43	LEU
1	С	59	ASP
1	С	70	LEU
1	С	149	ARG
1	С	161	LYS
1	С	197	VAL
1	С	228	ARG
1	С	239	ASP
1	С	246	LYS
1	С	347	ASP
1	С	404	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	66	ASN
1	А	97	ASN
1	А	184	ASN
1	А	321	GLN
1	А	353	GLN
1	А	393	HIS
1	А	433	ASN
1	В	66	ASN
1	В	97	ASN
1	В	184	ASN
1	В	353	GLN
1	В	393	HIS
1	В	418	GLN



0 0 1000								
\mathbf{Mol}	Chain	\mathbf{Res}	Type					
1	В	431	GLN					
1	С	66	ASN					
1	С	97	ASN					
1	С	98	GLN					
1	С	184	ASN					
1	С	353	GLN					
1	С	393	HIS					
1	С	443	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 $>$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	452/469~(96%)	0.12	11 (2%) 59 5	4	10, 24, 41, 58	0
1	В	450/469~(95%)	0.72	56 (12%) 4 3	3	15, 37, 59, 66	0
1	С	450/469~(95%)	0.35	32 (7%) 16 11	2	15, 30, 50, 59	0
All	All	1352/1407~(96%)	0.40	99 (7%) 15 1	1	10, 30, 53, 66	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	461	VAL	7.0
1	С	461	VAL	6.4
1	В	435	PRO	6.0
1	В	3	GLN	5.5
1	А	3	GLN	4.6
1	В	416	GLY	4.5
1	В	303	ASP	4.3
1	С	189	ASP	4.1
1	В	415	ARG	4.1
1	В	440	THR	4.1
1	С	435	PRO	3.7
1	В	169	VAL	3.6
1	С	181	PRO	3.6
1	В	295	TYR	3.5
1	В	302	GLY	3.5
1	А	189	ASP	3.5
1	В	319	ARG	3.5
1	В	189	ASP	3.3
1	С	111	GLY	3.3
1	В	443	GLN	3.3
1	В	98	GLN	3.3
1	В	315	LEU	3.3
1	В	181	PRO	3.3



Mol	Chain	Res	Type	RSRZ
1	С	98	GLN	3.3
1	В	249	GLU	3.2
1	В	97	ASN	3.2
1	В	459	ARG	3.1
1	А	98	GLN	3.1
1	С	295	TYR	3.1
1	А	118	VAL	3.0
1	В	96	GLY	3.0
1	В	439	GLY	3.0
1	С	364	LEU	3.0
1	В	314	THR	2.9
1	В	301	ALA	2.9
1	В	436	ALA	2.9
1	В	442	LEU	2.9
1	В	285	GLU	2.9
1	С	459	ARG	2.8
1	В	300	VAL	2.8
1	В	236	LEU	2.8
1	В	250	THR	2.8
1	В	238	ILE	2.8
1	В	118	VAL	2.8
1	С	228	ARG	2.8
1	С	415	ARG	2.8
1	С	297	THR	2.7
1	В	460	SER	2.7
1	С	249	GLU	2.7
1	С	3	GLN	2.7
1	А	97	ASN	2.7
1	В	458	ALA	2.7
1	А	112	GLY	2.7
1	С	303	ASP	2.6
1	В	433	ASN	2.6
1	С	431	GLN	2.6
1	А	111	GLY	2.6
1	В	339	THR	2.5
1	В	110	GLY	2.5
1	А	339	THR	2.4
1	В	112	GLY	2.4
1	С	96	GLY	2.4
1	В	338	ALA	2.4
1	В	298	ARG	2.4
1	С	443	GLN	2.4



Mol	Chain	Res	Type	RSRZ
1	В	430	VAL	2.4
1	В	343	ARG	2.3
1	В	362	ASP	2.3
1	В	404	GLU	2.3
1	С	460	SER	2.3
1	С	416	GLY	2.3
1	С	457	ARG	2.3
1	В	95	GLU	2.2
1	С	97	ASN	2.2
1	С	404	GLU	2.2
1	С	406	VAL	2.2
1	В	294	ASP	2.2
1	С	239	ASP	2.2
1	В	437	ALA	2.2
1	А	169	VAL	2.2
1	С	169	VAL	2.2
1	В	367	LYS	2.1
1	В	360	GLY	2.1
1	В	346	LEU	2.1
1	С	358	LEU	2.1
1	В	172	ALA	2.1
1	А	457	ARG	2.1
1	С	285	GLU	2.1
1	В	173	LEU	2.1
1	В	328	HIS	2.1
1	В	182	ASP	2.1
1	В	111	GLY	2.0
1	С	360	GLY	2.0
1	С	455	ARG	2.0
1	A	184	ASN	2.0
1	C	440	THR	2.0
1	В	432	VAL	2.0
1	В	80	GLU	2.0
1	C	318	THR	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
2	MG	А	1000	1/1	0.96	0.14	20,20,20,20	0
2	MG	В	2000	1/1	0.97	0.06	19, 19, 19, 19, 19	0
2	MG	С	3000	1/1	0.98	0.07	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.

