

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 4, 2024 - 01:48 pm BST

PDB ID	:	8CNL
Title	:	Lymphocytic choriomeningitis virus 3'-5' exonuclease domain of nucleoprotein
Authors	:	Spiliopoulou, M.; Papageorgiou, N.; Ferron, F.
Deposited on	:	2023-02-23
Resolution	:	2.80  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 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 02h-467
Vtais and (DL series)	•	1.025 101
Atriage (Pnenix)	:	1.15
$\mathrm{EDS}$	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

# 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 2.80 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 <sub>free</sub>	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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 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				
			10%				
1	А	218	71%	22%	7%		
			5%				
1	В	218	72%	22%	7%		
			6%				
1	С	218	71%	22%	7%		
			6%				
1	D	218	71%	22%	7%		
			22%				
1	Ε	218	69%	24%	7%		



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Mol	Chain	Length	Quality of chain				
			21%				
1	F	218	69%	24%	7%		
			23%				
1	G	218	69%	24%	7%		
			23%				
1	Н	218	69%	24%	7%		



#### 8CNL

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12976 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		At	oms			ZeroOcc	AltConf	Trace
1	1 D	202	Total	С	Ν	0	S	0	0	0
	D	203	1621	1028	279	303	11	0	0	0
1	Δ	203	Total	С	Ν	0	S	0	0	0
1	Л	203	1621	1028	279	303	11	0	0	0
1	С	203	Total	С	Ν	0	S	0	0	0
1	U	203	1621	1028	279	303	11	0	0	0
1		D 203	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	D		1621	1028	279	303	11	0	0	0
1	F	203	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
L	Ľ	205	1621	1028	279	303	11			
1	F	203	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	Ľ	200	1621	1028	279	303	11	0	0	0
1	C	203	Total	$\mathbf{C}$	Ν	0	$\mathbf{S}$	0	0	0
	G	200	1621	1028	279	303	11	0	0	0
1	1 U	203	Total	С	N	Ō	S	0	0	0
	203	1621	1028	279	303	11	0	0		

• Molecule 1 is a protein called Nucleoprotein.

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Zn 1 1	0	0
2	А	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	Е	1	Total Zn 1 1	0	0
2	$\mathbf{F}$	1	Total Zn 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	Н	1	Total Zn 1 1	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: Nucleoprotein



# 

# 1475 M479 743 749 8434 8434 8434 8434 8434 8434 8436 8436 8431 1505 1514 1514 1514 1515 1516 1516 1515 1516 1515 1516 1515 1515 1515 1515 1515 1515 1536 1537 1538 1533 1543 1536 1537 1543 1543 1543 1543 1543 1553 1544 1553 1553 1554 1553 1553 1553 <

 $\bullet$  Molecule 1: Nucleoprotein



## 

• Molecule 1: Nucleoprotein











# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	95.08Å 95.07Å 129.13Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $97.54^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	81.15 - 2.80	Depositor
Itesolution (A)	81.15 - 2.80	EDS
% Data completeness	99.7 (81.15-2.80)	Depositor
(in resolution range)	88.0 (81.15-2.80)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.72 (at 2.82 \text{\AA})$	Xtriage
Refinement program		Depositor
B B.	0.273 , $0.280$	Depositor
II, II free	0.275 , $0.278$	DCC
$R_{free}$ test set	54379 reflections $(3.56\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	48.8	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $43.0$	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12976	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: ZN

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	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.49	0/1656	0.67	0/2235
1	В	0.49	0/1656	0.68	0/2235
1	С	0.49	0/1656	0.67	0/2235
1	D	0.49	0/1656	0.68	0/2235
1	Е	0.49	0/1656	0.67	0/2235
1	F	0.49	0/1656	0.67	0/2235
1	G	0.49	0/1656	0.68	0/2235
1	Н	0.49	0/1656	0.67	0/2235
All	All	0.49	0/13248	0.67	0/17880

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1621	0	1615	79	5
1	В	1621	0	1615	70	6
1	С	1621	0	1615	75	7
1	D	1621	0	1615	78	7
1	Е	1621	0	1615	83	10



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1621	0	1615	73	11
1	G	1621	0	1613	79	9
1	Н	1621	0	1613	78	11
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
All	All	12976	0	12916	589	33

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 23.

All (589) 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:E:413:GLN:NE2	1:E:428:LEU:HD22	1.18	1.49
1:E:413:GLN:NE2	1:E:428:LEU:CD2	1.92	1.31
1:E:413:GLN:CD	1:E:428:LEU:CD2	1.99	1.30
1:E:413:GLN:OE1	1:E:428:LEU:CD2	1.82	1.27
1:D:491:VAL:HG12	1:D:521:MET:HE1	1.25	1.17
1:H:491:VAL:HG12	1:H:521:MET:HE1	1.19	1.17
1:F:491:VAL:HG12	1:F:521:MET:HE1	1.22	1.16
1:E:491:VAL:HG12	1:E:521:MET:HE3	1.16	1.15
1:D:375:PRO:HA	1:D:450:MET:CE	1.76	1.15
1:E:413:GLN:CD	1:E:428:LEU:HD21	1.61	1.14
1:C:356:VAL:HG12	1:C:357:GLY:H	1.03	1.14
1:G:356:VAL:HG12	1:G:357:GLY:H	1.03	1.14
1:D:356:VAL:HG12	1:D:357:GLY:H	1.03	1.13
1:F:356:VAL:HG12	1:F:357:GLY:H	1.03	1.13
1:E:413:GLN:OE1	1:E:428:LEU:HD21	0.94	1.10
1:E:356:VAL:HG12	1:E:357:GLY:H	1.03	1.10
1:G:491:VAL:HG12	1:G:521:MET:HE1	1.24	1.10
1:B:356:VAL:HG12	1:B:357:GLY:H	1.03	1.09
1:A:375:PRO:HA	1:A:450:MET:HE1	1.21	1.09
1:A:356:VAL:HG12	1:A:357:GLY:H	1.03	1.09
1:A:491:VAL:HG12	1:A:521:MET:HE1	1.14	1.09
1:H:356:VAL:HG12	1:H:357:GLY:H	1.03	1.08



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:386:ARG:NE	1:C:387:PHE:CD1	2.23	1.07
1:C:491:VAL:HG12	1:C:521:MET:HE1	1.13	1.07
1:F:386:ARG:NE	1:F:387:PHE:CD1	2.23	1.07
1:B:386:ARG:NE	1:B:387:PHE:CD1	2.23	1.06
1:B:491:VAL:HG12	1:B:521:MET:HE3	1.08	1.06
1:E:386:ARG:NE	1:E:387:PHE:CD1	2.23	1.06
1:D:386:ARG:NE	1:D:387:PHE:CD1	2.23	1.06
1:A:386:ARG:NE	1:A:387:PHE:CD1	2.23	1.06
1:G:386:ARG:NE	1:G:387:PHE:CD1	2.23	1.06
1:H:386:ARG:NE	1:H:387:PHE:CD1	2.23	1.05
1:D:492:TRP:HA	1:D:521:MET:HE2	1.05	1.05
1:E:413:GLN:HE22	1:E:428:LEU:CD2	1.62	1.04
1:F:492:TRP:HA	1:F:521:MET:HE2	1.04	1.03
1:A:491:VAL:HG12	1:A:521:MET:CE	1.88	1.03
1:E:491:VAL:HG12	1:E:521:MET:CE	1.88	1.03
1:H:491:VAL:HG12	1:H:521:MET:CE	1.88	1.03
1:D:375:PRO:HA	1:D:450:MET:HE3	1.38	1.03
1:C:491:VAL:HG12	1:C:521:MET:CE	1.88	1.02
1:F:491:VAL:HG12	1:F:521:MET:CE	1.88	1.02
1:G:491:VAL:HG12	1:G:521:MET:CE	1.88	1.02
1:E:492:TRP:HA	1:E:521:MET:HE1	1.03	1.02
1:B:492:TRP:HA	1:B:521:MET:HE1	1.02	1.02
1:B:491:VAL:HG12	1:B:521:MET:CE	1.88	1.01
1:C:492:TRP:HA	1:C:521:MET:HE2	1.03	1.01
1:D:491:VAL:HG12	1:D:521:MET:CE	1.88	1.01
1:G:492:TRP:HA	1:G:521:MET:HE2	1.05	1.01
1:H:492:TRP:HA	1:H:521:MET:HE2	1.04	1.01
1:A:492:TRP:HA	1:A:521:MET:HE2	1.03	1.01
1:B:492:TRP:CA	1:B:521:MET:HE1	1.90	1.01
1:C:447:PRO:HD2	1:C:450:MET:SD	2.01	1.01
1:H:492:TRP:CA	1:H:521:MET:HE2	1.91	1.01
1:C:413:GLN:HE22	1:G:387:PHE:HZ	1.05	1.00
1:C:492:TRP:CA	1:C:521:MET:HE2	1.91	1.00
1:H:356:VAL:HG12	1:H:357:GLY:N	1.77	0.99
1:G:492:TRP:CA	1:G:521:MET:HE2	1.93	0.99
1:A:492:TRP:CA	1:A:521:MET:HE2	1.91	0.99
1:E:492:TRP:CA	1:E:521:MET:HE1	1.91	0.99
1:G:356:VAL:HG12	1:G:357:GLY:N	1.77	0.98
1:E:356:VAL:HG12	1:E:357:GLY:N	1.77	0.98
1:C:492:TRP:HA	1:C:521:MET:CE	1.94	0.98
1:A:492:TRP:HA	1:A:521:MET:CE	1.94	0.98



