

Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 07:35 AM EDT

2GA6
The crystal structure of SARS nsp10 without zinc ion as additive
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2006-03-08
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	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m A}))$
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		
1	А	152	52%	23%	••	22%
1	В	152	2% 5 3%	21%		22%
1	С	152	47%	29%	••	22%
1	D	152	51%	23%	••	22%
1	Е	152	2% 5 1%	26%	•	22%



Mol	Chain	Length	Quality of chain					
1	F	152	45%	31%	••	21%		
1	G	152	2% 	28%	••	22%		
1	Н	152	51%	22%	••	22%		
1	Ι	152	49%	24%	••	22%		
1	J	152	3% 51%	24%	•	22%		
1	K	152	47%	29%	••	22%		
1	L	152	.% 5 6%	19%	••	22%		
1	М	152	3% 57%	15%	5%•	22%		
1	Ν	152	2% 	26%		22%		
1	Ο	152	3% 52%	22%	••	22%		
1	Р	152	2% 5 1%	24%	•	22%		
1	Q	152	5% 45%	28%	••	22%		
1	R	152	2% 46%	27%	••	23%		
1	S	152	45%	29%	•	22%		
1	Т	152	<u>6%</u> 50%	24%	••	22%		
1	U	152	% 5 5%	19%	••	22%		
1	V	152	% 51%	22%	••	22%		
1	W	152	49%	26%	•	22%		
1	X	152	3% 52%	22%	••	22%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21977 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	А	118	Total 873	C 544	N 147	0 167	S 15	0	0	0
1	В	119	Total 880	C 549	N 148	0 168	S 15	0	0	0
1	С	118	Total 873	С 544	N 147	0 167	S 15	0	0	0
1	D	118	Total 873	С 544	N 147	0 167	S 15	0	0	0
1	Е	118	Total 873	C 544	N 147	O 167	S 15	0	0	0
1	F	120	Total 883	C 551	N 148	O 169	S 15	0	0	0
1	G	118	Total 873	C 544	N 147	O 167	S 15	0	0	0
1	Н	118	Total 873	C 544	N 147	O 167	S 15	0	0	0
1	Ι	118	Total 873	C 544	N 147	O 167	S 15	0	0	0
1	J	118	Total 873	C 544	N 147	O 167	S 15	0	0	0
1	K	118	Total 873	С 544	N 147	0 167	S 15	0	0	0
1	L	118	Total 873	C 544	N 147	O 167	S 15	0	0	0
1	М	118	Total 873	C 544	N 147	O 167	S 15	0	0	0
1	Ν	119	Total 880	$\begin{array}{c} \mathrm{C} \\ 549 \end{array}$	N 148	O 168	$\begin{array}{c} \mathrm{S} \\ 15 \end{array}$	0	0	0
1	Ο	118	Total 873	С 544	N 147	0 167	S 15	0	0	0
1	Р	118	Total 873	C 544	N 147	0 167	S 15	0	0	0

• Molecule 1 is a protein called orf1a polyprotein.



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2	J.	Π	U

Mol	Chain	Residues	_	A	toms			ZeroOcc	AltConf	Trace
1	0	110	Total	С	Ν	0	S	0	0	0
	Q	110	873	544	147	167	15	0	0	0
1	В	117	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	п	111	863	538	144	166	15	0	0	0
1	q	118	Total	С	Ν	Ο	\mathbf{S}	0	0	0
T	a	110	873	544	147	167	15	0	0	0
1	т	118	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	L	110	873	544	147	167	15	0	0	0
1	II	118	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	U	0 110	873	544	147	167	15	0	0	0
1	V	118	Total	С	Ν	Ο	S	0	0	0
1	v	110	873	544	147	167	15	0	0	0
1	W	118	Total	С	Ν	Ο	S	0	0	0
1		110	873	544	147	167	15	0	0	0
1	v	118	Total	С	N	0	S	0	0	0
		110	873	544	147	167	15	0 0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0
2	В	2	Total Zn 2 2	0	0
2	С	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	Е	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	Н	2	Total Zn 2 2	0	0
2	Ι	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	К	2	Total Zn 2 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	2	Total Zn 2 2	0	0
2	М	2	Total Zn 2 2	0	0
2	Ν	2	Total Zn 2 2	0	0
2	О	2	Total Zn 2 2	0	0
2	Р	2	Total Zn 2 2	0	0
2	Q	2	Total Zn 2 2	0	0
2	R	2	Total Zn 2 2	0	0
2	S	2	Total Zn 2 2	0	0
2	Т	2	Total Zn 2 2	0	0
2	U	2	Total Zn 2 2	0	0
2	V	2	Total Zn 2 2	0	0
2	W	2	Total Zn 2 2	0	0
2	Х	2	$\begin{array}{ccc} \text{Total} & \overline{\text{Zn}} \\ 2 & 2 \end{array}$	0	0

Continued from previous page...

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	46	Total O 46 46	0	0
3	В	37	Total O 37 37	0	0
3	С	43	Total O 43 43	0	0
3	D	29	Total O 29 29	0	0
3	Ε	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0
3	F	44	Total O 44 44	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	48	Total O 48 48	0	0
3	Н	43	Total O 43 43	0	0
3	Ι	37	$\begin{array}{cc} \text{Total} & \text{O} \\ 37 & 37 \end{array}$	0	0
3	J	30	Total O 30 30	0	0
3	К	40	Total O 40 40	0	0
3	L	48	Total O 48 48	0	0
3	М	56	Total O 56 56	0	0
3	Ν	31	Total O 31 31	0	0
3	О	53	Total O 53 53	0	0
3	Р	51	Total O 51 51	0	0
3	Q	34	Total O 34 34	0	0
3	R	39	Total O 39 39	0	0
3	S	34	Total O 34 34	0	0
3	Т	33	Total O 33 33	0	0
3	U	26	Total O 26 26	0	0
3	V	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0
3	W	37	$\begin{array}{ccc} \text{Total} & \text{O} \\ 37 & 37 \end{array}$	0	0
3	Х	35	Total O 35 35	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: orf1a polyprotein















 \bullet Molecule 1: orf1a polyprotein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	159.74Å 322.70Å 162.15Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	50.00 - 2.70	Depositor
	45.78 - 2.70	EDS
% Data completeness	(Not available) $(50.00-2.70)$	Depositor
(in resolution range)	98.6 (45.78-2.70)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.52 (at 2.69 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
R R.	0.219 , 0.267	Depositor
II, II, <i>free</i>	0.225 , 0.271	DCC
R_{free} test set	10955 reflections $(4.92%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	34.7	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 55.0	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21977	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 21.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3121e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: 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).

Mol Chain		Bond lengths		Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.40	0/892	0.70	2/1211~(0.2%)	
1	В	0.44	0/900	0.80	4/1222~(0.3%)	
1	С	0.41	0/892	0.70	1/1211~(0.1%)	
1	D	0.41	0/892	0.71	2/1211~(0.2%)	
1	Е	0.43	0/892	0.68	1/1211~(0.1%)	
1	F	0.42	0/902	0.71	3/1224~(0.2%)	
1	G	0.44	0/892	0.73	2/1211~(0.2%)	
1	Н	0.41	0/892	0.71	2/1211~(0.2%)	
1	Ι	0.43	0/892	0.71	2/1211~(0.2%)	
1	J	0.41	0/892	0.67	1/1211~(0.1%)	
1	Κ	0.44	0/892	0.70	2/1211~(0.2%)	
1	L	0.43	0/892	0.74	3/1211~(0.2%)	
1	М	0.44	0/892	0.70	1/1211~(0.1%)	
1	Ν	0.40	0/900	0.78	3/1222~(0.2%)	
1	0	0.42	0/892	0.79	3/1211~(0.2%)	
1	Р	0.45	0/892	0.69	2/1211~(0.2%)	
1	Q	0.38	0/892	0.66	1/1211~(0.1%)	
1	R	0.43	0/880	0.69	1/1193~(0.1%)	
1	S	0.43	0/892	0.65	0/1211	
1	Т	0.42	0/892	0.69	2/1211~(0.2%)	
1	U	0.41	0/892	0.64	1/1211~(0.1%)	
1	V	0.43	0/892	0.71	2/1211~(0.2%)	
1	W	0.40	0/892	0.63	0/1211	
1	Х	0.42	0/892	0.68	1/1211~(0.1%)	
All	All	0.42	0/21422	0.70	42/29081~(0.1%)	

There are no bond length outliers.

All (42) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	L	90	CYS	CA-CB-SG	9.60	131.27	114.00
1	В	117	CYS	CA-CB-SG	9.40	130.92	114.00
1	В	90	CYS	CA-CB-SG	9.18	130.52	114.00
1	Ν	117	CYS	CA-CB-SG	8.84	129.91	114.00
1	G	90	CYS	CA-CB-SG	8.66	129.59	114.00
1	0	117	CYS	CA-CB-SG	8.27	128.88	114.00
1	D	90	CYS	CA-CB-SG	8.25	128.84	114.00
1	K	90	CYS	CA-CB-SG	8.08	128.55	114.00
1	R	90	CYS	CA-CB-SG	7.96	128.33	114.00
1	0	90	CYS	CA-CB-SG	7.78	128.00	114.00
1	Ν	90	CYS	CA-CB-SG	7.75	127.94	114.00
1	Ι	90	CYS	CA-CB-SG	6.48	125.66	114.00
1	D	74	CYS	CA-CB-SG	6.45	125.62	114.00
1	Р	90	CYS	CA-CB-SG	6.33	125.39	114.00
1	М	74	CYS	CA-CB-SG	6.18	125.12	114.00
1	С	74	CYS	CA-CB-SG	6.12	125.01	114.00
1	0	120	CYS	CA-CB-SG	6.07	124.92	114.00
1	Κ	74	CYS	CA-CB-SG	6.03	124.85	114.00
1	Т	90	CYS	CA-CB-SG	5.91	124.64	114.00
1	В	74	CYS	CA-CB-SG	5.89	124.60	114.00
1	U	74	CYS	CA-CB-SG	5.83	124.49	114.00
1	А	90	CYS	CA-CB-SG	5.83	124.48	114.00
1	F	74	CYS	CA-CB-SG	5.75	124.35	114.00
1	L	74	CYS	CA-CB-SG	5.67	124.21	114.00
1	Q	74	CYS	CA-CB-SG	5.59	124.07	114.00
1	Ι	74	CYS	CA-CB-SG	5.57	124.03	114.00
1	L	77	CYS	CA-CB-SG	-5.57	103.97	114.00
1	Ν	128	CYS	CA-CB-SG	5.57	124.02	114.00
1	V	90	CYS	CA-CB-SG	5.51	123.92	114.00
1	G	74	CYS	CA-CB-SG	5.35	123.63	114.00
1	Е	74	CYS	CA-CB-SG	5.33	123.60	114.00
1	А	74	CYS	CA-CB-SG	5.32	123.57	114.00
1	Н	74	CYS	CA-CB-SG	5.28	123.50	114.00
1	Н	90	CYS	CA-CB-SG	5.21	123.38	114.00
1	Р	74	CYS	CA-CB-SG	5.14	123.25	114.00
1	V	74	CYS	CA-CB-SG	5.14	123.25	114.00
1	Т	74	CYS	CA-CB-SG	5.10	123.18	114.00
1	В	120	CYS	CA-CB-SG	5.07	123.13	114.00
1	F	90	CYS	CA-CB-SG	5.06	123.11	114.00
1	J	74	CYS	CA-CB-SG	5.05	123.09	114.00
1	F	88	GLY	N-CA-C	5.05	125.72	113.10



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	74	CYS	CA-CB-SG	5.02	123.04	114.00

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	873	0	829	34	0
1	В	880	0	837	36	0
1	С	873	0	829	41	0
1	D	873	0	829	41	0
1	Е	873	0	829	37	0
1	F	883	0	845	40	0
1	G	873	0	829	40	0
1	Н	873	0	830	38	0
1	Ι	873	0	829	42	0
1	J	873	0	829	35	0
1	K	873	0	830	36	0
1	L	873	0	829	28	0
1	М	873	0	829	46	0
1	N	880	0	837	42	0
1	0	873	0	829	33	0
1	Р	873	0	829	33	0
1	Q	873	0	829	49	0
1	R	863	0	821	43	0
1	S	873	0	830	42	0
1	Т	873	0	829	42	0
1	U	873	0	829	38	0
1	V	873	0	829	38	0
1	W	873	0	829	36	0
1	Х	873	0	830	35	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0



	Choin	Non H	page	H(addad)	Clashog	Symm Clashes
	E				Clashes	Symm-Clasnes
	E	2	0	0	0	0
	F C	2	0	0	0	0
	G	2	0	0	0	0
	П	2	0	0	0	0
	I T	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2		2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	0	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	Т	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	Х	2	0	0	0	0
3	А	46	0	0	8	0
3	В	37	0	0	4	0
3	С	43	0	0	1	0
3	D	29	0	0	0	0
3	Е	42	0	0	3	0
3	F	44	0	0	6	0
3	G	48	0	0	6	0
3	Н	43	0	0	7	0
3	Ι	37	0	0	3	0
3	J	30	0	0	4	0
3	K	40	0	0	1	0
3	L	48	0	0	6	0
3	М	56	0	0	10	0
3	Ν	31	0	0	8	0
3	0	53	0	0	1	0
3	Р	51	0	0	3	0
3	Q	34	0	0	1	0
3	R	39	0	0	4	0
3	S	34	0	0	3	0
3	Т	33	0	0	4	0
3	U	26	0	0	7	0
3	V	47	0	0	6	0
		·	~			



	j	I I I I I I I I I I I I I I I I I I I	F 9			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	37	0	0	4	0
3	Х	35	0	0	2	0
All	All	21977	0	19924	882	0

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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 22.

