



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:32 PM GMT

PDB ID : 2GA6
Title : The crystal structure of SARS nsp10 without zinc ion as additive
Authors : Su, D.; Lou, Z.; Sun, F.; Zhai, Y.; Yang, H.; Rao, Z.
Deposited on : 2006-03-08
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

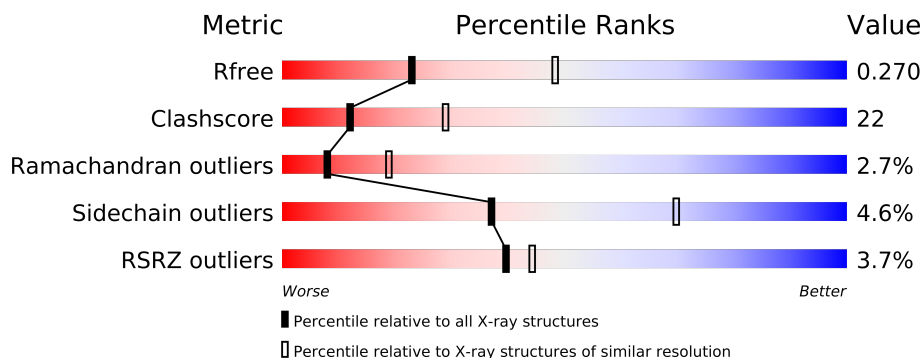
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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.







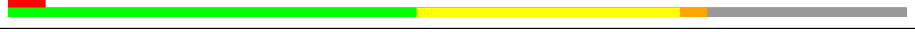




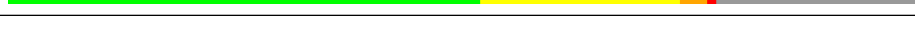
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	152	
1	B	152	
1	C	152	
1	D	152	
1	E	152	
1	F	152	
1	G	152	
1	H	152	
1	I	152	
1	J	152	
1	K	152	
1	L	152	
1	M	152	
1	N	152	

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Mol	Chain	Length	Quality of chain
1	O	152	
1	P	152	
1	Q	152	
1	R	152	
1	S	152	
1	T	152	
1	U	152	
1	V	152	
1	W	152	
1	X	152	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21977 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

- Molecule 1 is a protein called orfla polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	B	119	Total	C	N	O	S	0	0	0
			880	549	148	168	15			
1	C	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	D	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	E	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	F	120	Total	C	N	O	S	0	0	0
			883	551	148	169	15			
1	G	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	H	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	I	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	J	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	K	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	L	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	M	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	N	119	Total	C	N	O	S	0	0	0
			880	549	148	168	15			
1	O	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	P	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	R	117	Total	C	N	O	S	0	0	0
			863	538	144	166	15			
1	S	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	T	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	U	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	V	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	W	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			
1	X	118	Total	C	N	O	S	0	0	0
			873	544	147	167	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total	Zn	0	0
			2	2		
2	K	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	W	2	Total	Zn	0	0
			2	2		
2	N	2	Total	Zn	0	0
			2	2		
2	X	2	Total	Zn	0	0
			2	2		
2	S	2	Total	Zn	0	0
			2	2		
2	J	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	V	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	2	Total 2	Zn 2	0	0
2	M	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	U	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	Q	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	T	2	Total 2	Zn 2	0	0
2	O	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total 46	O 46	0	0
3	B	37	Total 37	O 37	0	0
3	C	43	Total 43	O 43	0	0
3	D	29	Total 29	O 29	0	0
3	E	42	Total 42	O 42	0	0
3	F	44	Total 44	O 44	0	0

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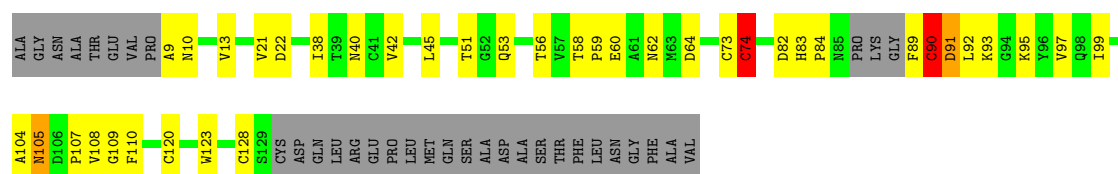
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	48	Total 48	O 48	0	0
3	H	43	Total 43	O 43	0	0
3	I	37	Total 37	O 37	0	0
3	J	30	Total 30	O 30	0	0
3	K	40	Total 40	O 40	0	0
3	L	48	Total 48	O 48	0	0
3	M	56	Total 56	O 56	0	0
3	N	31	Total 31	O 31	0	0
3	O	53	Total 53	O 53	0	0
3	P	51	Total 51	O 51	0	0
3	Q	34	Total 34	O 34	0	0
3	R	39	Total 39	O 39	0	0
3	S	34	Total 34	O 34	0	0
3	T	33	Total 33	O 33	0	0
3	U	26	Total 26	O 26	0	0
3	V	47	Total 47	O 47	0	0
3	W	37	Total 37	O 37	0	0
3	X	35	Total 35	O 35	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