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:492:TRP:HA	1:E:521:MET:CE	1.94	0.98
1:F:492:TRP:CA	1:F:521:MET:HE2	1.92	0.98
1:H:492:TRP:HA	1:H:521:MET:CE	1.94	0.97
1:G:492:TRP:HA	1:G:521:MET:CE	1.94	0.97
1:D:356:VAL:HG12	1:D:357:GLY:N	1.77	0.97
1:B:492:TRP:HA	1:B:521:MET:CE	1.94	0.97
1:A:356:VAL:HG12	1:A:357:GLY:N	1.77	0.97
1:D:492:TRP:HA	1:D:521:MET:CE	1.94	0.97
1:D:492:TRP:CA	1:D:521:MET:HE2	1.93	0.96
1:F:356:VAL:HG12	1:F:357:GLY:N	1.77	0.96
1:C:356:VAL:HG12	1:C:357:GLY:N	1.77	0.96
1:C:386:ARG:NE	1:C:387:PHE:CE1	2.33	0.96
1:F:386:ARG:NE	1:F:387:PHE:CE1	2.33	0.96
1:D:386:ARG:NE	1:D:387:PHE:CE1	2.33	0.96
1:E:386:ARG:NE	1:E:387:PHE:CE1	2.33	0.96
1:F:492:TRP:HA	1:F:521:MET:CE	1.94	0.96
1:B:386:ARG:NE	1:B:387:PHE:CE1	2.33	0.96
1:G:386:ARG:NE	1:G:387:PHE:CE1	2.33	0.95
1:B:386:ARG:HH21	1:B:462:LYS:NZ	1.65	0.95
1:D:386:ARG:HH21	1:D:462:LYS:NZ	1.65	0.95
1:E:386:ARG:HH21	1:E:462:LYS:NZ	1.65	0.95
1:B:356:VAL:HG12	1:B:357:GLY:N	1.77	0.95
1:H:386:ARG:NE	1:H:387:PHE:CE1	2.33	0.94
1:C:386:ARG:HH21	1:C:462:LYS:NZ	1.65	0.94
1:E:386:ARG:HE	1:E:387:PHE:HE1	1.11	0.94
1:B:386:ARG:HH21	1:B:462:LYS:HZ2	1.16	0.94
1:A:386:ARG:NE	1:A:387:PHE:CE1	2.33	0.94
1:F:386:ARG:HH21	1:F:462:LYS:NZ	1.65	0.94
1:H:386:ARG:HE	1:H:387:PHE:HE1	1.11	0.94
1:H:386:ARG:HH21	1:H:462:LYS:NZ	1.65	0.94
1:A:375:PRO:HA	1:A:450:MET:CE	1.97	0.94
1:G:386:ARG:HE	1:G:387:PHE:HE1	1.11	0.94
1:A:386:ARG:HH21	1:A:462:LYS:NZ	1.64	0.93
1:G:386:ARG:HH21	1:G:462:LYS:NZ	1.65	0.93
1:A:386:ARG:HE	1:A:387:PHE:HE1	1.11	0.93
1:B:386:ARG:HE	1:B:387:PHE:HE1	1.11	0.92
1:D:386:ARG:HE	1:D:387:PHE:HE1	1.11	0.92
1:C:386:ARG:HE	1:C:387:PHE:HE1	1.11	0.92
1:B:491:VAL:CG1	1:B:521:MET:HE3	2.00	0.92
1:G:386:ARG:NE	1:G:387:PHE:HD1	1.68	0.91
1:F:386:ARG:HE	1:F:387:PHE:HE1	1.11	0.90



	lo us pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:386:ARG:NE	1:D:387:PHE:HD1	1.68	0.90
1:D:386:ARG:HH22	1:D:462:LYS:HE3	1.37	0.90
1:F:386:ARG:NE	1:F:387:PHE:HD1	1.68	0.90
1:E:386:ARG:HH22	1:E:462:LYS:HE3	1.37	0.90
1:F:386:ARG:HH22	1:F:462:LYS:HE3	1.37	0.90
1:B:386:ARG:HH22	1:B:462:LYS:HE3	1.37	0.89
1:F:386:ARG:HH21	1:F:462:LYS:HZ2	1.10	0.89
1:A:386:ARG:HH22	1:A:462:LYS:HE3	1.37	0.89
1:E:386:ARG:HH21	1:E:462:LYS:HZ2	1.11	0.88
1:C:386:ARG:NE	1:C:387:PHE:HD1	1.68	0.88
1:C:386:ARG:HH22	1:C:462:LYS:HE3	1.37	0.88
1:C:386:ARG:NH2	1:C:462:LYS:HE3	1.89	0.88
1:E:411:VAL:CG1	1:H:428:LEU:HD23	2.03	0.88
1:G:386:ARG:HH22	1:G:462:LYS:HE3	1.37	0.88
1:D:386:ARG:NH2	1:D:462:LYS:HE3	1.89	0.88
1:H:386:ARG:HH22	1:H:462:LYS:HE3	1.37	0.88
1:H:386:ARG:NE	1:H:387:PHE:HD1	1.68	0.87
1:A:386:ARG:NH2	1:A:462:LYS:HE3	1.89	0.87
1:E:386:ARG:NE	1:E:387:PHE:HD1	1.68	0.87
1:B:386:ARG:NE	1:B:387:PHE:HD1	1.68	0.87
1:H:386:ARG:NH2	1:H:462:LYS:HE3	1.89	0.86
1:E:358:LEU:HD12	1:E:441:SER:OG	1.76	0.86
1:H:358:LEU:HD12	1:H:441:SER:OG	1.76	0.86
1:F:386:ARG:NH2	1:F:462:LYS:HE3	1.89	0.86
1:B:386:ARG:NH2	1:B:462:LYS:HE3	1.89	0.86
1:A:356:VAL:CG1	1:A:357:GLY:H	1.85	0.86
1:E:386:ARG:NH2	1:E:462:LYS:HE3	1.89	0.86
1:G:358:LEU:HD12	1:G:441:SER:OG	1.76	0.86
1:C:491:VAL:CG1	1:C:521:MET:HE1	2.04	0.86
1:G:386:ARG:NH2	1:G:462:LYS:HE3	1.89	0.86
1:B:358:LEU:HD12	1:B:441:SER:OG	1.76	0.85
1:D:375:PRO:HA	1:D:450:MET:HE1	1.58	0.85
1:D:358:LEU:HD12	1:D:441:SER:OG	1.76	0.85
1:C:358:LEU:HD12	1:C:441:SER:OG	1.76	0.85
1:F:358:LEU:HD12	1:F:441:SER:OG	1.76	0.85
1:C:508:ASP:OD2	1:C:514:ILE:HD11	1.77	0.85
1:A:386:ARG:NH2	1:A:462:LYS:NZ	2.25	0.84
1:A:386:ARG:NE	1:A:387:PHE:HD1	1.68	0.84
1:B:508:ASP:OD2	1:B:514:ILE:HD11	1.77	0.84
1:D:356:VAL:CG1	1:D:357:GLY:H	1.84	0.84
1:E:508:ASP:OD2	1:E:514:ILE:HD11	1.77	0.84