All (882) 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:N:90:CYS:HB3	1:N:93:LYS:H	1.21	1.04
1:G:90:CYS:HB3	1:G:93:LYS:H	1.21	1.03
1:M:105:ASN:HD22	1:M:105:ASN:H	1.03	1.02
1:D:90:CYS:HB3	1:D:93:LYS:H	1.18	1.02
1:J:45:LEU:HD21	1:M:48:HIS:HB2	1.41	1.01
1:P:105:ASN:HD22	1:P:105:ASN:H	1.14	0.95
1:S:105:ASN:HD22	1:S:105:ASN:H	1.15	0.94
1:B:90:CYS:HB3	1:B:93:LYS:H	1.34	0.92
1:K:90:CYS:HB3	1:K:93:LYS:H	1.34	0.91
1:S:84:PRO:HG2	1:S:85:ASN:H	1.38	0.89
1:S:47:THR:HG23	1:S:48:HIS:H	1.38	0.88
1:O:90:CYS:HB3	1:O:93:LYS:H	1.38	0.88
1:C:90:CYS:C	1:C:92:LEU:H	1.78	0.86
1:0:120:CYS:SG	1:0:128:CYS:HA	2.14	0.86
1:D:117:CYS:HB3	1:D:120:CYS:SG	2.16	0.85
1:L:90:CYS:HB3	1:L:93:LYS:HB2	1.59	0.85
1:S:90:CYS:SG	1:S:93:LYS:HB2	2.16	0.85
1:S:74:CYS:HB2	1:S:92:LEU:HD12	1.56	0.85
1:M:46:CYS:SG	1:M:48:HIS:HD2	1.99	0.84
1:D:74:CYS:HB2	1:D:92:LEU:HD12	1.59	0.84
1:T:43:LYS:HE3	1:T:66:GLU:HB3	1.60	0.84
1:B:90:CYS:HB2	1:B:93:LYS:HB2	1.58	0.84
1:G:90:CYS:C	1:G:92:LEU:H	1.81	0.84
1:Q:62:ASN:ND2	1:Q:63:MET:H	1.75	0.84
1:B:57:VAL:HG23	1:B:58:THR:HG23	1.58	0.83
1:H:90:CYS:C	1:H:92:LEU:H	1.82	0.83
1:M:105:ASN:HD22	1:M:105:ASN:N	1.76	0.83
1:I:90:CYS:HB3	1:I:93:LYS:HB2	1.63	0.81
1:B:120:CYS:SG	1:B:128:CYS:HA	2.21	0.81
1:V:90:CYS:C	1:V:92:LEU:H	1.83	0.81
1:H:105:ASN:H	1:H:105:ASN:HD22	1.26	0.80



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:117:CYS:HB2	1:D:124:LYS:HD2	1.63	0.80
1:H:74:CYS:HB2	1:H:92:LEU:HD12	1.62	0.79
1:X:105:ASN:HD22	1:X:105:ASN:H	1.28	0.79
1:N:90:CYS:HB2	1:N:93:LYS:HB2	1.65	0.79
1:R:105:ASN:HD22	1:R:105:ASN:H	1.27	0.79
1:G:90:CYS:HB2	1:G:93:LYS:HB2	1.65	0.79
1:L:57:VAL:HG23	1:L:58:THR:HG23	1.65	0.79
1:M:49:THR:HA	3:M:1010:HOH:O	1.82	0.78
1:P:44:MET:HE2	1:P:96:TYR:HE2	1.47	0.78
1:G:84:PRO:HG2	1:G:85:ASN:H	1.48	0.78
1:B:89:PHE:N	1:F:87:LYS:HE2	1.99	0.77
1:I:101:THR:O	1:M:101:THR:HG22	1.84	0.77
1:G:90:CYS:HB3	1:G:93:LYS:N	1.99	0.77
1:I:51:THR:HG23	1:I:60:GLU:OE1	1.87	0.74
1:A:90:CYS:C	1:A:92:LEU:H	1.89	0.74
1:I:74:CYS:HB2	1:I:92:LEU:HD12	1.70	0.74
1:J:84:PRO:HG2	1:J:85:ASN:H	1.51	0.74
1:N:90:CYS:C	1:N:92:LEU:H	1.90	0.74
1:G:90:CYS:CB	1:G:93:LYS:HB2	2.18	0.74
1:H:84:PRO:HG2	1:H:85:ASN:H	1.52	0.73
1:D:90:CYS:HB2	1:D:93:LYS:HB2	1.70	0.73
1:N:74:CYS:HB2	1:N:92:LEU:HD12	1.71	0.73
1:P:57:VAL:HG23	1:P:58:THR:HG23	1.69	0.73
1:T:49:THR:OG1	1:T:63:MET:HE1	1.87	0.73
1:X:39:THR:O	1:X:78:ARG:NH2	2.21	0.73
1:E:113:ARG:HH11	1:E:113:ARG:HB2	1.54	0.73
1:F:97:VAL:HB	3:F:1020:HOH:O	1.87	0.72
1:I:90:CYS:C	1:I:92:LEU:H	1.93	0.72
1:F:68:PHE:HB2	3:F:1020:HOH:O	1.88	0.72
1:D:84:PRO:HG2	1:D:85:ASN:H	1.56	0.71
1:L:74:CYS:HB2	1:L:92:LEU:HD12	1.73	0.70
1:N:90:CYS:HB3	1:N:93:LYS:N	2.02	0.70
1:S:105:ASN:HD22	1:S:105:ASN:N	1.88	0.70
1:L:76:TYR:HB2	1:L:83:HIS:CD2	2.26	0.70
1:T:90:CYS:C	1:T:92:LEU:H	1.92	0.70
1:Q:62:ASN:HB3	1:Q:65:GLN:HG3	1.72	0.70
1:J:46:CYS:O	1:M:49:THR:HG21	1.91	0.70
1:T:47:THR:O	1:T:48:HIS:HB2	1.91	0.70
1:X:41:CYS:HA	1:X:72:SER:HB3	1.72	0.70
1:D:90:CYS:HB3	1:D:93:LYS:N	2.01	0.70
1:Q:57:VAL:HG23	1:Q:58:THR:HG23	1.73	0.69



	A L	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:T:41:CYS:HA	1:T:72:SER:OG	1.92	0.69
1:Q:45:LEU:HD13	1:R:45:LEU:HD13	1.72	0.69
1:T:39:THR:O	1:T:40:ASN:HB2	1.93	0.69
1:F:57:VAL:HG23	1:F:58:THR:HG23	1.73	0.69
1:R:92:LEU:HD22	1:R:97:VAL:HG22	1.75	0.69
1:W:113:ARG:HH11	1:W:113:ARG:HB2	1.57	0.69
1:K:113:ARG:HH11	1:K:113:ARG:HB2	1.57	0.68
1:H:90:CYS:HB3	1:H:93:LYS:HB2	1.74	0.68
1:H:117:CYS:HA	1:H:124:LYS:HE2	1.76	0.68
1:N:39:THR:O	1:N:40:ASN:HB2	1.93	0.68
1:V:76:TYR:HB2	1:V:83:HIS:CD2	2.28	0.68
1:W:51:THR:OG1	1:W:53:GLN:HG3	1.93	0.68
1:P:44:MET:HE2	1:P:96:TYR:CE2	2.29	0.68
1:Q:98:GLN:NE2	1:Q:98:GLN:N	2.42	0.67
1:A:108:VAL:HB	3:A:1030:HOH:O	1.94	0.67
1:E:83:HIS:ND1	1:E:83:HIS:N	2.42	0.67
1:U:9:ALA:O	1:U:13:VAL:HG23	1.95	0.67
1:J:45:LEU:HD11	1:M:48:HIS:N	2.09	0.67
1:U:83:HIS:HD2	1:U:89:PHE:HA	1.59	0.67
1:W:57:VAL:HG23	1:W:58:THR:HG23	1.75	0.67
1:O:47:THR:HG23	1:O:49:THR:H	1.58	0.67
1:P:83:HIS:CD2	1:P:90:CYS:N	2.63	0.67
1:Q:98:GLN:N	1:Q:98:GLN:HE21	1.92	0.67
1:B:74:CYS:HB2	1:B:92:LEU:HD12	1.77	0.66
1:I:89:PHE:O	1:I:90:CYS:C	2.34	0.66
1:M:105:ASN:H	1:M:105:ASN:ND2	1.82	0.66
1:V:74:CYS:HB2	1:V:92:LEU:HD12	1.76	0.66
1:U:41:CYS:HA	1:U:72:SER:HB2	1.76	0.66
1:E:42:VAL:HG22	1:E:72:SER:OG	1.95	0.66
1:Q:51:THR:OG1	1:Q:53:GLN:HG2	1.94	0.66
1:Q:70:GLY:HA3	1:Q:92:LEU:O	1.96	0.66
1:D:41:CYS:HA	1:D:72:SER:HB3	1.77	0.66
1:I:105:ASN:HD22	1:I:105:ASN:H	1.45	0.65
1:F:85:ASN:ND2	1:F:90:CYS:HA	2.11	0.65
1:B:113:ARG:HH11	1:B:113:ARG:HB2	1.60	0.65
1:U:39:THR:O	1:U:40:ASN:HB2	1.96	0.65
1:H:89:PHE:O	1:H:90:CYS:C	2.34	0.65
1:N:90:CYS:CB	1:N:93:LYS:HB2	2.27	0.65
1:I:89:PHE:O	1:I:91:ASP:N	2.31	0.64
1:X:83:HIS:N	1:X:83:HIS:CD2	2.65	0.64
1:D:92:LEU:HD22	1:D:97:VAL:CG2	2.27	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:90:CYS:O	1:F:92:LEU:N	2.25	0.64
1:B:90:CYS:C	1:B:92:LEU:H	2.00	0.64
1:S:56:THR:HG21	1:S:60:GLU:HG3	1.78	0.64
1:G:57:VAL:HG23	1:G:58:THR:HG23	1.79	0.64
1:A:107:PRO:HB2	3:A:1016:HOH:O	1.97	0.64
1:Q:53:GLN:HB2	1:Q:56:THR:CG2	2.28	0.64
1:L:84:PRO:HG2	1:L:85:ASN:H	1.63	0.63
1:S:68:PHE:HB3	3:S:1015:HOH:O	1.97	0.63
1:E:41:CYS:HA	1:E:72:SER:HB3	1.79	0.63
1:C:90:CYS:C	1:C:92:LEU:N	2.44	0.63
1:F:92:LEU:HD22	1:F:97:VAL:HG21	1.80	0.63
1:G:74:CYS:HB2	1:G:92:LEU:HD12	1.79	0.63
1:J:109:GLY:HA3	3:J:1015:HOH:O	1.99	0.63
1:X:65:GLN:HG2	3:X:1018:HOH:O	1.97	0.63
1:B:90:CYS:HB3	1:B:93:LYS:N	2.11	0.63
1:N:57:VAL:HG23	1:N:58:THR:HG23	1.81	0.63
1:0:74:CYS:HB2	1:O:92:LEU:HD12	1.79	0.63
1:N:14:LEU:HD13	3:N:1022:HOH:O	1.98	0.63
1:O:90:CYS:C	1:O:92:LEU:H	2.00	0.63
1:S:45:LEU:HD13	1:T:45:LEU:HD13	1.78	0.63
1:T:90:CYS:C	1:T:92:LEU:N	2.51	0.63
1:E:92:LEU:O	1:E:95:LYS:HB2	1.99	0.63
1:D:48:HIS:HA	1:D:61:ALA:O	1.98	0.63
1:O:89:PHE:O	1:O:90:CYS:C	2.37	0.63
1:Q:40:ASN:HB3	1:X:21:VAL:HG11	1.79	0.63
1:U:90:CYS:C	1:U:92:LEU:H	2.01	0.63
1:T:69:GLY:O	1:T:72:SER:HB3	1.98	0.63
1:U:66:GLU:OE2	1:U:101:THR:HG23	1.99	0.63
1:D:106:ASP:OD2	1:D:113:ARG:NH2	2.31	0.62
1:L:113:ARG:HH11	1:L:113:ARG:HB2	1.64	0.62
1:T:90:CYS:HB3	1:T:93:LYS:H	1.63	0.62
1:X:62:ASN:OD1	1:X:65:GLN:HG3	1.99	0.62
1:V:90:CYS:C	1:V:92:LEU:N	2.52	0.62
1:I:41:CYS:HA	1:I:72:SER:HB3	1.81	0.62
1:X:117:CYS:HB3	1:X:124:LYS:CD	2.29	0.62
1:H:9:ALA:HB3	3:H:1015:HOH:O	1.99	0.62
1:J:45:LEU:HD11	1:M:47:THR:C	2.18	0.62
1:W:76:TYR:HB2	1:W:83:HIS:HD2	1.63	0.62
1:X:42:VAL:HG22	1:X:72:SER:OG	1.99	0.62
1:Q:98:GLN:HE21	1:Q:98:GLN:H	1.47	0.62
1:M:108:VAL:HA	3:M:1035:HOH:O	1.99	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:K:90:CYS:C	1:K:92:LEU:H	2.03	0.62
1:N:10:ASN:ND2	1:N:40:ASN:HD22	1.98	0.62
1:D:117:CYS:CB	1:D:120:CYS:SG	2.81	0.62
1:F:68:PHE:HB3	3:F:1027:HOH:O	2.00	0.62
1:E:50:GLY:HA3	1:E:60:GLU:HA	1.81	0.62
1:I:90:CYS:CB	1:I:93:LYS:HB2	2.28	0.62
1:I:90:CYS:C	1:I:92:LEU:N	2.54	0.61
1:X:39:THR:O	1:X:40:ASN:HB2	2.00	0.61
1:V:28:LYS:HG2	3:V:1022:HOH:O	1.99	0.61
1:W:98:GLN:NE2	1:W:98:GLN:N	2.47	0.61
1:E:51:THR:OG1	1:E:53:GLN:HG2	2.00	0.61
1:K:9:ALA:O	1:K:13:VAL:HG23	2.00	0.61
1:R:70:GLY:HA2	1:R:97:VAL:HG23	1.82	0.61
1:D:90:CYS:CB	1:D:93:LYS:HB2	2.28	0.61
1:S:84:PRO:HG2	1:S:85:ASN:N	2.14	0.61
1:A:38:ILE:HG12	3:A:1020:HOH:O	2.00	0.61
1:A:73:CYS:HA	3:A:1016:HOH:O	2.01	0.61
1:I:90:CYS:HB3	1:I:93:LYS:CB	2.30	0.61
1:V:39:THR:O	1:V:78:ARG:NH2	2.33	0.61
1:M:89:PHE:O	1:M:90:CYS:C	2.39	0.61
1:C:39:THR:O	1:C:40:ASN:HB2	2.00	0.61
1:L:44:MET:SD	3:L:1006:HOH:O	2.55	0.61
1:N:90:CYS:C	1:N:92:LEU:N	2.53	0.61
1:J:79:CYS:O	1:J:80:HIS:HB2	2.01	0.60
1:H:90:CYS:HB3	1:H:93:LYS:CB	2.31	0.60
1:U:39:THR:O	1:U:78:ARG:NH2	2.33	0.60
1:K:117:CYS:HB3	1:K:120:CYS:HB3	1.81	0.60
1:C:48:HIS:O	1:C:63:MET:HE2	2.01	0.60
1:G:9:ALA:O	1:G:13:VAL:HG23	2.01	0.60
1:D:90:CYS:C	1:D:92:LEU:H	2.05	0.59
1:G:14:LEU:HD21	1:G:38:ILE:HD13	1.84	0.59
1:H:90:CYS:C	1:H:92:LEU:N	2.50	0.59
1:L:68:PHE:HA	3:L:1006:HOH:O	2.02	0.59
1:W:99:ILE:HD13	1:W:107:PRO:HA	1.84	0.59
1:P:83:HIS:HD2	1:P:90:CYS:N	2.00	0.59
1:K:89:PHE:O	1:K:90:CYS:C	2.40	0.59
1:P:105:ASN:H	1:P:105:ASN:ND2	1.95	0.59
1:Q:69:GLY:O	1:Q:72:SER:HB2	2.02	0.59
1:U:106:ASP:OD2	1:U:109:GLY:HA3	2.02	0.59
1:G:43:LYS:HE2	1:G:66:GLU:OE1	2.01	0.59
1:V:51:THR:HG23	1:V:60:GLU:OE1	2.02	0.59