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:386:ARG:NH2	1:H:462:LYS:NZ	2.25	0.84
1:D:508:ASP:OD2	1:D:514:ILE:HD11	1.77	0.84
1:A:358:LEU:HD12	1:A:441:SER:OG	1.76	0.84
1:A:491:VAL:CG1	1:A:521:MET:HE1	2.05	0.84
1:G:508:ASP:OD2	1:G:514:ILE:HD11	1.77	0.84
1:H:508:ASP:OD2	1:H:514:ILE:HD11	1.77	0.84
1:E:386:ARG:NH2	1:E:462:LYS:NZ	2.25	0.84
1:G:386:ARG:NH2	1:G:462:LYS:NZ	2.25	0.84
1:A:508:ASP:OD2	1:A:514:ILE:HD11	1.77	0.83
1:C:386:ARG:NH2	1:C:462:LYS:NZ	2.25	0.83
1:E:356:VAL:CG1	1:E:357:GLY:H	1.85	0.83
1:D:358:LEU:HD12	1:D:441:SER:CB	2.09	0.83
1:D:386:ARG:NH2	1:D:462:LYS:NZ	2.25	0.83
1:E:412:ASP:OD1	1:H:429:ALA:HB2	1.79	0.83
1:B:356:VAL:CG1	1:B:357:GLY:H	1.85	0.83
1:C:386:ARG:NH2	1:C:462:LYS:CE	2.42	0.83
1:E:386:ARG:NH2	1:E:462:LYS:CE	2.42	0.83
1:F:508:ASP:OD2	1:F:514:ILE:HD11	1.77	0.83
1:B:386:ARG:NH2	1:B:462:LYS:NZ	2.25	0.83
1:A:386:ARG:NH2	1:A:462:LYS:CE	2.42	0.83
1:C:447:PRO:O	1:C:450:MET:HG3	1.79	0.83
1:C:358:LEU:HD12	1:C:441:SER:CB	2.09	0.83
1:D:386:ARG:NH2	1:D:462:LYS:CE	2.42	0.83
1:F:356:VAL:CG1	1:F:357:GLY:H	1.84	0.83
1:A:358:LEU:HD12	1:A:441:SER:CB	2.09	0.83
1:E:358:LEU:HD12	1:E:441:SER:CB	2.09	0.83
1:F:358:LEU:HD12	1:F:441:SER:CB	2.09	0.83
1:F:386:ARG:NH2	1:F:462:LYS:CE	2.42	0.83
1:G:358:LEU:HD12	1:G:441:SER:CB	2.09	0.83
1:H:358:LEU:HD12	1:H:441:SER:CB	2.09	0.83
1:F:386:ARG:NH2	1:F:462:LYS:NZ	2.25	0.82
1:B:386:ARG:NH2	1:B:462:LYS:CE	2.42	0.82
1:A:413:GLN:HE22	1:H:387:PHE:HZ	1.27	0.82
1:H:386:ARG:NH2	1:H:462:LYS:CE	2.42	0.82
1:G:356:VAL:CG1	1:G:357:GLY:H	1.84	0.82
1:G:447:PRO:HD2	1:G:450:MET:CE	2.09	0.82
1:E:491:VAL:CG1	1:E:521:MET:HE3	2.06	0.81
1:B:358:LEU:HD12	1:B:441:SER:CB	2.09	0.81
1:G:386:ARG:NH2	1:G:462:LYS:CE	2.42	0.81
1:D:375:PRO:O	1:D:450:MET:SD	2.39	0.81
1:C:447:PRO:CD	1:C:450:MET:SD	2.68	0.80



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:447:PRO:HD2	1:G:450:MET:HE1	1.63	0.80
1:D:386:ARG:HH21	1:D:462:LYS:HZ2	1.31	0.79
1:H:356:VAL:CG1	1:H:357:GLY:H	1.85	0.79
1:E:447:PRO:HD2	1:E:450:MET:HE1	1.65	0.78
1:H:447:PRO:HD2	1:H:450:MET:HE1	1.65	0.77
1:H:491:VAL:CG1	1:H:521:MET:HE1	2.09	0.76
1:C:413:GLN:NE2	1:G:387:PHE:HZ	1.82	0.76
1:C:356:VAL:CG1	1:C:357:GLY:H	1.85	0.75
1:D:491:VAL:CG1	1:D:521:MET:HE1	2.14	0.75
1:F:411:VAL:CG1	1:G:428:LEU:HD23	2.17	0.74
1:E:447:PRO:HD2	1:E:450:MET:CE	2.18	0.73
1:F:491:VAL:CG1	1:F:521:MET:HE1	2.11	0.72
1:B:404:ILE:HG12	1:B:543:ILE:HD11	1.69	0.71
1:C:386:ARG:HH21	1:C:462:LYS:HZ2	1.35	0.71
1:H:447:PRO:HD2	1:H:450:MET:CE	2.20	0.71
1:A:386:ARG:HH21	1:A:462:LYS:HZ2	1.39	0.69
1:A:375:PRO:CA	1:A:450:MET:HE1	2.12	0.69
1:D:358:LEU:CD1	1:D:441:SER:CB	2.71	0.69
1:E:358:LEU:CD1	1:E:441:SER:CB	2.71	0.69
1:G:358:LEU:CD1	1:G:441:SER:CB	2.71	0.69
1:G:491:VAL:CG1	1:G:521:MET:HE1	2.13	0.69
1:B:386:ARG:CZ	1:B:387:PHE:CD1	2.76	0.68
1:C:358:LEU:CD1	1:C:441:SER:CB	2.71	0.68
1:E:386:ARG:CZ	1:E:387:PHE:CD1	2.76	0.68
1:B:358:LEU:CD1	1:B:441:SER:CB	2.71	0.68
1:F:358:LEU:CD1	1:F:441:SER:CB	2.71	0.68
1:A:386:ARG:CZ	1:A:387:PHE:CD1	2.76	0.68
1:G:386:ARG:CZ	1:G:387:PHE:CD1	2.76	0.68
1:H:358:LEU:CD1	1:H:441:SER:CB	2.71	0.68
1:F:447:PRO:HD2	1:F:450:MET:HE1	1.76	0.68
1:H:386:ARG:CZ	1:H:387:PHE:CD1	2.76	0.68
1:A:358:LEU:CD1	1:A:441:SER:CB	2.71	0.68
1:C:386:ARG:CZ	1:C:387:PHE:CD1	2.76	0.68
1:D:386:ARG:CZ	1:D:387:PHE:CD1	2.76	0.67
1:E:518:CYS:HB3	1:E:521:MET:HB2	1.77	0.67
1:D:518:CYS:HB3	1:D:521:MET:HB2	1.76	0.67
1:G:518:CYS:HB3	1:G:521:MET:HB2	1.77	0.67
1:F:518:CYS:HB3	1:F:521:MET:HB2	1.77	0.67
1:F:386:ARG:CZ	1:F:387:PHE:CD1	2.76	0.67
1:H:518:CYS:HB3	1:H:521:MET:HB2	1.77	0.67
1:B:518:CYS:HB3	1:B:521:MET:HB2	1.76	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1·E·411·VAL·HG11	1.H.428.LEU.HD23	1 77	0.66
1:F:447:PRO:HD2	1:F:450:MET:CE	2.25	0.66
1:A:518:CYS:HB3	1·A·521·MET·HB2	1.77	0.66
1:G:356:VAL:CG1	1:G:357:GLY:N	2.52	0.65
1:A:386:ARG:NH2	1:A:462:LYS:HZ1	1.95	0.65
1:E:450:MET:SD	1:E:452:LEU:HD21	2.37	0.65
1:A:447:PRO:HB2	1:A:450:MET:SD	2.37	0.65
1:C:518:CYS:HB3	1:C:521:MET:HB2	1.77	0.64
1:D:375:PRO:CA	1:D:450:MET:CE	2.67	0.64
1:F:356:VAL:CG1	1:F:357:GLY:N	2.52	0.64
1:D:356:VAL:CG1	1:D:357:GLY:N	2.52	0.63
1:G:491:VAL:C	1:G:521:MET:HE1	2.19	0.63
1:A:356:VAL:O	1:H:414:LYS:NZ	2.32	0.63
1:C:447:PRO:HB2	1:C:450:MET:CG	2.30	0.62
1:D:491:VAL:C	1:D:521:MET:HE1	2.19	0.62
1:F:491:VAL:C	1:F:521:MET:HE1	2.20	0.62
1:D:375:PRO:CA	1:D:450:MET:HE1	2.28	0.62
1:C:386:ARG:CZ	1:C:387:PHE:HD1	2.13	0.62
1:A:386:ARG:CZ	1:A:387:PHE:HD1	2.13	0.61
1:E:386:ARG:CZ	1:E:387:PHE:HD1	2.13	0.61
1:D:386:ARG:CZ	1:D:387:PHE:HD1	2.13	0.61
1:E:386:ARG:HH22	1:E:462:LYS:CE	2.10	0.61
1:H:386:ARG:CZ	1:H:387:PHE:HD1	2.13	0.60
1:B:404:ILE:HG12	1:B:543:ILE:CD1	2.31	0.60
1:C:386:ARG:NH2	1:C:462:LYS:HZ1	1.99	0.60
1:G:447:PRO:HD2	1:G:450:MET:HE3	1.82	0.60
1:G:386:ARG:CZ	1:G:387:PHE:HD1	2.13	0.60
1:A:356:VAL:CG1	1:A:357:GLY:N	2.52	0.60
1:A:358:LEU:CD1	1:A:441:SER:HB2	2.32	0.60
1:D:358:LEU:CD1	1:D:441:SER:HB2	2.32	0.60
1:F:358:LEU:CD1	1:F:441:SER:HB2	2.32	0.60
1:G:358:LEU:CD1	1:G:441:SER:HB2	2.32	0.59
1:H:491:VAL:C	1:H:521:MET:HE1	2.21	0.59
1:B:492:TRP:CA	1:B:521:MET:CE	2.69	0.59
1:A:508:ASP:HB3	1:A:514:ILE:HD12	1.85	0.59
1:G:508:ASP:HB3	1:G:514:ILE:HD12	1.85	0.59
1:F:508:ASP:HB3	1:F:514:ILE:HD12	1.85	0.59
1:C:358:LEU:CD1	1:C:441:SER:HB2	2.32	0.59
1:D:508:ASP:HB3	1:D:514:ILE:HD12	1.85	0.59
1:E:358:LEU:CD1	1:E:441:SER:HB2	2.32	0.58
1:C:508:ASP:HB3	1:C:514:ILE:HD12	1.85	0.58