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:X:117:CYS:HB3	1:X:124:LYS:HD2	1.84	0.59
1:F:41:CYS:HA	1:F:72:SER:HB3	1.83	0.59
1:W:76:TYR:CB	1:W:83:HIS:HD2	2.15	0.59
1:E:38:ILE:HD12	1:E:108:VAL:HG11	1.83	0.59
1:G:52:GLY:HA2	1:G:65:GLN:OE1	2.02	0.59
1:Q:62:ASN:HB2	1:Q:65:GLN:OE1	2.03	0.59
1:C:44:MET:CE	1:D:42:VAL:HG12	2.33	0.58
1:Q:45:LEU:HB2	1:R:45:LEU:HB2	1.85	0.58
1:D:106:ASP:N	1:D:107:PRO:HD3	2.18	0.58
1:N:8:PRO:HG2	1:T:20:ALA:HA	1.85	0.58
1:C:53:GLN:HA	1:C:122:MET:HG2	1.84	0.58
1:C:70:GLY:HA2	1:C:97:VAL:HG23	1.85	0.58
1:K:90:CYS:HB3	1:K:93:LYS:N	2.12	0.58
1:C:96:TYR:OH	1:D:42:VAL:HG21	2.03	0.58
1:G:90:CYS:C	1:G:92:LEU:N	2.50	0.58
1:I:51:THR:OG1	1:I:53:GLN:HG2	2.03	0.58
1:R:39:THR:O	1:R:40:ASN:HB2	2.04	0.58
1:M:84:PRO:HG2	1:M:85:ASN:H	1.67	0.58
1:R:51:THR:HG23	1:R:60:GLU:OE1	2.04	0.58
1:F:92:LEU:HD22	1:F:97:VAL:CG2	2.33	0.58
1:W:98:GLN:H	1:W:98:GLN:HE21	1.51	0.58
1:F:47:THR:O	1:F:49:THR:N	2.36	0.58
1:H:47:THR:O	1:H:48:HIS:HB2	2.01	0.58
1:D:62:ASN:OD1	1:D:65:GLN:HG3	2.04	0.58
1:R:47:THR:O	1:R:49:THR:N	2.37	0.58
1:T:39:THR:O	1:T:78:ARG:NH2	2.35	0.58
1:V:76:TYR:HB2	1:V:83:HIS:HD2	1.69	0.58
1:K:42:VAL:HG22	1:K:72:SER:OG	2.04	0.57
1:I:45:LEU:HD13	1:J:45:LEU:HD13	1.87	0.57
1:I:48:HIS:CD2	1:N:45:LEU:HD11	2.39	0.57
1:H:105:ASN:HD22	1:H:105:ASN:N	1.97	0.57
1:I:90:CYS:HB3	1:I:93:LYS:H	1.69	0.57
1:Q:46:CYS:SG	1:Q:61:ALA:HB3	2.43	0.57
1:W:98:GLN:N	1:W:98:GLN:HE21	2.02	0.57
1:H:74:CYS:CB	1:H:92:LEU:HD12	2.32	0.57
1:Q:44:MET:CE	1:R:44:MET:SD	2.92	0.57
1:X:92:LEU:HD22	1:X:97:VAL:HG22	1.86	0.57
1:J:28:LYS:HG2	3:J:1001:HOH:O	2.02	0.57
1:X:89:PHE:O	1:X:91:ASP:N	2.37	0.57
1:X:105:ASN:H	1:X:105:ASN:ND2	2.01	0.57
1:F:61:ALA:HB2	1:F:67:SER:OG	2.05	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:51:THR:HG23	1:E:60:GLU:OE1	2.04	0.57
1:F:52:GLY:HA2	1:F:65:GLN:OE1	2.05	0.57
1:U:42:VAL:HG23	3:U:1006:HOH:O	2.05	0.57
1:D:89:PHE:O	1:D:90:CYS:C	2.42	0.57
1:K:90:CYS:CB	1:K:93:LYS:HB2	2.35	0.57
1:M:46:CYS:SG	1:M:48:HIS:CD2	2.91	0.57
1:A:21:VAL:HG11	1:C:40:ASN:HB3	1.86	0.57
1:N:120:CYS:SG	1:N:128:CYS:HA	2.45	0.57
1:J:70:GLY:HA3	1:J:92:LEU:O	2.05	0.56
1:J:90:CYS:HB2	3:J:1002:HOH:O	2.04	0.56
1:Q:13:VAL:O	1:Q:16:PHE:HB3	2.05	0.56
1:Q:39:THR:O	1:Q:40:ASN:HB2	2.05	0.56
1:X:75:LEU:HD22	1:X:112:LEU:HD11	1.87	0.56
1:E:113:ARG:HB2	1:E:113:ARG:NH1	2.19	0.56
1:G:89:PHE:O	1:G:90:CYS:C	2.43	0.56
1:J:51:THR:HG23	1:J:60:GLU:OE1	2.04	0.56
1:0:51:THR:OG1	1:O:53:GLN:HG3	2.05	0.56
1:A:90:CYS:C	1:A:92:LEU:N	2.57	0.56
1:S:32:ALA:C	1:S:34:GLY:H	2.09	0.56
1:A:105:ASN:HD22	1:A:105:ASN:H	1.53	0.56
1:J:57:VAL:HG23	1:J:58:THR:HG23	1.86	0.56
1:L:41:CYS:HA	1:L:72:SER:HB3	1.88	0.56
1:Q:96:TYR:OH	1:R:42:VAL:HG11	2.06	0.56
1:E:53:GLN:HB2	1:E:56:THR:CG2	2.35	0.56
1:K:39:THR:O	1:K:40:ASN:HB2	2.05	0.56
1:0:128:CYS:O	1:O:129:SER:HB2	2.04	0.56
1:S:41:CYS:HA	1:S:72:SER:OG	2.05	0.56
1:S:105:ASN:H	1:S:105:ASN:ND2	1.94	0.56
1:V:89:PHE:O	1:V:90:CYS:C	2.44	0.56
1:P:105:ASN:HD22	1:P:105:ASN:N	1.90	0.56
1:A:89:PHE:O	1:A:90:CYS:C	2.44	0.55
1:O:90:CYS:HB3	1:O:93:LYS:N	2.16	0.55
1:T:106:ASP:OD2	1:T:113:ARG:NH2	2.37	0.55
1:D:18:ALA:HB2	1:D:79:CYS:HB3	1.89	0.55
1:H:92:LEU:HD22	1:H:97:VAL:HG21	1.87	0.55
3:N:1022:HOH:O	1:T:19:PHE:HB3	2.06	0.55
1:R:57:VAL:HG23	1:R:58:THR:HG23	1.88	0.55
1:L:90:CYS:HB3	1:L:93:LYS:CB	2.35	0.55
1:N:10:ASN:HD21	1:N:40:ASN:HD22	1.55	0.55
1:B:77:CYS:SG	1:B:83:HIS:NE2	2.78	0.55
1:H:70:GLY:HA3	1:H:92:LEU:O	2.05	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:W:52:GLY:HA2	1:W:65:GLN:OE1	2.05	0.55
1:L:23:PRO:HG3	3:L:1039:HOH:O	2.07	0.55
1:E:109:GLY:HA3	3:E:1006:HOH:O	2.06	0.55
1:M:53:GLN:HG3	3:M:1044:HOH:O	2.06	0.55
1:Q:14:LEU:HD21	1:Q:38:ILE:HD13	1.88	0.55
1:C:44:MET:HE2	1:D:42:VAL:HG12	1.89	0.55
1:K:57:VAL:HG23	1:K:58:THR:HG23	1.89	0.55
1:R:10:ASN:ND2	1:R:40:ASN:HD22	2.04	0.55
1:R:68:PHE:HD1	3:R:1017:HOH:O	1.89	0.55
1:A:13:VAL:HB	3:A:1020:HOH:O	2.07	0.55
1:C:44:MET:HG2	1:C:67:SER:O	2.06	0.55
1:D:90:CYS:C	1:D:92:LEU:N	2.58	0.55
1:V:70:GLY:HA2	1:V:97:VAL:HG23	1.87	0.55
1:C:61:ALA:HB2	1:C:67:SER:OG	2.07	0.55
1:X:109:GLY:O	1:X:113:ARG:HG3	2.07	0.55
1:G:41:CYS:HA	1:G:72:SER:OG	2.07	0.55
1:U:113:ARG:NH1	1:U:113:ARG:HB2	2.22	0.55
1:A:9:ALA:O	1:A:13:VAL:HG23	2.06	0.54
1:R:105:ASN:HD22	1:R:105:ASN:N	1.98	0.54
1:V:58:THR:O	1:V:60:GLU:HG2	2.07	0.54
1:C:122:MET:HE2	1:C:127:GLY:HA3	1.89	0.54
1:I:101:THR:O	1:M:101:THR:CG2	2.55	0.54
1:K:61:ALA:HB2	1:K:67:SER:OG	2.07	0.54
1:M:105:ASN:N	1:M:105:ASN:ND2	2.48	0.54
1:W:10:ASN:ND2	1:W:40:ASN:HD22	2.05	0.54
1:M:40:ASN:HB3	1:R:21:VAL:HG11	1.89	0.54
1:C:92:LEU:HD22	1:C:97:VAL:CG2	2.38	0.54
1:F:82:ASP:HA	3:F:1030:HOH:O	2.08	0.54
1:H:41:CYS:HA	1:H:72:SER:OG	2.07	0.54
1:X:99:ILE:HD13	1:X:107:PRO:HA	1.89	0.54
1:E:50:GLY:HA3	1:E:60:GLU:CA	2.38	0.54
1:V:113:ARG:NE	3:V:1016:HOH:O	2.40	0.54
1:J:90:CYS:C	1:J:92:LEU:H	2.11	0.54
1:U:98:GLN:H	1:U:98:GLN:HE21	1.55	0.54
1:C:66:GLU:OE2	1:C:101:THR:HG23	2.08	0.53
1:C:103:CYS:C	1:C:105:ASN:H	2.12	0.53
1:K:62:ASN:OD1	1:K:65:GLN:HG3	2.08	0.53
1:K:90:CYS:C	1:K:92:LEU:N	2.61	0.53
1:E:47:THR:HG22	1:E:48:HIS:N	2.23	0.53
1:H:9:ALA:HB1	3:H:1034:HOH:O	2.06	0.53
1:I:53:GLN:HB2	1:I:56:THR:CG2	2.38	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:T:58:THR:O	1:T:60:GLU:HG2	2.08	0.53
1:C:9:ALA:HB3	3:C:1008:HOH:O	2.07	0.53
1:O:90:CYS:CB	1:O:93:LYS:HB2	2.38	0.53
1:0:27:TYR:0	1:O:30:TYR:HB3	2.08	0.53
1:T:28:LYS:HE3	3:T:1013:HOH:O	2.08	0.53
1:U:89:PHE:HB3	3:U:1008:HOH:O	2.09	0.53
1:U:98:GLN:N	1:U:98:GLN:NE2	2.57	0.53
1:B:90:CYS:CB	1:B:93:LYS:HB2	2.36	0.53
1:I:117:CYS:HB3	1:I:120:CYS:HB2	1.91	0.53
1:P:83:HIS:ND1	1:P:83:HIS:N	2.56	0.53
1:X:90:CYS:C	1:X:92:LEU:H	2.11	0.53
1:K:41:CYS:HA	1:K:72:SER:HB3	1.91	0.53
1:S:10:ASN:ND2	1:S:40:ASN:HD22	2.06	0.53
1:R:83:HIS:ND1	1:R:89:PHE:HA	2.24	0.53
1:T:48:HIS:CG	1:T:49:THR:H	2.27	0.53
1:M:92:LEU:HD22	1:M:97:VAL:CG2	2.38	0.53
1:O:99:ILE:HD13	1:O:107:PRO:HA	1.90	0.53
1:P:10:ASN:HB2	3:P:1045:HOH:O	2.09	0.53
1:Q:44:MET:HE3	1:R:44:MET:SD	2.49	0.53
1:T:84:PRO:HA	3:T:1015:HOH:O	2.09	0.53
1:W:110:PHE:HA	1:W:113:ARG:HH12	1.74	0.53
1:K:53:GLN:HA	1:K:122:MET:HG2	1.91	0.53
1:M:113:ARG:NE	3:M:1003:HOH:O	2.41	0.53
1:P:11:SER:HB2	3:P:1031:HOH:O	2.08	0.53
1:Q:53:GLN:HB2	1:Q:56:THR:HG21	1.90	0.53
1:R:14:LEU:HD21	1:R:38:ILE:HD13	1.89	0.53
1:U:74:CYS:HB2	1:U:92:LEU:HD12	1.91	0.53
1:K:52:GLY:HA2	1:K:65:GLN:OE1	2.09	0.52
1:R:92:LEU:HD22	1:R:97:VAL:CG2	2.38	0.52
1:J:48:HIS:HA	1:J:61:ALA:O	2.09	0.52
1:R:9:ALA:HA	3:R:1018:HOH:O	2.10	0.52
1:W:47:THR:O	1:W:49:THR:HG23	2.09	0.52
1:S:50:GLY:HA3	1:S:60:GLU:OE1	2.09	0.52
1:C:44:MET:HE2	1:D:42:VAL:CG1	2.39	0.52
1:G:84:PRO:HG2	1:G:85:ASN:N	2.23	0.52
1:J:10:ASN:ND2	1:J:40:ASN:HD22	2.07	0.52
1:S:9:ALA:HB3	3:S:1003:HOH:O	2.10	0.52
1:T:10:ASN:ND2	1:T:40:ASN:HD22	2.08	0.52
1:T:51:THR:HG23	1:T:60:GLU:OE1	2.08	0.52
1:T:51:THR:OG1	1:T:53:GLN:HG3	2.10	0.52
1:A:90:CYS:O	1:A:92:LEU:N	2.42	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:113:ARG:HB2	1:F:113:ARG:NH1	2.25	0.52
1:F:43:LYS:HE2	1:F:66:GLU:OE1	2.10	0.52
1:G:56:THR:HG21	1:G:60:GLU:HG3	1.92	0.52
1:D:52:GLY:O	1:D:122:MET:HG2	2.09	0.52
1:J:92:LEU:HD22	1:J:97:VAL:HG22	1.92	0.52
1:M:120:CYS:HB3	3:M:1022:HOH:O	2.09	0.52
1:R:43:LYS:HE2	1:R:66:GLU:OE1	2.10	0.52
1:R:10:ASN:HD21	1:R:40:ASN:HD22	1.58	0.52
1:W:113:ARG:NE	3:W:1021:HOH:O	2.43	0.52
1:B:47:THR:HG23	1:B:49:THR:H	1.76	0.52
1:D:74:CYS:CB	1:D:92:LEU:HD12	2.36	0.52
1:P:84:PRO:HG2	1:P:85:ASN:H	1.75	0.52
1:R:42:VAL:HG22	1:R:72:SER:OG	2.09	0.52
1:W:42:VAL:HG22	1:W:72:SER:OG	2.10	0.52
1:Q:50:GLY:HA3	1:Q:60:GLU:C	2.29	0.51
1:U:57:VAL:HG23	1:U:58:THR:HG23	1.92	0.51
1:M:47:THR:O	1:M:49:THR:OG1	2.26	0.51
1:O:10:ASN:ND2	1:O:40:ASN:ND2	2.57	0.51
1:Q:44:MET:HG3	1:Q:96:TYR:HD2	1.74	0.51
1:R:47:THR:HB	1:R:49:THR:OG1	2.10	0.51
1:A:97:VAL:HB	3:A:1029:HOH:O	2.11	0.51
1:N:83:HIS:HB3	3:N:1016:HOH:O	2.10	0.51
1:V:97:VAL:HB	3:V:1035:HOH:O	2.10	0.51
1:E:39:THR:O	1:E:40:ASN:HB2	2.10	0.51
1:K:9:ALA:N	3:K:1027:HOH:O	2.43	0.51
1:0:10:ASN:ND2	1:O:40:ASN:HD22	2.09	0.51
1:Q:61:ALA:HB2	1:Q:67:SER:OG	2.11	0.51
1:V:117:CYS:SG	1:V:120:CYS:HB2	2.49	0.51
1:C:90:CYS:O	1:C:92:LEU:N	2.44	0.51
1:L:105:ASN:H	1:L:105:ASN:HD22	1.58	0.51
1:Q:62:ASN:ND2	1:Q:63:MET:N	2.52	0.51
1:S:76:TYR:HB2	1:S:83:HIS:CD2	2.45	0.51
1:T:99:ILE:HD13	1:T:107:PRO:HA	1.92	0.51
1:J:52:GLY:HA2	1:J:65:GLN:OE1	2.10	0.51
1:P:106:ASP:OD2	1:P:113:ARG:NH2	2.44	0.51
1:G:47:THR:OG1	1:G:48:HIS:CD2	2.64	0.51
1:K:48:HIS:HB2	1:K:63:MET:HE1	1.91	0.51
1:X:9:ALA:O	1:X:13:VAL:HG23	2.11	0.51
1:L:39:THR:O	1:L:40:ASN:HB2	2.11	0.51
1:B:39:THR:O	1:B:40:ASN:HB2	2.10	0.51
1:E:47:THR:O	1:E:48:HIS:HB2	2.09	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:T:62:ASN:HB2	1:T:65:GLN:HG3	1.91	0.51
1:A:74:CYS:HB2	1:A:92:LEU:HD12	1.93	0.50
1:A:89:PHE:O	1:A:91:ASP:N	2.43	0.50
1:D:92:LEU:HD22	1:D:97:VAL:HG21	1.93	0.50
1:E:110:PHE:HA	1:E:113:ARG:HH12	1.75	0.50
1:C:45:LEU:HD23	1:D:43:LYS:HD3	1.92	0.50
1:G:69:GLY:O	1:G:72:SER:HB3	2.12	0.50
1:N:47:THR:O	1:N:49:THR:HG23	2.10	0.50
1:Q:47:THR:O	1:Q:49:THR:N	2.44	0.50
1:S:84:PRO:CG	1:S:85:ASN:N	2.73	0.50
1:X:106:ASP:OD2	1:X:113:ARG:NH2	2.44	0.50
1:B:52:GLY:HA2	1:B:65:GLN:OE1	2.11	0.50
1:F:91:ASP:N	1:F:91:ASP:OD2	2.45	0.50
1:M:48:HIS:HE1	1:M:66:GLU:OE2	1.95	0.50
1:S:105:ASN:N	1:S:105:ASN:ND2	2.57	0.50
1:S:106:ASP:OD2	1:S:113:ARG:NH2	2.44	0.50
1:B:89:PHE:O	1:F:87:LYS:HD3	2.12	0.50
1:F:9:ALA:O	1:F:13:VAL:HG23	2.11	0.50
1:F:72:SER:HB2	3:F:1027:HOH:O	2.11	0.50
1:N:58:THR:O	1:N:60:GLU:HG2	2.12	0.50
1:N:89:PHE:O	1:N:90:CYS:C	2.48	0.50
1:V:24:ALA:O	1:V:28:LYS:HG3	2.12	0.50
1:Q:44:MET:HE1	1:R:44:MET:SD	2.52	0.50
1:B:47:THR:HG21	3:B:1030:HOH:O	2.11	0.50
1:E:9:ALA:HB3	3:E:1020:HOH:O	2.11	0.50
1:M:47:THR:O	1:M:47:THR:OG1	2.29	0.50
1:N:42:VAL:HG23	3:N:1003:HOH:O	2.12	0.50
1:P:39:THR:O	1:P:40:ASN:HB2	2.12	0.50
1:Q:44:MET:HG3	1:Q:96:TYR:CD2	2.47	0.50
1:I:117:CYS:HB2	1:I:124:LYS:HD2	1.93	0.50
1:Q:76:TYR:HB2	1:Q:83:HIS:HD2	1.77	0.50
1:V:90:CYS:HB3	1:V:93:LYS:HB2	1.93	0.50
1:H:108:VAL:HA	3:H:1027:HOH:O	2.12	0.49
1:I:98:GLN:NE2	1:I:98:GLN:N	2.59	0.49
1:O:90:CYS:C	1:O:92:LEU:N	2.65	0.49
1:T:92:LEU:HD22	1:T:97:VAL:CG2	2.42	0.49
1:U:44:MET:SD	3:U:1006:HOH:O	2.59	0.49
1:E:14:LEU:HD21	1:E:38:ILE:HD13	1.94	0.49
1:E:90:CYS:C	1:E:92:LEU:H	2.15	0.49
1:P:83:HIS:CD2	1:P:90:CYS:H	2.30	0.49
1:A:120:CYS:SG	1:A:128:CYS:HA	2.52	0.49