	, and page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:491:VAL:C	1:E:521:MET:HE3	2.23	0.58
1:B:358:LEU:CD1	1:B:441:SER:HB2	2.32	0.58
1:A:375:PRO:O	1:A:450:MET:CE	2.51	0.58
1:C:356:VAL:CG1	1:C:357:GLY:N	2.52	0.58
1:E:508:ASP:HB3	1:E:514:ILE:HD12	1.85	0.58
1:F:492:TRP:CA	1:F:521:MET:CE	2.69	0.58
1:A:359:SER:OG	1:A:362:GLN:HG3	2.04	0.58
1:H:358:LEU:CD1	1:H:441:SER:HB2	2.32	0.58
1:H:508:ASP:HB3	1:H:514:ILE:HD12	1.85	0.58
1:D:492:TRP:CA	1:D:521:MET:CE	2.69	0.58
1:E:412:ASP:OD1	1:H:429:ALA:CB	2.51	0.58
1:B:447:PRO:HD2	1:B:450:MET:CE	2.34	0.58
1:A:491:VAL:C	1:A:521:MET:HE1	2.24	0.58
1:B:508:ASP:HB3	1:B:514:ILE:HD12	1.85	0.58
1:F:359:SER:OG	1:F:362:GLN:HG3	2.04	0.58
1:C:359:SER:OG	1:C:362:GLN:HG3	2.04	0.57
1:G:359:SER:OG	1:G:362:GLN:HG3	2.03	0.57
1:B:356:VAL:CG1	1:B:357:GLY:N	2.52	0.57
1:B:359:SER:OG	1:B:362:GLN:HG3	2.04	0.57
1:D:359:SER:OG	1:D:362:GLN:HG3	2.04	0.57
1:H:359:SER:OG	1:H:362:GLN:HG3	2.04	0.57
1:B:386:ARG:CD	1:B:387:PHE:CD1	2.88	0.57
1:G:386:ARG:NH2	1:G:462:LYS:HZ1	2.03	0.57
1:D:386:ARG:CD	1:D:387:PHE:CD1	2.88	0.57
1:E:359:SER:OG	1:E:362:GLN:HG3	2.04	0.57
1:C:491:VAL:C	1:C:521:MET:HE1	2.25	0.57
1:F:386:ARG:CD	1:F:387:PHE:CD1	2.88	0.57
1:B:479:MET:HE1	1:B:484:SER:HB2	1.87	0.57
1:E:386:ARG:CD	1:E:387:PHE:CD1	2.88	0.56
1:A:386:ARG:CD	1:A:387:PHE:CD1	2.88	0.56
1:F:450:MET:SD	1:F:452:LEU:HD21	2.45	0.56
1:G:386:ARG:CD	1:G:387:PHE:CD1	2.88	0.56
1:C:356:VAL:O	1:G:414:LYS:NZ	2.39	0.56
1:C:492:TRP:CA	1:C:521:MET:CE	2.69	0.56
1:E:356:VAL:CG1	1:E:357:GLY:N	2.52	0.56
1:B:386:ARG:CZ	1:B:387:PHE:HD1	2.13	0.56
1:C:386:ARG:CD	1:C:387:PHE:CD1	2.88	0.56
1:G:378:PRO:HD2	1:G:399:GLN:NE2	2.21	0.56
1:D:386:ARG:HH22	1:D:462:LYS:CE	2.10	0.55
1:F:378:PRO:HD2	1:F:399:GLN:NE2	2.21	0.55
1:H:386:ARG:CD	1:H:387:PHE:CD1	2.88	0.55



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:451:VAL:CG1	1:B:475:ILE:HD11	2.37	0.55
1:D:386:ARG:NH2	1:D:462:LYS:HZ1	2.03	0.55
1:F:404:ILE:HG23	1:F:544:LEU:HD11	1.88	0.55
1:B:378:PRO:HD2	1:B:399:GLN:NE2	2.21	0.55
1:A:358:LEU:HD11	1:A:441:SER:HB2	1.89	0.55
1:B:386:ARG:HH22	1:B:462:LYS:CE	2.10	0.55
1:E:378:PRO:HD2	1:E:399:GLN:NE2	2.20	0.55
1:A:378:PRO:HD2	1:A:399:GLN:NE2	2.21	0.55
1:A:451:VAL:CG1	1:A:475:ILE:HD11	2.37	0.55
1:D:451:VAL:CG1	1:D:475:ILE:HD11	2.37	0.55
1:F:386:ARG:CZ	1:F:387:PHE:HD1	2.13	0.55
1:G:451:VAL:CG1	1:G:475:ILE:HD11	2.37	0.55
1:C:451:VAL:CG1	1:C:475:ILE:HD11	2.36	0.55
1:F:451:VAL:CG1	1:F:475:ILE:HD11	2.37	0.55
1:B:404:ILE:HG23	1:B:544:LEU:HD11	1.88	0.55
1:G:450:MET:SD	1:G:452:LEU:HD21	2.46	0.55
1:C:358:LEU:HD11	1:C:441:SER:HB2	1.89	0.55
1:G:492:TRP:CA	1:G:521:MET:CE	2.69	0.55
1:A:375:PRO:HA	1:A:450:MET:SD	2.47	0.55
1:D:508:ASP:HB3	1:D:514:ILE:CD1	2.37	0.55
1:E:451:VAL:CG1	1:E:475:ILE:HD11	2.37	0.55
1:G:404:ILE:HG23	1:G:544:LEU:HD11	1.88	0.55
1:E:411:VAL:HG12	1:H:428:LEU:HD23	1.87	0.55
1:E:492:TRP:CA	1:E:521:MET:CE	2.69	0.55
1:C:508:ASP:HB3	1:C:514:ILE:CD1	2.38	0.54
1:F:358:LEU:HD11	1:F:441:SER:HB2	1.89	0.54
1:D:358:LEU:HD11	1:D:441:SER:HB2	1.89	0.54
1:B:508:ASP:HB3	1:B:514:ILE:CD1	2.37	0.54
1:E:508:ASP:HB3	1:E:514:ILE:CD1	2.37	0.54
1:G:508:ASP:HB3	1:G:514:ILE:CD1	2.37	0.54
1:H:451:VAL:CG1	1:H:475:ILE:HD11	2.37	0.54
1:E:358:LEU:HD11	1:E:441:SER:HB2	1.89	0.54
1:A:508:ASP:HB3	1:A:514:ILE:CD1	2.38	0.54
1:F:508:ASP:HB3	1:F:514:ILE:CD1	2.38	0.54
1:H:356:VAL:CG1	1:H:357:GLY:N	2.52	0.54
1:H:358:LEU:HD11	1:H:441:SER:HB2	1.89	0.54
1:D:404:ILE:HG23	1:D:544:LEU:HD11	1.88	0.54
1:A:386:ARG:CD	1:A:387:PHE:HD1	2.21	0.54
1:E:404:ILE:HG23	1:E:544:LEU:HD11	1.88	0.54
1:B:358:LEU:HD11	1:B:441:SER:HB2	1.89	0.54
1:A:404:ILE:HG23	1:A:544:LEU:HD11	1.88	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:404:ILE:HG23	1:H:544:LEU:HD11	1.89	0.54
1:H:551:ARG:NH2	1:H:554:ASN:OD1	2.41	0.54
1:C:386:ARG:CD	1:C:387:PHE:HD1	2.21	0.53
1:C:404:ILE:HG23	1:C:544:LEU:HD11	1.89	0.53
1:F:386:ARG:CD	1:F:387:PHE:HD1	2.21	0.53
1:B:386:ARG:CD	1:B:387:PHE:HD1	2.21	0.53
1:G:358:LEU:HD11	1:G:441:SER:HB2	1.89	0.53
1:H:508:ASP:HB3	1:H:514:ILE:CD1	2.38	0.53
1:B:491:VAL:C	1:B:521:MET:HE3	2.28	0.53
1:D:386:ARG:CD	1:D:387:PHE:HD1	2.21	0.53
1:B:404:ILE:HG23	1:B:544:LEU:CD1	2.39	0.53
1:C:413:GLN:HB2	1:G:462:LYS:NZ	2.24	0.53
1:H:450:MET:SD	1:H:452:LEU:HD21	2.48	0.53
1:B:450:MET:SD	1:B:452:LEU:HD21	2.49	0.53
1:E:404:ILE:HG23	1:E:544:LEU:CD1	2.39	0.53
1:A:492:TRP:CA	1:A:521:MET:CE	2.69	0.52
1:H:404:ILE:HG23	1:H:544:LEU:CD1	2.39	0.52
1:G:386:ARG:CD	1:G:387:PHE:HD1	2.21	0.52
1:D:479:MET:HE1	1:D:484:SER:HB2	1.91	0.52
1:B:447:PRO:HD2	1:B:450:MET:HE1	1.91	0.52
1:C:404:ILE:HG23	1:C:544:LEU:CD1	2.40	0.52
1:E:479:MET:HE1	1:E:484:SER:HB2	1.90	0.52
1:H:479:MET:HE1	1:H:484:SER:HB2	1.91	0.52
1:C:518:CYS:O	1:C:518:CYS:SG	2.68	0.52
1:D:518:CYS:SG	1:D:518:CYS:O	2.68	0.52
1:A:404:ILE:HG23	1:A:544:LEU:CD1	2.39	0.52
1:E:518:CYS:SG	1:E:518:CYS:O	2.68	0.52
1:B:518:CYS:SG	1:B:518:CYS:O	2.68	0.52
1:H:386:ARG:CD	1:H:387:PHE:HD1	2.21	0.52
1:C:447:PRO:N	1:C:450:MET:SD	2.83	0.51
1:F:404:ILE:HG23	1:F:544:LEU:CD1	2.39	0.51
1:G:404:ILE:HG23	1:G:544:LEU:CD1	2.39	0.51
1:D:404:ILE:HG23	1:D:544:LEU:CD1	2.39	0.51
1:A:518:CYS:O	1:A:518:CYS:SG	2.68	0.51
1:H:518:CYS:O	1:H:518:CYS:SG	2.68	0.51
1:F:412:ASP:OD1	1:G:429:ALA:HB2	2.10	0.51
1:F:518:CYS:O	1:F:518:CYS:SG	2.68	0.51
1:H:492:TRP:CA	1:H:521:MET:CE	2.69	0.51
1:G:518:CYS:SG	1:G:518:CYS:O	2.68	0.51
1:E:386:ARG:CD	1:E:387:PHE:HD1	2.21	0.50
1:A:479:MET:HE1	1:A:484:SER:HB2	1.94	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:447:PRO:HB2	1:D:450:MET:HE1	1.94	0.50
1:A:375:PRO:O	1:A:450:MET:HE3	2.12	0.49
1:H:386:ARG:NH2	1:H:462:LYS:HZ1	2.11	0.48
1:D:467:GLN:OE1	1:H:558:LEU:HG	2.14	0.48
1:F:536:ASP:C	1:F:537:LEU:HD23	2.34	0.48
1:A:536:ASP:C	1:A:537:LEU:HD23	2.35	0.48
1:C:536:ASP:C	1:C:537:LEU:HD23	2.35	0.48
1:A:375:PRO:CA	1:A:450:MET:SD	3.02	0.47
1:E:536:ASP:C	1:E:537:LEU:HD23	2.34	0.47
1:G:479:MET:HE1	1:G:484:SER:HB2	1.95	0.47
1:B:536:ASP:C	1:B:537:LEU:HD23	2.34	0.47
1:D:467:GLN:OE1	1:H:558:LEU:CD1	2.62	0.47
1:D:536:ASP:C	1:D:537:LEU:HD23	2.35	0.47
1:D:386:ARG:CZ	1:D:387:PHE:CE1	2.98	0.47
1:H:536:ASP:C	1:H:537:LEU:HD23	2.34	0.47
1:B:451:VAL:HG11	1:B:475:ILE:HD11	1.97	0.47
1:A:467:GLN:OE1	1:E:558:LEU:HD12	2.15	0.47
1:F:451:VAL:HG11	1:F:475:ILE:HD11	1.97	0.47
1:C:447:PRO:HB2	1:C:450:MET:SD	2.55	0.47
1:E:413:GLN:HE22	1:E:428:LEU:HD22	0.66	0.47
1:G:536:ASP:C	1:G:537:LEU:HD23	2.34	0.47
1:A:467:GLN:OE1	1:E:558:LEU:CD1	2.62	0.46
1:D:451:VAL:HG11	1:D:475:ILE:HD11	1.97	0.46
1:E:451:VAL:HG11	1:E:475:ILE:HD11	1.97	0.46
1:G:451:VAL:HG11	1:G:475:ILE:HD11	1.97	0.46
1:E:386:ARG:CZ	1:E:387:PHE:CE1	2.98	0.46
1:G:386:ARG:CZ	1:G:387:PHE:CE1	2.98	0.46
1:C:451:VAL:HG11	1:C:475:ILE:HD11	1.97	0.46
1:C:479:MET:HE1	1:C:484:SER:HB2	1.97	0.46
1:H:451:VAL:HG11	1:H:475:ILE:HD11	1.97	0.46
1:F:411:VAL:HG11	1:G:428:LEU:HD23	1.98	0.46
1:E:404:ILE:HG12	1:E:543:ILE:HG12	1.98	0.46
1:C:404:ILE:HG12	1:C:543:ILE:HG12	1.98	0.46
1:A:451:VAL:HG11	1:A:475:ILE:HD11	1.97	0.45
1:D:404:ILE:HG12	1:D:543:ILE:HG12	1.98	0.45
1:F:404:ILE:HG12	1:F:543:ILE:HG12	1.98	0.45
1:C:413:GLN:NE2	1:G:387:PHE:CZ	2.69	0.45
1:A:404:ILE:HG12	1:A:543:ILE:HG12	1.98	0.45
1:D:491:VAL:HG12	1:D:521:MET:HE3	1.89	0.45
1:F:447:PRO:HD2	1:F:450:MET:HE3	1.99	0.45
1:H:404:ILE:HG12	1:H:543:ILE:HG12	1.98	0.45