	A L	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:113:ARG:HB2	1:B:113:ARG:NH1	2.28	0.49
1:F:75:LEU:HD22	1:F:112:LEU:HD11	1.92	0.49
1:L:11:SER:HB2	3:L:1028:HOH:O	2.11	0.49
1:L:13:VAL:HG22	1:L:30:TYR:CZ	2.47	0.49
1:W:10:ASN:ND2	1:W:40:ASN:ND2	2.61	0.49
1:C:117:CYS:HB2	1:C:124:LYS:HD2	1.95	0.49
1:D:51:THR:HG23	1:D:60:GLU:OE1	2.11	0.49
1:H:109:GLY:HA3	3:H:1019:HOH:O	2.12	0.49
1:M:52:GLY:HA2	1:M:65:GLN:OE1	2.12	0.49
1:V:39:THR:O	1:V:40:ASN:HB2	2.13	0.49
1:X:38:ILE:HG22	1:X:78:ARG:NH2	2.28	0.49
1:M:83:HIS:ND1	1:M:89:PHE:HB3	2.27	0.49
1:O:44:MET:CE	1:P:42:VAL:HG13	2.42	0.49
1:V:31:LEU:HD13	3:V:1016:HOH:O	2.13	0.49
1:H:92:LEU:HD22	1:H:97:VAL:CG2	2.43	0.49
1:M:83:HIS:CE1	1:M:89:PHE:HB3	2.47	0.49
1:W:110:PHE:HA	1:W:113:ARG:NH1	2.28	0.49
1:X:73:CYS:HA	1:X:108:VAL:HG22	1.95	0.49
1:I:53:GLN:NE2	1:I:121:GLY:HA3	2.28	0.49
1:L:113:ARG:NE	3:L:1000:HOH:O	2.45	0.49
1:P:89:PHE:N	1:P:89:PHE:CD2	2.81	0.49
1:E:113:ARG:HH11	1:E:113:ARG:CB	2.24	0.49
1:K:113:ARG:HB2	1:K:113:ARG:NH1	2.25	0.49
1:M:47:THR:O	1:M:49:THR:N	2.46	0.49
1:T:48:HIS:CD2	1:T:49:THR:H	2.31	0.49
1:J:43:LYS:HG2	1:J:68:PHE:CE2	2.48	0.48
3:M:1042:HOH:O	1:T:25:LYS:HE2	2.11	0.48
1:W:53:GLN:HA	1:W:122:MET:HG2	1.94	0.48
1:W:70:GLY:HA3	1:W:92:LEU:O	2.12	0.48
1:W:13:VAL:HG22	1:W:30:TYR:CZ	2.49	0.48
1:X:91:ASP:HB2	3:X:1011:HOH:O	2.12	0.48
1:C:103:CYS:O	1:C:105:ASN:N	2.46	0.48
1:D:42:VAL:HG23	1:D:72:SER:OG	2.12	0.48
1:L:58:THR:O	1:L:60:GLU:HG2	2.13	0.48
1:P:75:LEU:HD22	1:P:112:LEU:HD11	1.96	0.48
1:Q:47:THR:O	1:Q:49:THR:HG23	2.13	0.48
1:Q:62:ASN:HB3	1:Q:65:GLN:CG	2.42	0.48
1:Q:100:PRO:HG2	1:Q:126:TYR:CD2	2.49	0.48
1:W:103:CYS:C	1:W:105:ASN:H	2.17	0.48
1:C:91:ASP:OD2	1:C:91:ASP:N	2.47	0.48
1:O:119:VAL:HG22	1:V:124:LYS:HD3	1.95	0.48