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:386:ARG:CZ	1:A:387:PHE:CE1	2.98	0.45	
1:A:479:MET:CE	1:A:484:SER:HB2	2.47	0.45	
1:E:492:TRP:N	1:E:521:MET:CE	2.80	0.45	
1:F:479:MET:CE	1:F:484:SER:HB2	2.47	0.45	
1:F:492:TRP:N	1:F:521:MET:CE	2.80	0.45	
1:G:492:TRP:N	1:G:521:MET:CE	2.80	0.45	
1:B:479:MET:CE	1:B:484:SER:HB2	2.47	0.44	
1:H:407:TYR:CZ	1:H:501:MET:HG3	2.53	0.44	
1:B:407:TYR:CZ	1:B:501:MET:HG3	2.53	0.44	
1:A:375:PRO:CA	1:A:450:MET:CE	2.82	0.44	
1:A:407:TYR:CZ	1:A:501:MET:HG3	2.53	0.44	
1:C:479:MET:CE	1:C:484:SER:HB2	2.47	0.44	
1:D:479:MET:CE	1:D:484:SER:HB2	2.47	0.44	
1:G:407:TYR:CZ	1:G:501:MET:HG3	2.53	0.44	
1:G:404:ILE:HG12	1:G:543:ILE:HG12	1.98	0.44	
1:H:492:TRP:N	1:H:521:MET:CE	2.80	0.44	
1:C:386:ARG:CZ	1:C:387:PHE:CE1	2.98	0.44	
1:E:447:PRO:HD2	1:E:450:MET:HE3	1.97	0.44	
1:G:479:MET:CE	1:G:484:SER:HB2	2.47	0.44	
1:A:447:PRO:O	1:A:450:MET:HG2	2.17	0.44	
1:F:450:MET:O	1:F:472:ILE:HG23	2.17	0.44	
1:G:491:VAL:HG12	1:G:521:MET:HE3	1.90	0.44	
1:D:386:ARG:HG3	1:D:387:PHE:CD1	2.53	0.44	
1:B:467:GLN:OE1	1:G:558:LEU:CD1	2.66	0.44	
1:A:492:TRP:N	1:A:521:MET:CE	2.80	0.44	
1:D:467:GLN:OE1	1:H:558:LEU:HD12	2.17	0.44	
1:D:554:ASN:OD1	1:D:555:VAL:N	2.51	0.44	
1:F:407:TYR:CZ	1:F:501:MET:HG3	2.53	0.44	
1:H:479:MET:CE	1:H:484:SER:HB2	2.47	0.44	
1:C:492:TRP:N	1:C:521:MET:CE	2.80	0.43	
1:D:407:TYR:CZ	1:D:501:MET:HG3	2.53	0.43	
1:F:554:ASN:OD1	1:F:555:VAL:N	2.51	0.43	
1:H:514:ILE:HG22	1:H:515:THR:N	2.33	0.43	
1:B:386:ARG:HG3	1:B:387:PHE:CD1	2.53	0.43	
1:B:492:TRP:N	1:B:521:MET:CE	2.80	0.43	
1:A:413:GLN:NE2	1:H:387:PHE:HZ	2.04	0.43	
1:C:407:TYR:CZ	1:C:501:MET:HG3	2.53	0.43	
1:G:514:ILE:HG22	1:G:515:THR:N	2.33	0.43	
1:H:386:ARG:CZ	1:H:387:PHE:CE1	2.98	0.43	
1:D:492:TRP:N	1:D:521:MET:CE	2.80	0.43	
1:E:407:TYR:CZ	1:E:501:MET:HG3	2.53	0.43	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:554:ASN:OD1	1:A:555:VAL:N	2.52	0.43
1:E:514:ILE:HG22	1:E:515:THR:N	2.34	0.43
1:G:554:ASN:OD1	1:G:555:VAL:N	2.51	0.43
1:F:514:ILE:HG22	1:F:515:THR:N	2.34	0.43
1:A:378:PRO:HD2	1:A:399:GLN:CD	2.39	0.43
1:A:386:ARG:HG3	1:A:387:PHE:CD1	2.53	0.43
1:D:514:ILE:HG22	1:D:515:THR:N	2.33	0.43
1:E:479:MET:CE	1:E:484:SER:HB2	2.47	0.43
1:H:386:ARG:HG3	1:H:387:PHE:CD1	2.53	0.43
1:B:554:ASN:OD1	1:B:555:VAL:N	2.51	0.43
1:C:386:ARG:HG3	1:C:387:PHE:CD1	2.53	0.43
1:E:404:ILE:CG2	1:E:544:LEU:HD11	2.49	0.43
1:F:386:ARG:HG3	1:F:387:PHE:CD1	2.53	0.43
1:G:378:PRO:HD2	1:G:399:GLN:CD	2.39	0.43
1:B:467:GLN:OE1	1:G:558:LEU:HD12	2.18	0.43
1:D:404:ILE:CG2	1:D:544:LEU:HD11	2.48	0.43
1:E:531:LYS:HA	1:E:531:LYS:HD3	1.91	0.43
1:B:514:ILE:HG22	1:B:515:THR:N	2.33	0.43
1:C:554:ASN:OD1	1:C:555:VAL:N	2.51	0.43
1:E:386:ARG:HG3	1:E:387:PHE:CD1	2.53	0.43
1:G:386:ARG:HG3	1:G:387:PHE:CD1	2.53	0.43
1:C:467:GLN:OE1	1:F:558:LEU:HD12	2.19	0.42
1:C:514:ILE:HG22	1:C:515:THR:N	2.33	0.42
1:E:378:PRO:HD2	1:E:399:GLN:CD	2.39	0.42
1:H:390:PRO:O	1:H:408:ARG:HB3	2.19	0.42
1:A:390:PRO:O	1:A:408:ARG:HB3	2.19	0.42
1:C:505:ILE:HG23	1:C:513:GLU:HG3	2.01	0.42
1:D:531:LYS:HA	1:D:531:LYS:HD3	1.91	0.42
1:A:514:ILE:HG22	1:A:515:THR:N	2.33	0.42
1:F:378:PRO:HD2	1:F:399:GLN:CD	2.39	0.42
1:G:404:ILE:CG2	1:G:544:LEU:HD11	2.49	0.42
1:G:505:ILE:HG23	1:G:513:GLU:HG3	2.02	0.42
1:C:404:ILE:CG2	1:C:544:LEU:HD11	2.49	0.42
1:E:505:ILE:HG23	1:E:513:GLU:HG3	2.02	0.42
1:E:554:ASN:OD1	1:E:555:VAL:N	2.51	0.42
1:F:491:VAL:HG12	1:F:521:MET:HE3	1.92	0.42
1:A:505:ILE:HG23	1:A:513:GLU:HG3	2.01	0.42
1:D:420:SER:O	1:D:425:GLY:HA2	2.20	0.42
1:H:404:ILE:CG2	1:H:544:LEU:HD11	2.49	0.42
1:F:420:SER:O	1:F:425:GLY:HA2	2.20	0.42
1:F:505:ILE:HG23	1:F:513:GLU:HG3	2.02	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:H:505:ILE:HG23	1:H:513:GLU:HG3	2.02	0.42	
1:B:447:PRO:HD2	1:B:450:MET:HE3	1.99	0.42	
1:A:420:SER:O	1:A:425:GLY:HA2	2.20	0.42	
1:C:390:PRO:O	1:C:408:ARG:HB3	2.19	0.42	
1:C:467:GLN:OE1	1:F:558:LEU:CD1	2.68	0.42	
1:F:390:PRO:O	1:F:408:ARG:HB3	2.20	0.42	
1:G:390:PRO:O	1:G:408:ARG:HB3	2.19	0.42	
1:G:536:ASP:O	1:G:537:LEU:HD23	2.20	0.42	
1:A:536:ASP:O	1:A:537:LEU:HD23	2.20	0.42	
1:D:536:ASP:O	1:D:537:LEU:HD23	2.20	0.42	
1:F:386:ARG:CZ	1:F:387:PHE:CE1	2.98	0.42	
1:C:455:GLN:HE21	1:C:479:MET:HB3	1.85	0.42	
1:D:390:PRO:O	1:D:408:ARG:HB3	2.19	0.42	
1:D:455:GLN:HE21	1:D:479:MET:HB3	1.85	0.42	
1:E:455:GLN:HE21	1:E:479:MET:HB3	1.85	0.42	
1:F:455:GLN:HE21	1:F:479:MET:HB3	1.85	0.42	
1:F:514:ILE:CG2	1:F:515:THR:N	2.83	0.42	
1:G:455:GLN:HE21	1:G:479:MET:HB3	1.85	0.42	
1:H:420:SER:O	1:H:425:GLY:HA2	2.20	0.42	
1:D:505:ILE:HG23	1:D:513:GLU:HG3	2.02	0.41	
1:F:536:ASP:O	1:F:537:LEU:HD23	2.20	0.41	
1:B:404:ILE:CG2	1:B:544:LEU:HD11	2.48	0.41	
1:A:404:ILE:CG2	1:A:544:LEU:HD11	2.49	0.41	
1:A:455:GLN:HE21	1:A:479:MET:HB3	1.85	0.41	
1:A:490:LYS:HB3	1:A:534:LEU:CD1	2.51	0.41	
1:H:450:MET:O	1:H:472:ILE:HG23	2.20	0.41	
1:H:514:ILE:CG2	1:H:515:THR:N	2.83	0.41	
1:B:386:ARG:CZ	1:B:387:PHE:CE1	2.98	0.41	
1:B:536:ASP:O	1:B:537:LEU:HD23	2.20	0.41	
1:G:514:ILE:CG2	1:G:515:THR:N	2.83	0.41	
1:D:514:ILE:CG2	1:D:515:THR:N	2.83	0.41	
1:E:390:PRO:O	1:E:408:ARG:HB3	2.19	0.41	
1:G:420:SER:O	1:G:425:GLY:HA2	2.20	0.41	
1:G:450:MET:O	1:G:472:ILE:HG23	2.20	0.41	
1:H:536:ASP:O	1:H:537:LEU:HD23	2.20	0.41	
1:B:378:PRO:HD2	1:B:399:GLN:CD	2.39	0.41	
1:B:455:GLN:HE21	1:B:479:MET:HB3	1.85	0.41	
1:A:514:ILE:CG2	1:A:515:THR:N	2.83	0.41	
1:H:531:LYS:HA	1:H:531:LYS:HD3	1.91	0.41	
1:B:390:PRO:O	1:B:408:ARG:HB3	2.20	0.41	
1:C:420:SER:O	1:C:425:GLY:HA2	2.20	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:440:SER:HB3	1:H:558:LEU:H	1.85	0.41
1:E:420:SER:O	1:E:425:GLY:HA2	2.20	0.41
1:E:490:LYS:HB3	1:E:534:LEU:CD1	2.51	0.41
1:H:455:GLN:HE21	1:H:479:MET:HB3	1.85	0.41
1:B:420:SER:O	1:B:425:GLY:HA2	2.20	0.41
1:B:490:LYS:HB3	1:B:534:LEU:CD1	2.51	0.41
1:E:536:ASP:O	1:E:537:LEU:HD23	2.20	0.41
1:F:404:ILE:CG2	1:F:544:LEU:HD11	2.49	0.41
1:F:490:LYS:HB3	1:F:534:LEU:CD1	2.51	0.41
1:D:375:PRO:HB3	1:D:447:PRO:HB3	2.03	0.41
1:E:386:ARG:HG3	1:E:387:PHE:N	2.36	0.41
1:G:386:ARG:HG3	1:G:387:PHE:N	2.36	0.41
1:B:386:ARG:HG3	1:B:387:PHE:N	2.36	0.41
1:A:360:TYR:O	1:A:364:MET:HG2	2.21	0.41
1:C:490:LYS:HB3	1:C:534:LEU:CD1	2.51	0.41
1:C:536:ASP:O	1:C:537:LEU:HD23	2.20	0.41
1:D:360:TYR:O	1:D:364:MET:HG2	2.21	0.41
1:E:514:ILE:CG2	1:E:515:THR:N	2.83	0.41
1:B:514:ILE:CG2	1:B:515:THR:N	2.83	0.41
1:D:386:ARG:HG3	1:D:387:PHE:N	2.36	0.41
1:F:386:ARG:HG3	1:F:387:PHE:N	2.36	0.41
1:H:360:TYR:O	1:H:364:MET:HG2	2.21	0.41
1:B:360:TYR:O	1:B:364:MET:HG2	2.21	0.40
1:G:360:TYR:O	1:G:364:MET:HG2	2.21	0.40
1:G:490:LYS:HB3	1:G:534:LEU:CD1	2.51	0.40
1:H:490:LYS:HB3	1:H:534:LEU:CD1	2.51	0.40
1:C:514:ILE:CG2	1:C:515:THR:N	2.83	0.40
1:D:375:PRO:HB3	1:D:447:PRO:CB	2.51	0.40
1:C:360:TYR:O	1:C:364:MET:HG2	2.21	0.40
1:C:531:LYS:HD3	1:C:531:LYS:HA	1.91	0.40
1:D:490:LYS:HB3	1:D:534:LEU:CD1	2.51	0.40
1:A:386:ARG:HG3	1:A:387:PHE:N	2.36	0.40
1:H:386:ARG:HG3	1:H:387:PHE:N	2.36	0.40
1:F:360:TYR:O	1:F:364:MET:HG2	2.21	0.40

All (33) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:478:GLU:OE1	$1:G:478:GLU:OE1[1_455]$	0.95	1.25



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:F:478:GLU:OE1	$1:H:478:GLU:OE1[1_545]$	0.98	1.22
1:B:475:ILE:CD1	$1:E:497:TRP:CH2[2_546]$	1.47	0.73
1:C:475:ILE:CD1	1:F:497:TRP:CH2[2_655]	1.48	0.72
1:D:475:ILE:CD1	1:H:497:TRP:CH2[2_545]	1.52	0.68
1:A:475:ILE:CD1	1:G:497:TRP:CH2[2_656]	1.56	0.64
1:C:461:ARG:NE	1:F:538:LYS:CE[2_655]	1.61	0.59
1:A:461:ARG:NE	1:G:538:LYS:CE[2_656]	1.64	0.56
1:B:461:ARG:NE	1:E:538:LYS:CE[2_546]	1.67	0.53
1:D:461:ARG:NE	1:H:538:LYS:CE[2_545]	1.72	0.48
1:E:478:GLU:CB	1:G:478:GLU:CB[1_455]	1.77	0.43
1:F:478:GLU:CB	1:H:478:GLU:CB[1_545]	1.78	0.42
1:A:465:ASP:OD1	1:G:538:LYS:NZ[2_656]	1.81	0.39
1:C:465:ASP:OD1	1:F:538:LYS:NZ[2_655]	1.82	0.38
1:B:465:ASP:OD1	1:E:538:LYS:NZ[2_546]	1.84	0.36
1:D:465:ASP:OD1	1:H:538:LYS:NZ[2_545]	1.87	0.33
1:B:475:ILE:CD1	1:E:497:TRP:CZ3[2_546]	1.89	0.31
1:D:475:ILE:CD1	1:H:497:TRP:CZ3[2_545]	1.89	0.31
1:C:475:ILE:CD1	1:F:497:TRP:CZ3[2_655]	1.93	0.27
1:B:473:LYS:CE	1:E:494:LYS:CE[2_546]	1.94	0.26
1:A:475:ILE:CD1	1:G:497:TRP:CZ3[2_656]	1.95	0.25
1:C:461:ARG:CD	1:F:538:LYS:CE[2_655]	2.01	0.19
1:A:461:ARG:CD	1:G:538:LYS:CE[2_656]	2.03	0.17
1:B:461:ARG:CD	1:E:538:LYS:CE[2_546]	2.05	0.15
1:D:461:ARG:CD	1:H:538:LYS:CE[2_545]	2.05	0.15
1:D:473:LYS:NZ	1:H:494:LYS:CE[2_545]	2.05	0.15
1:E:478:GLU:CD	1:G:478:GLU:OE1[1_455]	2.05	0.15
1:F:478:GLU:CD	1:H:478:GLU:OE1[1_545]	2.06	0.14
1:D:473:LYS:CE	1:H:494:LYS:CE[2_545]	2.07	0.13
1:E:478:GLU:OE1	1:G:478:GLU:CD[1_455]	2.13	0.07
1:C:461:ARG:CZ	1:F:538:LYS:CE[2_655]	2.16	0.04
1:C:473:LYS:NZ	1:F:494:LYS:CG[2_655]	2.16	0.04
1:F:478:GLU:OE1	1:H:478:GLU:CD[1_545]	2.16	0.04

## 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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	201/218~(92%)	192 (96%)	9 (4%)	0	100	100
1	В	201/218~(92%)	192 (96%)	9 (4%)	0	100	100
1	С	201/218~(92%)	191 (95%)	10 (5%)	0	100	100
1	D	201/218~(92%)	193 (96%)	8 (4%)	0	100	100
1	Ε	201/218~(92%)	193 (96%)	8 (4%)	0	100	100
1	F	201/218~(92%)	193 (96%)	8 (4%)	0	100	100
1	G	201/218~(92%)	193 (96%)	8 (4%)	0	100	100
1	Н	201/218~(92%)	193 (96%)	8 (4%)	0	100	100
All	All	1608/1744~(92%)	1540 (96%)	68 (4%)	0	100	100

analysed, and the total number of residues.

There are no Ramachandran outliers to report.

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	181/191~(95%)	181 (100%)	0	100 100
1	В	181/191~(95%)	181 (100%)	0	100 100
1	С	181/191~(95%)	181 (100%)	0	100 100
1	D	181/191~(95%)	181 (100%)	0	100 100
1	Ε	181/191~(95%)	181 (100%)	0	100 100
1	F	181/191~(95%)	181 (100%)	0	100 100
1	G	181/191~(95%)	181 (100%)	0	100 100
1	Н	181/191~(95%)	181 (100%)	0	100 100
All	All	1448/1528~(95%)	1448 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.



#### 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 oligosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	203/218~(93%)	0.72	21 (10%) 13 10	37, 57, 99, 231	0
1	В	203/218~(93%)	0.52	11 (5%) 32 25	34, 57, 97, 230	0
1	С	203/218~(93%)	0.64	13 (6%) 27 20	36, 58, 98, 231	0
1	D	203/218~(93%)	0.58	13 (6%) 27 20	36, 58, 100, 232	0
1	Е	203/218~(93%)	1.40	47 (23%) 2 3	43, 65, 111, 236	0
1	F	203/218~(93%)	1.38	46 (22%) 3 3	43, 66, 114, 237	0
1	G	203/218~(93%)	1.52	51 (25%) 2 2	42, 68, 113, 238	0
1	Н	203/218~(93%)	1.48	51 (25%) 2 2	45, 69, 114, 239	0
All	All	1624/1744~(93%)	1.03	253 (15%) 6 5	34, 62, 112, 239	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	555	VAL	8.0
1	А	557	THR	7.7
1	F	555	VAL	7.6
1	G	557	THR	7.4
1	D	555	VAL	7.4
1	Е	555	VAL	7.2
1	F	557	THR	6.9
1	Н	555	VAL	6.7
1	В	555	VAL	6.7
1	G	495	TYR	6.7
1	Н	483	ALA	6.6
1	Е	557	THR	6.5
1	С	557	THR	6.4
1	Н	495	TYR	6.4
1	С	555	VAL	6.4
1	G	555	VAL	6.3