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:U:83:HIS:CD2	1:U:89:PHE:HA	2.46	0.48
1:V:22:ASP:OD2	1:V:25:LYS:HE3	2.13	0.48
1:W:41:CYS:HA	1:W:72:SER:HB3	1.96	0.48
1:J:90:CYS:O	1:J:92:LEU:N	2.45	0.48
1:K:55:ILE:HG22	1:K:95:LYS:HD3	1.96	0.48
1:N:74:CYS:CB	1:N:92:LEU:HD12	2.42	0.48
1:V:66:GLU:HG2	1:V:101:THR:CG2	2.44	0.48
1:X:91:ASP:N	1:X:91:ASP:OD2	2.46	0.48
1:W:96:TYR:OH	1:X:42:VAL:HG21	2.14	0.48
1:A:51:THR:HG23	1:A:60:GLU:OE1	2.13	0.48
1:D:91:ASP:OD2	1:D:91:ASP:N	2.47	0.48
1:F:83:HIS:CD2	1:F:83:HIS:N	2.80	0.48
1:I:105:ASN:H	1:I:105:ASN:ND2	2.11	0.48
1:A:110:PHE:HE2	1:A:123:TRP:CE2	2.31	0.48
1:I:54:ALA:HB1	1:I:123:TRP:CE2	2.49	0.48
1:J:117:CYS:SG	1:J:119:VAL:HB	2.54	0.48
1:M:44:MET:SD	3:M:1015:HOH:O	2.61	0.48
1:T:44:MET:HG3	1:T:96:TYR:HD2	1.78	0.48
1:T:112:LEU:HD13	3:T:1013:HOH:O	2.14	0.48
1:V:90:CYS:HB3	1:V:93:LYS:CB	2.44	0.48
1:B:90:CYS:CB	1:B:93:LYS:H	2.16	0.48
1:H:69:GLY:O	1:H:72:SER:HB3	2.13	0.48
1:N:115:THR:HG22	1:N:116:VAL:N	2.28	0.48
1:S:70:GLY:HA3	1:S:92:LEU:O	2.14	0.48
1:X:117:CYS:HB3	1:X:124:LYS:CE	2.44	0.48
1:L:62:ASN:OD1	1:L:65:GLN:HG3	2.14	0.47
1:N:44:MET:SD	3:N:1003:HOH:O	2.61	0.47
1:0:11:SER:O	1:0:15:SER:HB2	2.13	0.47
1:T:41:CYS:HA	1:T:72:SER:HG	1.78	0.47
1:B:115:THR:CG2	1:B:116:VAL:N	2.77	0.47
1:B:76:TYR:HB2	1:B:83:HIS:CD2	2.49	0.47
1:R:119:VAL:HB	3:R:1025:HOH:O	2.14	0.47
1:V:49:THR:HG23	1:V:62:ASN:HA	1.96	0.47
1:V:66:GLU:HG2	1:V:101:THR:HG22	1.95	0.47
1:D:84:PRO:HG2	1:D:85:ASN:N	2.27	0.47
1:M:83:HIS:CD2	1:M:83:HIS:N	2.82	0.47
1:W:103:CYS:O	1:W:105:ASN:N	2.48	0.47
1:C:74:CYS:HB2	1:C:92:LEU:HD12	1.96	0.47
1:H:129:SER:HA	3:H:1042:HOH:O	2.15	0.47
1:E:14:LEU:HD11	1:E:78:ARG:NH1	2.30	0.47
1:U:10:ASN:ND2	1:U:40:ASN:HD22	2.12	0.47



	A O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:X:90:CYS:O	1:X:92:LEU:N	2.46	0.47
1:B:39:THR:O	1:B:78:ARG:NH2	2.37	0.47
1:B:55:ILE:HD13	1:B:92:LEU:HD23	1.97	0.47
1:C:92:LEU:HD22	1:C:97:VAL:HG22	1.95	0.47
1:F:42:VAL:HG23	1:F:42:VAL:O	2.13	0.47
1:O:13:VAL:HG13	1:O:14:LEU:N	2.29	0.47
1:O:75:LEU:HD22	1:O:112:LEU:HD11	1.97	0.47
1:O:106:ASP:OD2	1:O:113:ARG:NH2	2.47	0.47
1:P:70:GLY:HA3	1:P:92:LEU:O	2.14	0.47
1:R:83:HIS:HB2	3:R:1022:HOH:O	2.14	0.47
1:X:128:CYS:O	1:X:129:SER:HB2	2.15	0.47
1:F:32:ALA:C	1:F:34:GLY:H	2.17	0.47
1:K:58:THR:O	1:K:60:GLU:HG2	2.14	0.47
1:Q:45:LEU:HB2	1:R:45:LEU:HD13	1.97	0.47
1:H:117:CYS:HB2	1:H:124:LYS:HD2	1.97	0.47
1:S:66:GLU:HB2	1:S:68:PHE:CE1	2.50	0.47
1:U:90:CYS:C	1:U:92:LEU:N	2.68	0.47
1:A:42:VAL:HG23	1:A:42:VAL:O	2.14	0.47
1:I:48:HIS:HA	1:I:61:ALA:O	2.14	0.47
1:N:110:PHE:HE2	1:N:123:TRP:CE2	2.33	0.47
1:O:55:ILE:HG22	1:O:95:LYS:HD2	1.97	0.47
1:Q:90:CYS:SG	1:Q:90:CYS:O	2.72	0.47
1:B:129:SER:HA	3:B:1036:HOH:O	2.15	0.46
1:D:105:ASN:HD22	1:D:105:ASN:H	1.63	0.46
1:H:76:TYR:HB2	1:H:83:HIS:CD2	2.50	0.46
1:P:48:HIS:HA	1:P:61:ALA:O	2.15	0.46
1:S:47:THR:HG23	1:S:48:HIS:N	2.18	0.46
1:U:9:ALA:HB3	3:U:1011:HOH:O	2.14	0.46
1:S:117:CYS:HB3	1:S:120:CYS:HB3	1.96	0.46
1:D:76:TYR:HB2	1:D:83:HIS:CD2	2.51	0.46
1:L:90:CYS:CB	1:L:93:LYS:HB2	2.38	0.46
1:N:69:GLY:N	3:N:1003:HOH:O	2.48	0.46
1:S:117:CYS:HB2	1:S:124:LYS:HD2	1.97	0.46
1:U:90:CYS:O	1:U:92:LEU:N	2.39	0.46
1:N:92:LEU:HD22	1:N:97:VAL:CG2	2.45	0.46
1:T:78:ARG:HD2	3:T:1020:HOH:O	2.15	0.46
1:W:50:GLY:C	1:W:52:GLY:H	2.19	0.46
1:B:56:THR:O	1:B:95:LYS:HB3	2.15	0.46
1:J:83:HIS:ND1	1:J:83:HIS:N	2.62	0.46
1:K:90:CYS:HB2	1:K:93:LYS:HB2	1.97	0.46
1:O:44:MET:HE1	1:P:42:VAL:CG1	2.46	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:R:84:PRO:HG2	1:R:85:ASN:H	1.80	0.46
1:T:48:HIS:CG	1:T:49:THR:N	2.84	0.46
1:C:110:PHE:HE2	1:C:123:TRP:CE2	2.32	0.46
1:D:39:THR:O	1:D:40:ASN:HB2	2.15	0.46
1:G:40:ASN:HB2	3:G:1046:HOH:O	2.15	0.46
1:I:108:VAL:HA	3:I:1020:HOH:O	2.16	0.46
1:V:76:TYR:CB	1:V:83:HIS:CD2	2.97	0.46
1:W:79:CYS:O	1:W:80:HIS:HB2	2.15	0.46
1:A:99:ILE:HD13	1:A:107:PRO:HA	1.98	0.46
1:F:120:CYS:SG	1:F:128:CYS:HA	2.56	0.46
1:K:61:ALA:HA	1:K:98:GLN:HG3	1.98	0.46
1:L:105:ASN:HD22	1:L:105:ASN:N	2.14	0.46
1:X:18:ALA:HB2	1:X:79:CYS:HB3	1.98	0.46
1:C:39:THR:O	1:C:78:ARG:NH2	2.42	0.46
1:C:90:CYS:SG	1:C:93:LYS:HB2	2.56	0.46
1:P:99:ILE:HD13	1:P:107:PRO:HA	1.97	0.46
1:Q:74:CYS:N	3:Q:1029:HOH:O	2.48	0.46
1:C:38:ILE:HD12	1:C:108:VAL:HG11	1.96	0.46
1:K:43:LYS:HG3	1:K:68:PHE:CE2	2.51	0.46
1:O:51:THR:HG23	1:O:60:GLU:OE1	2.15	0.46
1:S:44:MET:SD	1:T:44:MET:CE	3.04	0.46
1:S:92:LEU:HD22	1:S:97:VAL:CG2	2.46	0.46
1:F:14:LEU:HD21	1:F:38:ILE:HD13	1.97	0.45
1:K:113:ARG:HH11	1:K:113:ARG:CB	2.25	0.45
1:N:52:GLY:O	1:N:122:MET:HE2	2.15	0.45
1:N:82:ASP:C	1:N:83:HIS:ND1	2.69	0.45
1:Q:51:THR:HG23	1:Q:60:GLU:OE1	2.16	0.45
1:A:92:LEU:HD22	1:A:97:VAL:CG2	2.46	0.45
1:C:109:GLY:HA3	1:C:113:ARG:HH21	1.81	0.45
1:E:54:ALA:HB1	1:E:123:TRP:CE2	2.50	0.45
1:H:90:CYS:CB	1:H:93:LYS:HB2	2.42	0.45
1:A:56:THR:O	1:A:95:LYS:HB3	2.16	0.45
1:F:89:PHE:CD2	1:F:89:PHE:N	2.82	0.45
1:G:76:TYR:HB2	1:G:83:HIS:CD2	2.52	0.45
1:E:113:ARG:NH2	3:E:1006:HOH:O	2.48	0.45
1:H:90:CYS:HB3	1:H:93:LYS:H	1.82	0.45
1:I:58:THR:O	1:I:60:GLU:HG2	2.17	0.45
1:I:61:ALA:HB2	1:I:67:SER:OG	2.16	0.45
1:P:9:ALA:O	1:P:13:VAL:HG23	2.17	0.45
1:V:68:PHE:HB2	3:V:1035:HOH:O	2.16	0.45
1:F:58:THR:O	1:F:60:GLU:HG2	2.16	0.45



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:92:LEU:HD22	1:G:97:VAL:CG2	2.47	0.45
1:U:69:GLY:N	3:U:1006:HOH:O	2.49	0.45
1:U:113:ARG:CB	1:U:113:ARG:HH11	2.29	0.45
1:R:99:ILE:HD13	1:R:107:PRO:HA	1.97	0.45
1:S:32:ALA:O	1:S:34:GLY:N	2.50	0.45
1:S:97:VAL:CG1	1:S:99:ILE:HD11	2.46	0.45
1:U:82:ASP:C	1:U:83:HIS:ND1	2.70	0.45
1:V:61:ALA:HB2	1:V:67:SER:OG	2.17	0.45
1:C:13:VAL:HG13	1:C:14:LEU:N	2.32	0.45
1:C:99:ILE:HD13	1:C:107:PRO:HA	1.99	0.45
1:J:91:ASP:OD2	1:J:91:ASP:N	2.50	0.45
1:A:21:VAL:HG23	1:A:22:ASP:N	2.32	0.45
1:A:51:THR:OG1	1:A:53:GLN:HG3	2.16	0.45
1:M:53:GLN:HA	1:M:53:GLN:HE21	1.80	0.45
1:O:92:LEU:HD22	1:O:97:VAL:CG2	2.46	0.45
1:Q:39:THR:O	1:Q:78:ARG:NH2	2.46	0.45
1:S:14:LEU:HD21	1:S:38:ILE:HD13	1.99	0.45
1:S:69:GLY:O	1:S:72:SER:HB3	2.17	0.45
1:X:92:LEU:HD22	1:X:97:VAL:CG2	2.46	0.45
1:P:55:ILE:HG22	1:P:95:LYS:HD2	1.98	0.45
1:S:99:ILE:HD12	1:S:110:PHE:CD2	2.52	0.45
1:V:90:CYS:HB3	1:V:93:LYS:H	1.82	0.45
1:V:113:ARG:NH1	3:V:1001:HOH:O	2.49	0.45
1:W:90:CYS:C	1:W:92:LEU:H	2.20	0.45
1:X:55:ILE:HG22	1:X:95:LYS:HD2	1.99	0.45
1:B:14:LEU:HD22	1:B:79:CYS:SG	2.57	0.45
1:E:44:MET:HG2	1:E:67:SER:O	2.17	0.45
1:G:62:ASN:OD1	1:G:65:GLN:HG3	2.17	0.45
1:I:66:GLU:HB2	1:I:68:PHE:CE1	2.53	0.45
1:J:84:PRO:HG2	1:J:85:ASN:N	2.27	0.45
1:L:76:TYR:CE2	1:L:84:PRO:HD3	2.52	0.45
1:N:84:PRO:O	1:N:85:ASN:C	2.54	0.45
1:O:30:TYR:HE2	1:O:36:GLN:O	2.00	0.45
1:B:89:PHE:O	1:B:90:CYS:C	2.55	0.44
1:I:91:ASP:N	1:I:91:ASP:OD2	2.50	0.44
1:J:84:PRO:CG	1:J:85:ASN:H	2.25	0.44
1:M:110:PHE:CE1	1:M:114:ASN:ND2	2.86	0.44
1:B:90:CYS:HB2	1:B:93:LYS:CB	2.39	0.44
1:G:90:CYS:HB3	1:G:93:LYS:HB2	1.96	0.44
1:I:106:ASP:N	1:I:107:PRO:HD3	2.31	0.44
1:I:120:CYS:HB3	1:I:122:MET:H	1.82	0.44