Mol	Chain	Res	Type	RSRZ
1	В	557	THR	5.9
1	G	477	VAL	5.8
1	F	495	TYR	5.8
1	G	541	HIS	5.8
1	Е	495	TYR	5.7
1	D	557	THR	5.7
1	Е	556	VAL	5.6
1	Н	557	THR	5.6
1	Н	480	THR	5.5
1	Н	477	VAL	5.5
1	А	556	VAL	5.4
1	G	479	MET	5.3
1	С	558	LEU	5.3
1	Н	540	VAL	5.2
1	Н	556	VAL	5.1
1	Е	497	TRP	5.1
1	А	558	LEU	5.1
1	G	483	ALA	5.1
1	F	556	VAL	5.1
1	Е	482	GLU	5.0
1	F	356	VAL	5.0
1	G	556	VAL	5.0
1	F	494	LYS	4.8
1	G	540	VAL	4.8
1	Е	483	ALA	4.8
1	Н	497	TRP	4.7
1	G	558	LEU	4.6
1	А	450	MET	4.6
1	Е	480	THR	4.6
1	E	477	VAL	4.6
1	H	479	MET	4.6
1	E	486	GLU	4.5
1	C	356	VAL	4.5
1	H	486	GLU	4.5
1	E	479	MET	4.5
1	F	479	MET	4.5
1	F	541	HIS	4.4
1	F	540	VAL	4.4
1	В	558	LEU	4.4
1	G	480	THR	4.4
1	F	477	VAL	4.4
1	G	537	LEU	4.4



Mol	Chain	Res	Type	RSRZ
1	Е	540	VAL	4.3
1	Е	541	HIS	4.3
1	D	558	LEU	4.3
1	F	493	ASP	4.3
1	Е	356	VAL	4.3
1	А	553	PRO	4.3
1	F	497	TRP	4.3
1	F	558	LEU	4.3
1	G	494	LYS	4.2
1	Н	541	HIS	4.2
1	В	356	VAL	4.2
1	G	356	VAL	4.2
1	Е	526	PHE	4.1
1	F	480	THR	4.1
1	Е	494	LYS	4.1
1	Н	494	LYS	4.1
1	Е	558	LEU	4.1
1	В	553	PRO	4.1
1	F	537	LEU	4.1
1	Е	537	LEU	4.0
1	G	497	TRP	4.0
1	Н	356	VAL	4.0
1	Н	537	LEU	4.0
1	G	517	HIS	3.9
1	С	556	VAL	3.9
1	Н	482	GLU	3.9
1	F	386	ARG	3.9
1	С	553	PRO	3.9
1	G	493	ASP	3.8
1	D	553	PRO	3.8
1	F	553	PRO	3.8
1	F	526	PHE	3.8
1	F	482	GLU	3.7
1	А	356	VAL	3.7
1	F	413	GLN	3.7
1	Н	558	LEU	3.6
1	F	478	GLU	3.6
1	С	450	MET	3.6
1	Е	517	HIS	3.6
1	G	478	GLU	3.5
1	F	483	ALA	3.5
1	Е	413	GLN	3.5



Mol	Chain	Res	Type	RSRZ
1	Е	478	GLU	3.5
1	Н	484	SER	3.5
1	В	556	VAL	3.4
1	Е	493	ASP	3.4
1	Е	386	ARG	3.4
1	D	356	VAL	3.4
1	F	475	ILE	3.4
1	Н	493	ASP	3.4
1	Н	553	PRO	3.4
1	Н	459	ASP	3.3
1	D	556	VAL	3.3
1	Е	553	PRO	3.3
1	G	386	ARG	3.3
1	Е	534	LEU	3.2
1	D	554	ASN	3.2
1	Н	386	ARG	3.2
1	G	415	GLN	3.2
1	D	514	ILE	3.1
1	Е	552	GLY	3.1
1	В	386	ARG	3.1
1	G	457	SER	3.1
1	Н	357	GLY	3.1
1	С	386	ARG	3.1
1	Н	478	GLU	3.1
1	G	531	LYS	3.1
1	С	536	ASP	3.1
1	Н	503	THR	3.0
1	F	486	GLU	3.0
1	G	459	ASP	3.0
1	Н	426	MET	3.0
1	G	484	SER	3.0
1	Н	415	GLN	2.9
1	Н	554	ASN	2.9
1	Н	399	GLN	2.9
1	А	386	ARG	2.9
1	G	486	GLU	2.9
1	E	509	LYS	2.8
1	G	399	GLN	2.8
1	E	414	LYS	2.8
1	G	526	PHE	2.8
1	F	517	HIS	2.8
1	F	534	LEU	2.8



Mol	Chain	Res	Type	RSRZ
1	Е	399	GLN	2.8
1	G	482	82 GLU 2	
1	G	503	3 THR 2	
1	Н	552	GLY	2.8
1	Н	466	SER	2.7
1	Е	459	ASP	2.7
1	А	514	ILE	2.7
1	Е	530	SER	2.7
1	С	513	GLU	2.7
1	G	475	ILE	2.7
1	F	552	GLY	2.7
1	D	386	ARG	2.7
1	G	554	ASN	2.7
1	Н	400	ASN	2.7
1	F	415	GLN	2.7
1	Н	422	TYR	2.7
1	G	498	LEU	2.7
1	F	503	THR	2.7
1	Н	546	HIS	2.7
1	G	552	GLY	2.7
1	F	399	GLN	2.6
1	Н	387	PHE	2.6
1	D	450	MET	2.6
1	А	552	GLY	2.6
1	G	387	PHE	2.6
1	Н	360	TYR	2.6
1	А	399	GLN	2.5
1	Е	417	LYS	2.5
1	F	509	LYS	2.5
1	А	387	PHE	2.5
1	С	399	GLN	2.5
1	Н	498	LEU	2.5
1	Н	539	THR	2.5
1	G	360	TYR	2.5
1	Е	415	GLN	2.5
1	Н	517	HIS	2.5
1	F	357	GLY	2.5
1	G	534	LEU	2.5
1	Е	357	GLY	2.5
1	G	533	ARG	2.4
1	В	358	LEU	2.4
1	Е	400	ASN	2.4



Mol	Chain	Res	Type	RSRZ
1	Н	532	ALA	2.4
1	Е	503	503 THR 2.	
1	G	553	PRO	2.4
1	Н	450	MET	2.4
1	А	468	ASN	2.4
1	А	554	ASN	2.4
1	Е	554	ASN	2.4
1	Е	539	THR	2.4
1	В	514	ILE	2.4
1	Е	484	SER	2.3
1	С	515	THR	2.3
1	F	455	GLN	2.3
1	Н	457	SER	2.3
1	F	532	ALA	2.3
1	Н	526	PHE	2.3
1	Е	358	LEU	2.3
1	F	450	MET	2.3
1	Н	487	TYR	2.3
1	G	492	TRP	2.3
1	D	358	LEU	2.3
1	F	539	THR	2.3
1	F	400	ASN	2.3
1	Е	487	TYR	2.3
1	F	466	SER	2.3
1	F	484	SER	2.3
1	G	500	LYS	2.3
1	В	513	GLU	2.2
1	Н	536	ASP	2.2
1	F	417	LYS	2.2
1	F	487	TYR	2.2
1	E	481	ARG	2.2
1	H	481	ARG	2.2
1	A	485	ARG	2.2
1	Е	485	ARG	2.2
1	G	422	TYR	2.2
1	A	429	ALA	2.2
1	E	532	ALA	2.2
1	A	414	LYS	2.2
1	D	513	GLU	2.2
1	A	413	GLN	2.1
1	A	503	THR	2.1
1	Н	417	LYS	2.1



Mol	Chain	Res	Type	RSRZ
1	А	551 ARG		2.1
1	F	459	ASP	2.1
1	G	458	ASP	2.1
1	G	521	MET	2.1
1	С	485	ARG	2.1
1	F	432	PHE	2.1
1	G	538	LYS	2.1
1	Н	427	ASP	2.1
1	G	402	GLN	2.1
1	Н	534	LEU	2.1
1	F	360	TYR	2.1
1	Н	506	VAL	2.1
1	F	481	ARG	2.1
1	G	481	ARG	2.1
1	В	552	GLY	2.1
1	А	512	LYS	2.1
1	Е	455	GLN	2.0
1	G	539	THR	2.0
1	Е	514	ILE	2.0
1	Е	516	PRO	2.0
1	F	554	ASN	2.0
1	G	426	MET	2.0
1	G	450	MET	2.0
1	G	507	ARG	2.0
1	D	552	GLY	2.0
1	Н	521	MET	2.0
1	G	431	LEU	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 monosaccharides 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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
2	ZN	F	900	1/1	0.95	0.06	$57,\!57,\!57,\!57$	0
2	ZN	G	900	1/1	0.95	0.10	79,79,79,79	0
2	ZN	D	900	1/1	0.96	0.05	49,49,49,49	0
2	ZN	Н	900	1/1	0.96	0.09	75,75,75,75	0
2	ZN	В	900	1/1	0.97	0.05	$55,\!55,\!55,\!55$	0
2	ZN	Е	900	1/1	0.98	0.06	56, 56, 56, 56	0
2	ZN	А	900	1/1	0.98	0.03	48,48,48,48	0
2	ZN	С	900	1/1	0.99	0.02	42,42,42,42	0

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.

## 6.5 Other polymers (i)

There are no such residues in this entry.