	1 + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:N:90:CYS:HB2	1:N:93:LYS:CB	2.42	0.44
1:R:79:CYS:O	1:R:80:HIS:HB2	2.17	0.44
1:U:102:THR:HB	3:U:1023:HOH:O	2.16	0.44
1:W:58:THR:O	1:W:60:GLU:HG2	2.17	0.44
1:C:103:CYS:C	1:C:105:ASN:N	2.70	0.44
1:G:89:PHE:O	1:G:91:ASP:N	2.49	0.44
1:J:46:CYS:C	1:M:49:THR:HG21	2.37	0.44
1:S:42:VAL:HG23	1:S:42:VAL:O	2.17	0.44
1:W:42:VAL:HG23	3:W:1030:HOH:O	2.17	0.44
1:A:73:CYS:O	1:A:108:VAL:HG22	2.17	0.44
1:B:115:THR:HG22	1:B:116:VAL:N	2.32	0.44
1:E:10:ASN:ND2	1:E:40:ASN:HD22	2.15	0.44
1:F:39:THR:O	1:F:40:ASN:HB2	2.17	0.44
1:L:43:LYS:HE2	1:L:68:PHE:CZ	2.52	0.44
1:S:120:CYS:SG	1:S:128:CYS:HA	2.57	0.44
1:F:13:VAL:HG22	1:F:30:TYR:CZ	2.53	0.44
1:G:58:THR:O	1:G:60:GLU:HG2	2.18	0.44
1:H:84:PRO:CG	1:H:85:ASN:H	2.27	0.44
1:M:40:ASN:CB	1:R:21:VAL:HG11	2.47	0.44
1:N:103:CYS:C	1:N:105:ASN:H	2.20	0.44
1:R:58:THR:O	1:R:60:GLU:HG2	2.18	0.44
1:R:70:GLY:HA3	1:R:92:LEU:O	2.17	0.44
1:T:41:CYS:CA	1:T:72:SER:OG	2.64	0.44
1:I:129:SER:HA	3:I:1023:HOH:O	2.18	0.44
1:J:10:ASN:ND2	1:J:40:ASN:ND2	2.66	0.44
1:L:42:VAL:HG22	1:L:72:SER:OG	2.17	0.44
1:E:70:GLY:HA3	1:E:92:LEU:O	2.18	0.44
1:J:54:ALA:HB1	1:J:123:TRP:CE2	2.53	0.44
1:M:45:LEU:HB2	1:N:45:LEU:HD13	1.99	0.44
3:O:1039:HOH:O	1:Q:57:VAL:HG11	2.17	0.44
1:P:61:ALA:HB2	1:P:67:SER:OG	2.18	0.44
1:T:28:LYS:HE2	1:T:113:ARG:HG2	2.00	0.44
1:T:44:MET:HG3	1:T:96:TYR:CD2	2.53	0.44
1:T:55:ILE:HD13	1:T:92:LEU:CD2	2.48	0.44
1:C:44:MET:CE	1:D:42:VAL:CG1	2.96	0.44
1:Q:79:CYS:O	1:Q:80:HIS:HB2	2.17	0.44
1:I:51:THR:OG1	1:I:53:GLN:CG	2.66	0.44
1:Q:62:ASN:CG	1:Q:63:MET:H	2.20	0.44
1:B:62:ASN:OD1	1:B:65:GLN:HG3	2.17	0.43
1:E:47:THR:CG2	1:E:48:HIS:N	2.81	0.43
1:F:70:GLY:HA3	1:F:92:LEU:O	2.18	0.43



	t i cas page	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
1:G:92:LEU:HD22	1:G:97:VAL:HG22	2.00	0.43	
1:H:39:THR:O	1:H:40:ASN:HB2	2.17	0.43	
1:I:42:VAL:HG22	1:I:72:SER:OG	2.18	0.43	
1:O:76:TYR:CZ	1:O:84:PRO:HG3	2.53	0.43	
1:S:44:MET:SD	1:T:44:MET:HE1	2.58	0.43	
1:V:13:VAL:HG22	1:V:30:TYR:CZ	2.53	0.43	
1:A:90:CYS:HB3	1:A:93:LYS:HB2	2.00	0.43	
1:C:30:TYR:HE2	1:C:36:GLN:O	2.01	0.43	
1:J:92:LEU:HD22	1:J:97:VAL:CG2	2.48	0.43	
1:K:76:TYR:HB2	1:K:83:HIS:CD2	2.53	0.43	
1:M:45:LEU:HA	1:N:45:LEU:HD13	2.00	0.43	
1:U:113:ARG:HB2	1:U:113:ARG:HH11	1.82	0.43	
1:N:99:ILE:HD13	1:N:107:PRO:HA	2.00	0.43	
1:P:76:TYR:CE2	1:P:84:PRO:HD3	2.53	0.43	
1:Q:45:LEU:HB2	1:R:45:LEU:CB	2.46	0.43	
1:T:89:PHE:O	1:T:90:CYS:C	2.57	0.43	
1:E:44:MET:HE3	1:F:44:MET:SD	2.59	0.43	
1:F:84:PRO:O	1:F:85:ASN:C	2.57	0.43	
1:H:28:LYS:HG2	3:H:1028:HOH:O	2.17	0.43	
1:J:83:HIS:HE1	3:J:1010:HOH:O	2.00	0.43	
1:K:106:ASP:N	1:K:107:PRO:HD3	2.33	0.43	
1:E:110:PHE:HA	1:E:113:ARG:NH1	2.34	0.43	
1:P:128:CYS:HB3	3:P:1021:HOH:O	2.19	0.43	
1:F:54:ALA:HB1	1:F:123:TRP:CE2	2.54	0.43	
1:H:83:HIS:HB3	1:H:84:PRO:HD2	2.00	0.43	
1:I:39:THR:O	1:I:40:ASN:HB2	2.19	0.43	
1:M:63:MET:HA	3:M:1021:HOH:O	2.17	0.43	
1:N:41:CYS:HA	1:N:72:SER:HB2	1.99	0.43	
1:D:92:LEU:HD22	1:D:97:VAL:HG22	1.98	0.43	
1:F:80:HIS:N	3:F:1036:HOH:O	2.50	0.43	
1:M:48:HIS:HB3	3:M:1021:HOH:O	2.17	0.43	
1:X:105:ASN:HD22	1:X:105:ASN:N	2.08	0.43	
1:I:98:GLN:N	1:I:98:GLN:HE21	2.14	0.43	
1:N:100:PRO:HG2	1:N:126:TYR:CD2	2.53	0.43	
3:N:1018:HOH:O	1:T:21:VAL:HG22	2.18	0.43	
1:R:61:ALA:HB2	1:R:67:SER:OG	2.17	0.43	
1:R:89:PHE:O	1:R:90:CYS:C	2.56	0.43	
1:U:47:THR:O	1:U:49:THR:HG23	2.19	0.43	
1:U:92:LEU:HD22	1:U:97:VAL:CG2	2.49	0.43	
1:V:91:ASP:OD2	1:V:91:ASP:N	2.51	0.43	
1:W:27:TYR:CE2	1:W:31:LEU:HD11	2.54	0.43	



	• • • • • •	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:F:47:THR:HG22	1:F:49:THR:HG23	2.00	0.43	
1:G:53:GLN:O	1:G:98:GLN:NE2	2.45	0.43	
1:J:51:THR:OG1	1:J:53:GLN:HG3	2.19	0.43	
1:K:92:LEU:HD22	1:K:97:VAL:HG22	2.00	0.43	
1:O:45:LEU:HD23	1:P:43:LYS:HE2	2.00	0.43	
1:Q:92:LEU:HD22	1:Q:97:VAL:CG2	2.48	0.43	
1:S:51:THR:OG1	1:S:53:GLN:HG3	2.19	0.43	
1:A:58:THR:O	1:A:59:PRO:C	2.57	0.43	
1:M:113:ARG:NH1	3:M:1001:HOH:O	2.50	0.43	
1:R:62:ASN:O	1:R:64:ASP:N	2.52	0.43	
1:S:92:LEU:N	3:S:1005:HOH:O	2.50	0.43	
1:V:55:ILE:HD13	1:V:92:LEU:HD23	2.01	0.43	
1:J:99:ILE:HD13	1:J:107:PRO:HA	2.00	0.42	
1:K:48:HIS:CB	1:K:63:MET:HE1	2.48	0.42	
1:M:113:ARG:HH11	1:M:113:ARG:HB2	1.84	0.42	
1:Q:27:TYR:CE2	1:Q:31:LEU:HD11	2.54	0.42	
1:U:98:GLN:HE21	1:U:98:GLN:N	2.14	0.42	
1:H:79:CYS:O	1:H:81:ILE:HG23	2.19	0.42	
1:I:52:GLY:HA2	1:I:65:GLN:OE1	2.18	0.42	
1:I:106:ASP:OD2	1:I:113:ARG:NH2	2.52	0.42	
1:0:91:ASP:OD2	1:O:91:ASP:N	2.52	0.42	
1:P:13:VAL:HG22	1:P:30:TYR:CZ	2.54	0.42	
1:W:73:CYS:HB3	3:W:1023:HOH:O	2.19	0.42	
1:C:89:PHE:O	1:C:90:CYS:C	2.58	0.42	
1:E:14:LEU:HD11	1:E:78:ARG:HH12	1.83	0.42	
1:L:106:ASP:N	1:L:107:PRO:HD3	2.34	0.42	
1:Q:106:ASP:N	1:Q:107:PRO:HD3	2.35	0.42	
1:V:13:VAL:O	1:V:16:PHE:HB3	2.19	0.42	
1:A:109:GLY:N	3:A:1030:HOH:O	2.52	0.42	
1:B:113:ARG:NE	3:B:1018:HOH:O	2.51	0.42	
1:M:48:HIS:C	1:M:49:THR:HG23	2.40	0.42	
1:G:84:PRO:CG	1:G:85:ASN:H	2.18	0.42	
1:I:39:THR:O	1:I:78:ARG:NH2	2.45	0.42	
1:L:84:PRO:CG	1:L:85:ASN:H	2.31	0.42	
1:A:83:HIS:ND1	1:A:83:HIS:N	2.67	0.42	
1:C:56:THR:HG21	1:C:60:GLU:HB2	2.01	0.42	
1:F:79:CYS:O	1:F:80:HIS:HB2	2.20	0.42	
1:G:10:ASN:ND2	3:G:1046:HOH:O	2.53	0.42	
1:J:47:THR:O	1:J:48:HIS:HB2	2.20	0.42	
1:L:117:CYS:HB2	1:L:124:LYS:HD2	2.00	0.42	
1:Q:58:THR:O	1:Q:60:GLU:HG2	2.20	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:58:THR:O	1:A:60:GLU:HG2	2.20	0.42	
1:D:39:THR:O	1:D:78:ARG:NH2	2.34	0.42	
1:G:11:SER:O	1:G:15:SER:HB2	2.19	0.42	
1:G:42:VAL:O	1:G:68:PHE:HA	2.18	0.42	
1:H:106:ASP:N	1:H:107:PRO:HD3	2.34	0.42	
1:P:106:ASP:N	1:P:107:PRO:HD3	2.35	0.42	
1:W:55:ILE:HD13	1:W:92:LEU:CD2	2.50	0.42	
1:P:62:ASN:OD1	1:P:65:GLN:HG3	2.20	0.42	
1:R:16:PHE:CE2	1:R:26:ALA:HB1	2.55	0.42	
1:S:97:VAL:HG11	1:S:99:ILE:HD11	2.02	0.42	
1:U:62:ASN:OD1	1:U:65:GLN:HG3	2.19	0.42	
1:V:79:CYS:O	1:V:80:HIS:HB2	2.20	0.42	
1:W:69:GLY:N	3:W:1030:HOH:O	2.52	0.42	
1:A:45:LEU:HD23	1:B:43:LYS:HD2	2.01	0.42	
1:F:90:CYS:C	1:F:92:LEU:H	2.16	0.42	
1:O:90:CYS:HB3	1:O:93:LYS:HB2	2.01	0.42	
1:Q:54:ALA:HB1	1:Q:123:TRP:CE2	2.55	0.42	
1:S:32:ALA:C	1:S:34:GLY:N	2.71	0.42	
1:V:25:LYS:HE3	1:V:25:LYS:HB2	1.86	0.42	
1:K:44:MET:HB2	1:K:67:SER:HB2	2.02	0.41	
1:K:47:THR:O	1:K:48:HIS:HB2	2.19	0.41	
1:M:98:GLN:NE2	1:M:98:GLN:N	2.68	0.41	
1:O:60:GLU:OE2	1:V:25:LYS:NZ	2.52	0.41	
1:W:113:ARG:HH11	1:W:113:ARG:CB	2.29	0.41	
1:B:53:GLN:HA	1:B:122:MET:HG2	2.01	0.41	
1:C:52:GLY:HA2	1:C:65:GLN:OE1	2.19	0.41	
1:R:22:ASP:OD1	1:R:22:ASP:C	2.58	0.41	
1:S:39:THR:O	1:S:40:ASN:HB2	2.20	0.41	
1:D:25:LYS:HE3	1:D:25:LYS:HB2	1.93	0.41	
1:G:72:SER:HB2	3:G:1001:HOH:O	2.20	0.41	
1:H:82:ASP:HA	3:H:1020:HOH:O	2.21	0.41	
1:I:89:PHE:N	3:I:1032:HOH:O	2.53	0.41	
1:L:82:ASP:HA	3:L:1018:HOH:O	2.18	0.41	
1:M:9:ALA:O	1:M:13:VAL:HG23	2.21	0.41	
1:M:51:THR:OG1	1:M:53:GLN:HG2	2.20	0.41	
1:N:84:PRO:HD2	3:N:1016:HOH:O	2.18	0.41	
1:A:108:VAL:HG23	3:A:1016:HOH:O	2.20	0.41	
1:G:85:ASN:HB2	3:G:1025:HOH:O	2.19	0.41	
1:G:91:ASP:OD2	1:G:91:ASP:C	2.59	0.41	
1:H:105:ASN:N	1:H:105:ASN:ND2	2.68	0.41	
1:Q:69:GLY:O	1:Q:70:GLY:C	2.57	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:J:98:GLN:NE2	1:J:98:GLN:N	2.69	0.41
1:P:106:ASP:CG	1:P:113:ARG:HH22	2.23	0.41
1:A:10:ASN:ND2	1:A:40:ASN:HD22	2.18	0.41
1:C:83:HIS:ND1	1:C:83:HIS:N	2.69	0.41
1:G:89:PHE:N	3:G:1017:HOH:O	2.54	0.41
1:L:113:ARG:HB2	1:L:113:ARG:NH1	2.32	0.41
1:R:105:ASN:N	1:R:105:ASN:ND2	2.65	0.41
1:U:83:HIS:ND1	1:U:83:HIS:N	2.67	0.41
1:V:90:CYS:O	1:V:92:LEU:N	2.54	0.41
1:C:51:THR:HG23	1:C:60:GLU:OE1	2.21	0.41
1:F:87:LYS:HA	1:F:87:LYS:HD2	1.65	0.41
1:N:83:HIS:ND1	1:N:83:HIS:N	2.69	0.41
1:O:90:CYS:HB3	1:O:93:LYS:CB	2.50	0.41
1:F:17:CYS:SG	1:F:27:TYR:HB2	2.61	0.41
1:I:13:VAL:HG22	1:I:30:TYR:CZ	2.56	0.41
1:K:62:ASN:OD1	1:K:64:ASP:N	2.48	0.41
1:S:22:ASP:C	1:S:22:ASP:OD1	2.59	0.41
1:T:49:THR:HG23	1:T:63:MET:HE3	2.02	0.41
1:V:74:CYS:CB	1:V:92:LEU:HD12	2.48	0.41
1:W:58:THR:O	1:W:59:PRO:C	2.58	0.41
1:B:113:ARG:HH11	1:B:113:ARG:CB	2.30	0.41
1:E:10:ASN:HD21	1:E:40:ASN:HD22	1.68	0.41
1:E:105:ASN:ND2	1:E:105:ASN:H	2.19	0.41
1:E:106:ASP:N	1:E:107:PRO:HD3	2.35	0.41
1:G:36:GLN:HA	1:G:37:PRO:HD3	2.00	0.41
1:G:53:GLN:HB2	1:G:56:THR:CG2	2.51	0.41
1:M:90:CYS:C	1:M:92:LEU:H	2.24	0.41
1:O:47:THR:HG23	1:O:49:THR:N	2.30	0.41
1:S:128:CYS:O	1:S:129:SER:C	2.59	0.41
1:T:84:PRO:O	1:T:85:ASN:C	2.59	0.41
1:U:10:ASN:HD21	1:U:40:ASN:HD22	1.69	0.41
1:U:13:VAL:HG22	1:U:30:TYR:CZ	2.56	0.41
1:U:69:GLY:O	1:U:72:SER:OG	2.36	0.41
1:U:91:ASP:OD2	1:U:91:ASP:N	2.54	0.41
1:D:32:ALA:C	1:D:34:GLY:H	2.25	0.41
1:G:117:CYS:O	1:G:121:GLY:HA2	2.21	0.41
1:N:113:ARG:NH1	1:N:113:ARG:HB2	2.36	0.41
1:U:13:VAL:O	1:U:16:PHE:HB3	2.21	0.41
1:X:117:CYS:CB	1:X:124:LYS:HE2	2.50	0.41
1:A:62:ASN:OD1	1:A:64:ASP:N	2.51	0.40
1:B:9:ALA:HA	3:B:1024:HOH:O	2.19	0.40



A + amo 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:57:VAL:HG23	1:E:58:THR:HG23	2.02	0.40
1:H:48:HIS:O	1:H:49:THR:C	2.58	0.40
1:J:73:CYS:HA	1:J:108:VAL:HG22	2.04	0.40
1:D:47:THR:O	1:D:48:HIS:HB2	2.21	0.40
1:E:36:GLN:HA	1:E:37:PRO:HD3	1.94	0.40
1:M:45:LEU:C	1:M:45:LEU:HD12	2.42	0.40
1:N:39:THR:O	1:N:78:ARG:NH2	2.41	0.40
1:W:90:CYS:C	1:W:92:LEU:N	2.74	0.40
1:E:25:LYS:HE3	1:E:25:LYS:HB2	1.95	0.40
1:H:90:CYS:O	1:H:92:LEU:N	2.53	0.40
1:K:92:LEU:HD22	1:K:97:VAL:CG2	2.51	0.40
1:N:14:LEU:HD21	1:N:38:ILE:HD13	2.04	0.40
1:N:98:GLN:NE2	1:N:98:GLN:N	2.70	0.40
1:R:9:ALA:O	1:R:13:VAL:HG23	2.22	0.40
1:X:105:ASN:ND2	1:X:105:ASN:N	2.69	0.40
1:B:25:LYS:HE3	1:B:25:LYS:HB2	1.91	0.40
1:C:90:CYS:HB3	1:C:93:LYS:CB	2.51	0.40
1:G:109:GLY:HA3	3:G:1009:HOH:O	2.22	0.40
1:H:25:LYS:HG2	1:H:29:ASP:OD2	2.22	0.40
1:K:103:CYS:C	1:K:105:ASN:H	2.24	0.40
1:R:53:GLN:HA	1:R:122:MET:HG2	2.03	0.40
1:U:98:GLN:H	1:U:98:GLN:NE2	2.15	0.40
1:X:14:LEU:HD21	1:X:38:ILE:HD13	2.04	0.40
1:B:90:CYS:C	1:B:92:LEU:N	2.67	0.40
1:D:84:PRO:CG	1:D:85:ASN:N	2.84	0.40
1:H:43:LYS:HE2	1:H:68:PHE:CZ	2.57	0.40
1:K:36:GLN:HA	1:K:37:PRO:HD3	1.96	0.40
1:P:13:VAL:O	1:P:16:PHE:HB3	2.21	0.40
1:Q:106:ASP:OD2	1:Q:113:ARG:NH2	2.49	0.40
1:T:50:GLY:HA3	1:T:60:GLU:C	2.41	0.40
1:U:91:ASP:HA	3:U:1013:HOH:O	2.20	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	114/152~(75%)	100 (88%)	9~(8%)	5~(4%)	2 5
1	В	115/152~(76%)	103~(90%)	8 (7%)	4 (4%)	3 8
1	С	114/152~(75%)	100 (88%)	12 (10%)	2(2%)	8 21
1	D	114/152~(75%)	100 (88%)	12 (10%)	2(2%)	8 21
1	Е	114/152~(75%)	100 (88%)	12 (10%)	2(2%)	8 21
1	F	116/152~(76%)	99~(85%)	14 (12%)	3 (3%)	5 13
1	G	114/152~(75%)	104 (91%)	7 (6%)	3(3%)	5 13
1	Н	114/152~(75%)	96 (84%)	13 (11%)	5(4%)	2 5
1	Ι	114/152~(75%)	101 (89%)	12 (10%)	1 (1%)	17 40
1	J	114/152~(75%)	103 (90%)	8 (7%)	3(3%)	5 13
1	Κ	114/152~(75%)	104 (91%)	7 (6%)	3(3%)	5 13
1	L	114/152~(75%)	106 (93%)	7~(6%)	1 (1%)	17 40
1	М	114/152~(75%)	104 (91%)	6 (5%)	4 (4%)	3 8
1	Ν	115/152~(76%)	100 (87%)	12 (10%)	3~(3%)	5 13
1	Ο	114/152~(75%)	101 (89%)	10 (9%)	3~(3%)	5 13
1	Р	114/152~(75%)	106 (93%)	7~(6%)	1 (1%)	17 40
1	Q	114/152~(75%)	96 (84%)	11 (10%)	7~(6%)	1 2
1	R	111/152~(73%)	99~(89%)	10 (9%)	2(2%)	8 21
1	S	114/152~(75%)	99~(87%)	11 (10%)	4 (4%)	3 8
1	Т	114/152~(75%)	99~(87%)	10 (9%)	5(4%)	2 5
1	U	114/152~(75%)	105 (92%)	7 (6%)	2(2%)	8 21
1	V	114/152~(75%)	103 (90%)	8 (7%)	3 (3%)	5 13
1	W	$\overline{114/152}\ (75\%)$	95~(83%)	15 (13%)	4 (4%)	3 8
1	Х	114/152~(75%)	102 (90%)	9 (8%)	3 (3%)	5 13
All	All	2737/3648 (75%)	2425 (89%)	237 (9%)	75 (3%)	5 12

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	90	CYS
1	D	84	PRO
1	F	91	ASP



Mol	Chain	Res	Type
1	G	84	PRO
1	Ι	90	CYS
1	J	91	ASP
1	М	48	HIS
1	М	84	PRO
1	М	90	CYS
1	Q	48	HIS
1	S	47	THR
1	S	48	HIS
1	S	84	PRO
1	W	84	PRO
1	Х	91	ASP
1	А	91	ASP
1	С	104	ALA
1	Е	91	ASP
1	F	86	PRO
1	F	87	LYS
1	Н	49	THR
1	Н	84	PRO
1	Н	90	CYS
1	J	84	PRO
1	К	84	PRO
1	K	104	ALA
1	Q	71	ALA
1	Q	91	ASP
1	R	63	MET
1	S	33	SER
1	Т	40	ASN
1	Т	48	HIS
1	Т	90	CYS
1	U	91	ASP
1	V	84	PRO
1	V	90	CYS
1	W	51	THR
1	W	104	ALA
1	Х	84	PRO
1	Х	90	CYS
1	С	91	ASP
1	E	72	SER
1	J	82	ASP
1	М	91	ASP
1	N	40	ASN



Mol	Chain	Res	Type
1	0	90	CYS
1	Р	104	ALA
1	Q	40	ASN
1	Q	50	GLY
1	Q	90	CYS
1	Т	84	PRO
1	W	74	CYS
1	А	82	ASP
1	В	84	PRO
1	Н	91	ASP
1	K	90	CYS
1	N	84	PRO
1	0	84	PRO
1	0	104	ALA
1	R	40	ASN
1	U	40	ASN
1	А	104	ALA
1	В	54	ALA
1	В	128	CYS
1	G	90	CYS
1	N	90	CYS
1	Т	50	GLY
1	V	91	ASP
1	Н	70	GLY
1	L	84	PRO
1	G	70	GLY
1	Q	70	GLY
1	В	70	GLY
1	D	127	GLY
1	A	84	PRO

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	eric Outliers Percent	
1	А	97/123~(79%)	94~(97%)	3~(3%)	40 69



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	В	98/123~(80%)	95~(97%)	3 (3%)	40	69
1	С	97/123~(79%)	95~(98%)	2 (2%)	53	80
1	D	97/123~(79%)	93~(96%)	4 (4%)	30	59
1	Е	97/123~(79%)	95~(98%)	2 (2%)	53	80
1	F	98/123~(80%)	93~(95%)	5 (5%)	24	50
1	G	97/123~(79%)	93~(96%)	4 (4%)	30	59
1	Н	97/123~(79%)	90~(93%)	7 (7%)	14	34
1	Ι	97/123~(79%)	90 (93%)	7 (7%)	14	34
1	J	97/123~(79%)	92~(95%)	5 (5%)	23	49
1	Κ	97/123~(79%)	93~(96%)	4 (4%)	30	59
1	L	97/123~(79%)	95~(98%)	2 (2%)	53	80
1	М	97/123~(79%)	90~(93%)	7 (7%)	14	34
1	Ν	98/123~(80%)	93~(95%)	5(5%)	24	50
1	Ο	97/123~(79%)	94~(97%)	3~(3%)	40	69
1	Р	97/123~(79%)	93~(96%)	4 (4%)	30	59
1	Q	97/123~(79%)	92~(95%)	5(5%)	23	49
1	R	96/123~(78%)	89~(93%)	7 (7%)	14	33
1	S	97/123~(79%)	91~(94%)	6 (6%)	18	40
1	Т	97/123~(79%)	95~(98%)	2(2%)	53	80
1	U	97/123~(79%)	92~(95%)	5(5%)	23	49
1	V	97/123~(79%)	89 (92%)	8 (8%)	11	26
1	W	97/123~(79%)	93~(96%)	4 (4%)	30	59
1	Х	97/123~(79%)	93~(96%)	4 (4%)	30	59
All	All	$23\overline{30/2952}$ (79%)	2222 (95%)	108 (5%)	27	54

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All (108) residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	74	CYS
1	А	90	CYS
1	А	105	ASN
1	В	74	CYS
1	В	84	PRO
1	В	129	SER



Mol	Chain	Res	Type
1	С	74	CYS
1	С	90	CYS
1	D	74	CYS
1	D	90	CYS
1	D	91	ASP
1	D	105	ASN
1	Е	83	HIS
1	Е	124	LYS
1	F	74	CYS
1	F	83	HIS
1	F	90	CYS
1	F	102	THR
1	F	129	SER
1	G	74	CYS
1	G	90	CYS
1	G	118	THR
1	G	129	SER
1	Н	16	PHE
1	Н	44	MET
1	Н	74	CYS
1	Н	90	CYS
1	Н	91	ASP
1	Н	105	ASN
1	Н	120	CYS
1	Ι	53	GLN
1	Ι	74	CYS
1	Ι	84	PRO
1	Ι	89	PHE
1	Ι	90	CYS
1	Ι	98	GLN
1	Ι	105	ASN
1	J	21	VAL
1	J	47	THR
1	J	74	CYS
1	J	83	HIS
1	J	89	PHE
1	K	21	VAL
1	K	74	CYS
1	K	89	PHE
1	K	90	CYS
1	L	74	CYS
1	L	105	ASN

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Mol	Chain	Res	Type
1	М	45	LEU
1	М	47	THR
1	М	53	GLN
1	М	74	CYS
1	М	83	HIS
1	М	90	CYS
1	М	105	ASN
1	Ν	74	CYS
1	N	90	CYS
1	N	98	GLN
1	N	105	ASN
1	N	129	SER
1	0	47	THR
1	0	74	CYS
1	0	90	CYS
1	Р	74	CYS
1	Р	83	HIS
1	Р	101	THR
1	Р	105	ASN
1	Q	74	CYS
1	Q	83	HIS
1	Q	90	CYS
1	Q	98	GLN
1	Q	118	THR
1	R	39	THR
1	R	74	CYS
1	R	83	HIS
1	R	89	PHE
1	R	90	CYS
1	R	105	ASN
1	R	120	CYS
1	S	63	MET
1	S	73	CYS
1	S	74	CYS
1	S	77	CYS
1	S	89	PHE
1	S	105	ASN
1	T	74	CYS
1	T	90	CYS
1	U	72	SER
1	U	74	CYS
1	U	83	HIS



Mol	Chain	Res	Type
1	U	98	GLN
1	U	124	LYS
1	V	29	ASP
1	V	46	CYS
1	V	74	CYS
1	V	84	PRO
1	V	89	PHE
1	V	90	CYS
1	V	101	THR
1	V	120	CYS
1	W	83	HIS
1	W	98	GLN
1	W	113	ARG
1	W	129	SER
1	Х	74	CYS
1	Х	83	HIS
1	Х	90	CYS
1	Х	105	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	40	ASN
1	А	85	ASN
1	А	105	ASN
1	В	40	ASN
1	В	48	HIS
1	В	53	GLN
1	В	85	ASN
1	С	40	ASN
1	С	53	GLN
1	D	40	ASN
1	D	53	GLN
1	D	105	ASN
1	D	114	ASN
1	Е	40	ASN
1	Е	53	GLN
1	Е	62	ASN
1	Е	105	ASN
1	F	40	ASN
1	F	53	GLN
1	F	83	HIS



Mol	Chain	Res	Type
1	F	85	ASN
1	F	114	ASN
1	G	48	HIS
1	G	105	ASN
1	Н	53	GLN
1	Н	62	ASN
1	Н	105	ASN
1	Ι	40	ASN
1	Ι	48	HIS
1	Ι	53	GLN
1	Ι	105	ASN
1	Ι	114	ASN
1	J	40	ASN
1	J	48	HIS
1	J	53	GLN
1	K	40	ASN
1	Κ	53	GLN
1	L	40	ASN
1	L	53	GLN
1	L	105	ASN
1	М	48	HIS
1	М	53	GLN
1	М	105	ASN
1	М	114	ASN
1	Ν	40	ASN
1	N	48	HIS
1	Ν	53	GLN
1	0	40	ASN
1	Р	105	ASN
1	Р	114	ASN
1	Q	40	ASN
1	Q	53	GLN
1	Q	62	ASN
1	Q	83	HIS
1	Q	85	ASN
1	Q	105	ASN
1	R	40	ASN
1	R	53	GLN
1	R	85	ASN
1	R	105	ASN
1	S	40	ASN
1	S	48	HIS



Mol	Chain	Res	Type
1	S	53	GLN
1	S	105	ASN
1	S	114	ASN
1	Т	40	ASN
1	Т	48	HIS
1	Т	62	ASN
1	U	40	ASN
1	U	53	GLN
1	U	83	HIS
1	V	53	GLN
1	V	105	ASN
1	W	10	ASN
1	W	40	ASN
1	W	53	GLN
1	W	83	HIS
1	W	114	ASN
1	Х	40	ASN
1	Х	105	ASN
1	Х	114	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)

Of 48 ligands modelled in this entry, 48 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 $>$	$\#RSRZ{>}2$	$OWAB(Å^2)$	Q<0.9
1	А	118/152~(77%)	-0.20	0 100 100	22, 32, 52, 67	0
1	В	119/152~(78%)	0.02	3 (2%) 57 59	21, 36, 53, 82	0
1	С	118/152~(77%)	0.01	4 (3%) 45 45	24, 36, 53, 73	0
1	D	118/152~(77%)	0.02	5 (4%) 36 35	25, 36, 54, 77	0
1	Е	118/152~(77%)	0.05	3 (2%) 57 59	23, 34, 56, 79	0
1	F	120/152~(78%)	0.10	7 (5%) 23 22	19, 35, 59, 75	0
1	G	118/152~(77%)	0.04	3 (2%) 57 59	24, 33, 53, 70	0
1	Н	118/152~(77%)	0.07	0 100 100	22, 36, 58, 76	0
1	Ι	118/152~(77%)	-0.03	2 (1%) 70 72	23, 34, 53, 66	0
1	J	118/152~(77%)	-0.00	5 (4%) 36 35	22, 35, 54, 76	0
1	K	118/152~(77%)	0.02	4 (3%) 45 45	21, 33, 55, 75	0
1	L	118/152~(77%)	-0.12	1 (0%) 86 87	19, 31, 48, 61	0
1	М	118/152~(77%)	0.08	5 (4%) 36 35	18, 32, 55, 81	0
1	Ν	119/152~(78%)	0.08	3 (2%) 57 59	23, 38, 57, 81	0
1	Ο	118/152~(77%)	-0.01	5 (4%) 36 35	17, 31, 49, 71	0
1	Р	118/152~(77%)	-0.16	3 (2%) 57 59	18, 29, 47, 67	0
1	Q	118/152~(77%)	0.33	8 (6%) 17 15	30, 42, 69, 97	0
1	R	117/152~(76%)	-0.03	3 (2%) 56 57	20, 33, 56, 74	0
1	S	118/152~(77%)	0.02	5 (4%) 36 35	18, 32, 62, 83	0
1	Т	118/152~(77%)	0.27	9 (7%) 13 12	24, 38, 62, 75	0
1	U	118/152~(77%)	0.09	2 (1%) 70 72	24, 39, 53, 69	0
1	V	$1\overline{18/152}\ (77\%)$	0.02	2 (1%) 70 72	22, 32, 55, 73	0
1	W	118/152~(77%)	0.14	4 (3%) 45 45	29, 42, 60, 75	0
1	X	118/152 (77%)	0.21	5 (4%) 36 35	25, 40, 56, 66	0
				(Continued on new	rt page



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
All	All	2835/3648~(77%)	0.04	91 (3%) 47 48	17, 35, 57, 97	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	М	48	HIS	12.2
1	S	85	ASN	5.9
1	Т	85	ASN	5.7
1	N	8	PRO	5.7
1	Ν	89	PHE	5.6
1	Е	89	PHE	5.3
1	D	85	ASN	5.2
1	S	48	HIS	5.1
1	R	89	PHE	5.1
1	Q	48	HIS	4.8
1	0	89	PHE	4.8
1	W	89	PHE	4.7
1	М	47	THR	4.6
1	В	8	PRO	4.5
1	С	85	ASN	4.4
1	W	85	ASN	4.3
1	F	87	LYS	4.2
1	Х	85	ASN	4.0
1	J	89	PHE	4.0
1	S	47	THR	3.8
1	V	85	ASN	3.8
1	F	88	GLY	3.6
1	0	129	SER	3.6
1	G	89	PHE	3.6
1	Q	85	ASN	3.6
1	Е	85	ASN	3.4
1	R	85	ASN	3.4
1	В	85	ASN	3.3
1	Q	126	TYR	3.3
1	L	85	ASN	3.2
1	Т	16	PHE	3.2
1	J	32	ALA	3.1
1	J	34	GLY	3.1
1	D	89	PHE	3.1
1	К	90	CYS	3.1
1	N	85	ASN	3.1
1	S	90	CYS	3.1



Mol	Chain	Res	Type	RSRZ
1	U	89	PHE	3.1
1	K	85	ASN	2.9
1	М	49	THR	2.9
1	В	89	PHE	2.9
1	D	90	CYS	2.9
1	Ι	129	SER	2.8
1	K	89	PHE	2.8
1	Х	30	TYR	2.8
1	G	85	ASN	2.8
1	J	90	CYS	2.7
1	Х	89	PHE	2.7
1	Ι	34	GLY	2.6
1	Q	32	ALA	2.6
1	Т	126	TYR	2.6
1	Т	48	HIS	2.6
1	S	89	PHE	2.6
1	Q	33	SER	2.6
1	С	90	CYS	2.5
1	Т	33	SER	2.5
1	F	86	PRO	2.5
1	U	84	PRO	2.5
1	G	32	ALA	2.5
1	F	33	SER	2.5
1	Т	125	GLY	2.5
1	0	90	CYS	2.5
1	Р	89	PHE	2.5
1	D	32	ALA	2.4
1	Т	49	THR	2.4
1	Κ	34	GLY	2.4
1	Ο	34	GLY	2.4
1	Р	85	ASN	2.4
1	Ο	85	ASN	2.4
1	Р	90	CYS	2.4
1	R	84	PRO	2.4
1	С	89	PHE	2.3
1	V	89	PHE	2.3
1	Q	47	THR	2.3
1	С	34	GLY	2.3
1	М	85	ASN	2.3
1	D	129	SER	2.2
1	М	90	CYS	2.2
1	F	85	ASN	2.2



Mol	Chain	Res	Type	RSRZ
1	Т	63	MET	2.2
1	Q	89	PHE	2.2
1	Q	91	ASP	2.1
1	W	84	PRO	2.1
1	Х	90	CYS	2.1
1	Т	91	ASP	2.1
1	Е	84	PRO	2.1
1	F	89	PHE	2.1
1	J	84	PRO	2.1
1	W	125	GLY	2.0
1	F	90	CYS	2.0
1	Х	16	PHE	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, 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	B-factors(Å ²)	Q < 0.9
2	ZN	N	998	1/1	0.90	0.16	62,62,62,62	0
2	ZN	Х	999	1/1	0.92	0.09	$54,\!54,\!54,\!54$	0
2	ZN	Р	998	1/1	0.93	0.13	76,76,76,76	0
2	ZN	K	998	1/1	0.94	0.11	66, 66, 66, 66	0
2	ZN	D	998	1/1	0.94	0.14	75,75,75,75	0
2	ZN	Ι	998	1/1	0.95	0.16	67,67,67,67	0
2	ZN	0	999	1/1	0.95	0.11	$67,\!67,\!67,\!67$	0
2	ZN	В	998	1/1	0.95	0.10	67,67,67,67	0
2	ZN	Т	998	1/1	0.95	0.19	78,78,78,78	0
2	ZN	L	998	1/1	0.95	0.18	74,74,74,74	0
2	ZN	В	999	1/1	0.96	0.10	74,74,74,74	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(A ²)	Q<0.9			
2	ŹN	0	998	1/1	0.96	0.11	84,84,84,84	0			
2	ZN	N	999	1/1	0.96	0.10	79,79,79,79	0			
2	ZN	Q	999	1/1	0.97	0.07	49,49,49,49	0			
2	ZN	0	998	1/1	0.97	0.13	55,55,55,55	0			
2	ZN	G	998	1/1	0.97	0.10	$51,\!51,\!51,\!51$	0			
2	ZN	V	998	1/1	0.97	0.13	83,83,83,83	0			
2	ZN	Х	998	1/1	0.97	0.14	$72,\!72,\!72,\!72$	0			
2	ZN	А	998	1/1	0.97	0.10	$72,\!72,\!72,\!72$	0			
2	ZN	С	998	1/1	0.98	0.13	84,84,84,84	0			
2	ZN	Ι	999	1/1	0.98	0.08	46, 46, 46, 46	0			
2	ZN	J	998	1/1	0.98	0.11	85,85,85,85	0			
2	ZN	Р	999	1/1	0.98	0.09	40,40,40,40	0			
2	ZN	Q	998	1/1	0.98	0.08	76,76,76,76	0			
2	ZN	D	999	1/1	0.98	0.12	63,63,63,63	0			
2	ZN	R	998	1/1	0.98	0.11	64,64,64,64	0			
2	ZN	R	999	1/1	0.98	0.08	46,46,46,46	0			
2	ZN	S	998	1/1	0.98	0.14	49,49,49,49	0			
2	ZN	S	999	1/1	0.98	0.07	39,39,39,39	0			
2	ZN	Е	998	1/1	0.98	0.11	$73,\!73,\!73,\!73$	0			
2	ZN	М	998	1/1	0.98	0.14	$62,\!62,\!62,\!62$	0			
2	ZN	U	999	1/1	0.98	0.07	$50,\!50,\!50,\!50$	0			
2	ZN	М	999	1/1	0.98	0.08	42,42,42,42	0			
2	ZN	V	999	1/1	0.98	0.06	42,42,42,42	0			
2	ZN	W	998	1/1	0.98	0.11	80,80,80,80	0			
2	ZN	W	999	1/1	0.98	0.07	48,48,48,48	0			
2	ZN	С	999	1/1	0.98	0.06	45,45,45,45	0			
2	ZN	Н	998	1/1	0.98	0.14	78,78,78,78	0			
2	ZN	G	999	1/1	0.99	0.06	46,46,46,46	0			
2	ZN	Т	999	1/1	0.99	0.05	$35,\!35,\!35,\!35$	0			
2	ZN	Κ	999	1/1	0.99	0.08	46,46,46,46	0			
2	ZN	Е	999	1/1	0.99	0.10	44,44,44,44	0			
2	ZN	L	999	1/1	0.99	0.09	40,40,40,40	0			
2	ZN	Н	999	1/1	0.99	0.09	41,41,41,41	0			
2	ZN	F	998	1/1	0.99	0.16	73,73,73,73	0			
2	ZN	F	999	1/1	0.99	0.07	42,42,42,42	0			
2	ZN	A	999	1/1	0.99	0.08	43,43,43,43	0			
2	ZN	J	999	1/1	0.99	0.07	40,40,40,40	0			

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Other polymers (i)6.5

There are no such residues in this entry.