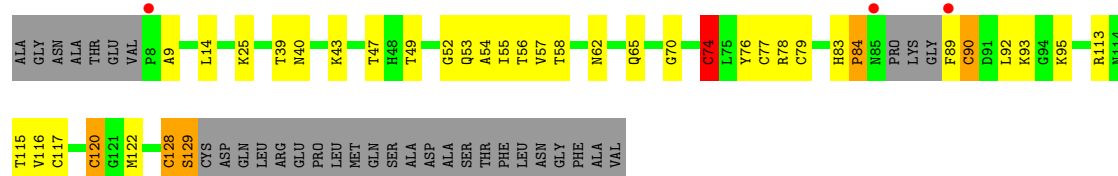
• Molecule 1: orf1a polypeptide

Chain A:



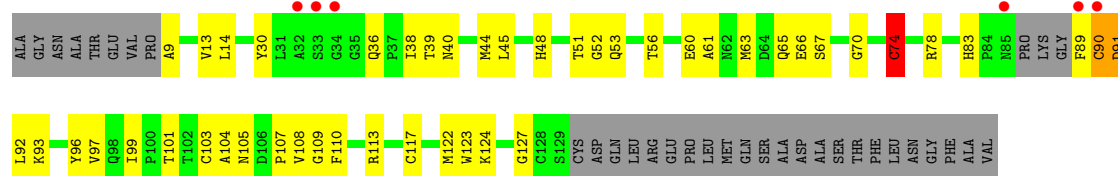
• Molecule 1: orf1a polypeptide

Chain B:



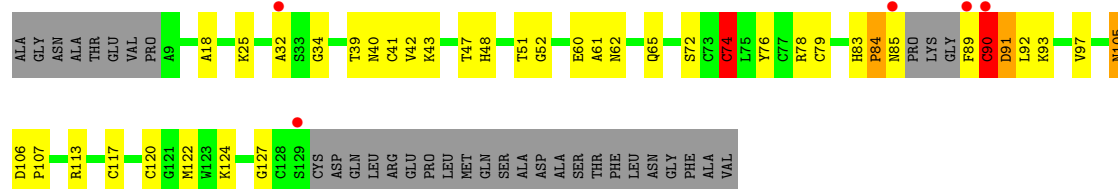
• Molecule 1: orf1a polypeptide

Chain C:

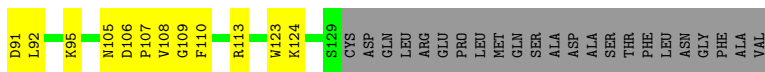


• Molecule 1: orf1a polypeptide

Chain D:



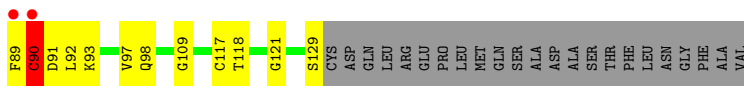
• Molecule 1: orf1a polypeptide



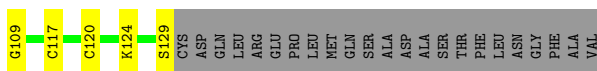
- Molecule 1: orf1a polypeptide



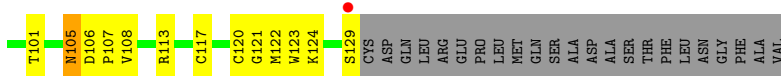
- Molecule 1: orf1a polyprotein



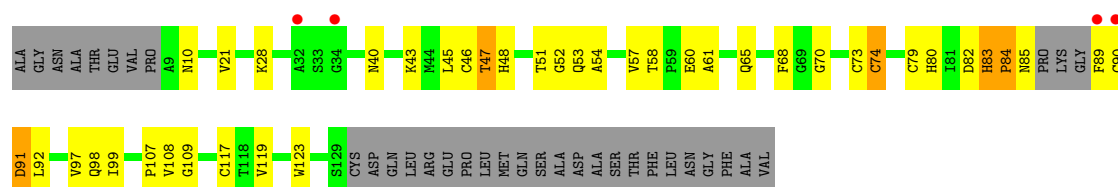
- Molecule 1: orf1a polypeptide



- Molecule 1: orf1a polyprotein

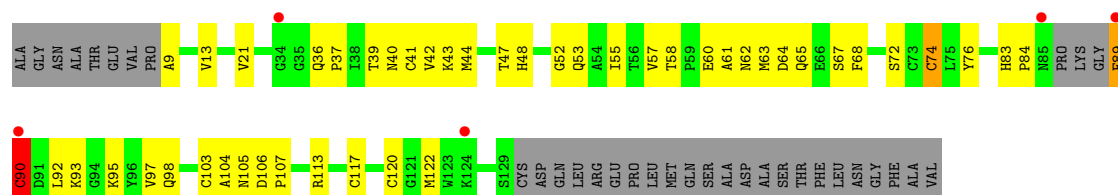


- Molecule 1: orf1a polyprotein



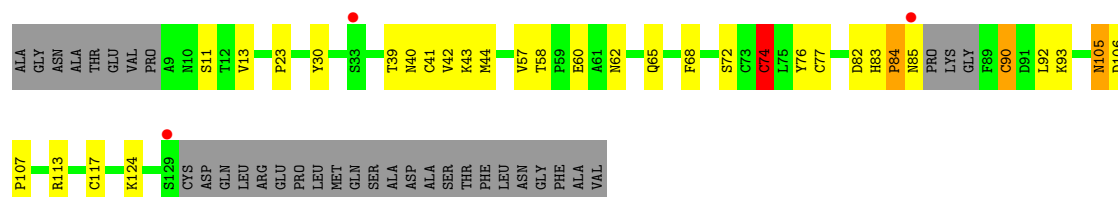
- Molecule 1: orf1a polypeptide

Chain K:



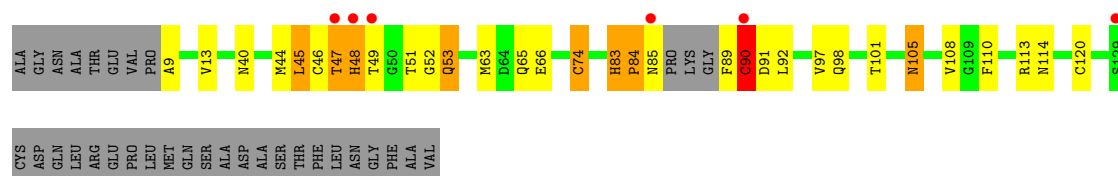
- Molecule 1: orf1a polypeptide

Chain L:



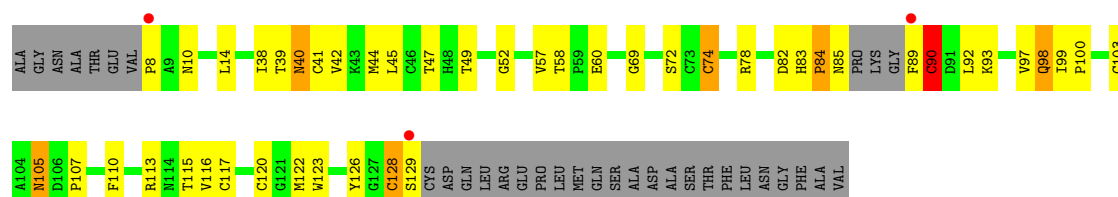
- Molecule 1: orf1a polypeptide

Chain M:



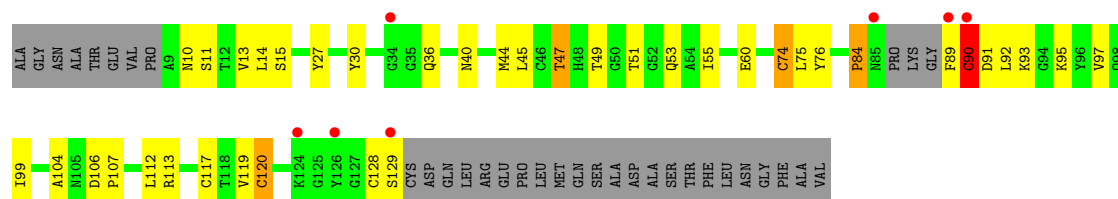
- Molecule 1: orf1a polypeptide

Chain N:



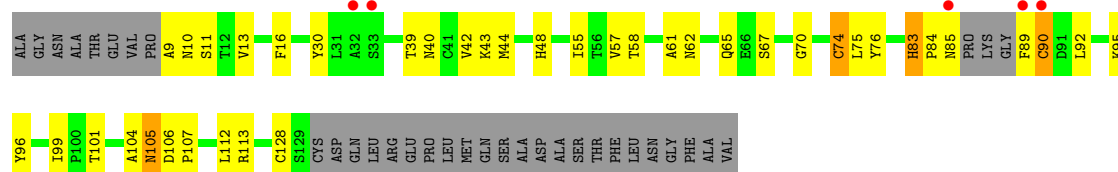
- Molecule 1: orf1a polypeptide

Chain O:



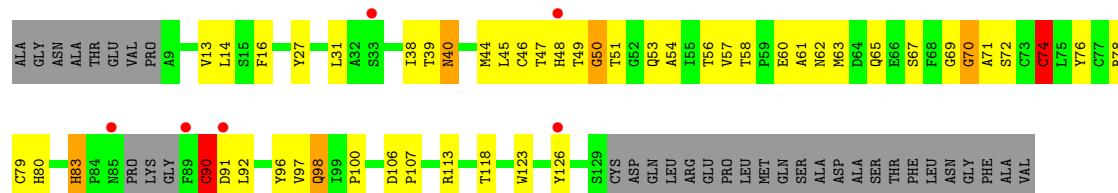
• Molecule 1: orf1a polypeptide

Chain P:



• Molecule 1: orf1a polypeptide

Chain Q:



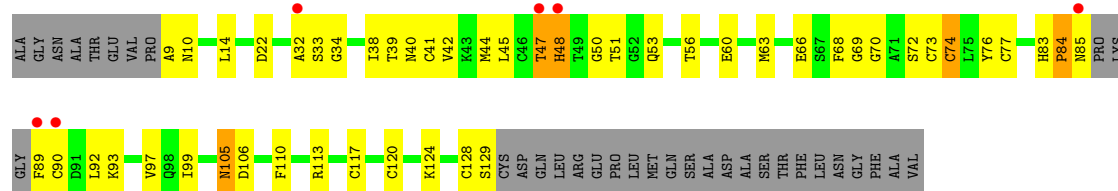
• Molecule 1: orf1a polypeptide

Chain R:



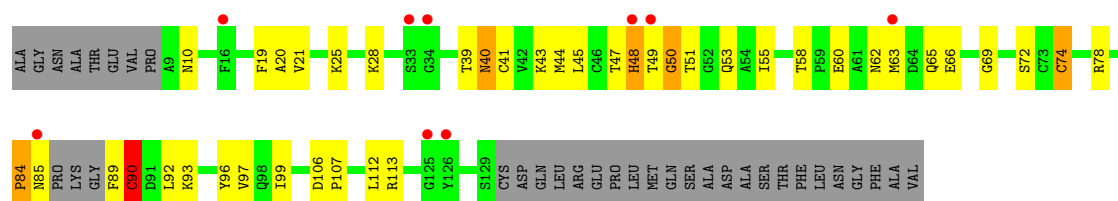
• Molecule 1: orf1a polypeptide

Chain S:



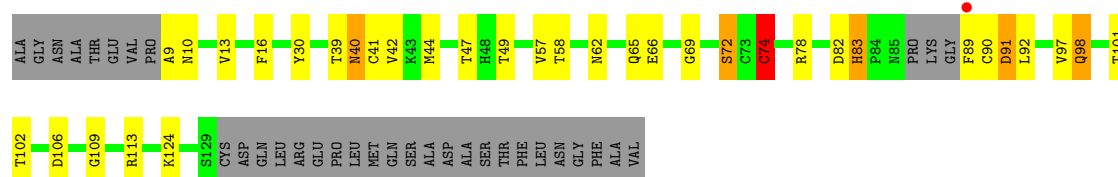
• Molecule 1: orf1a polypeptide

Chain T:



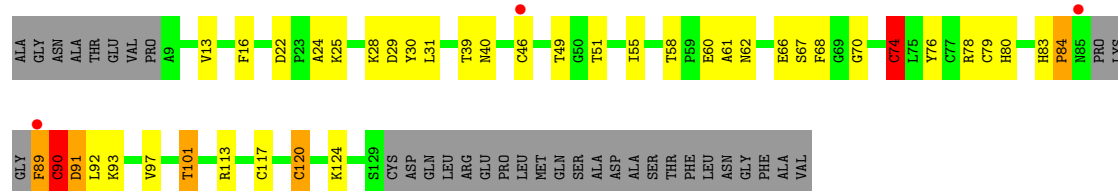
• Molecule 1: orf1a polypeptide

Chain U:



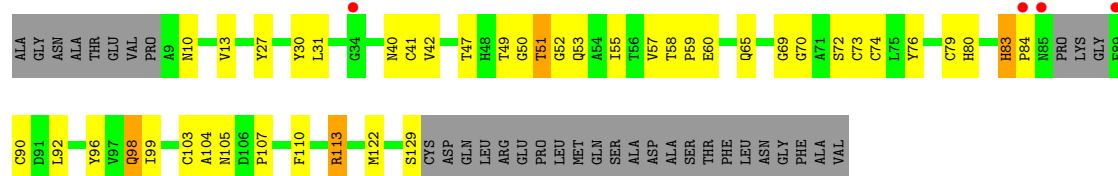
• Molecule 1: orf1a polypeptide

Chain V:



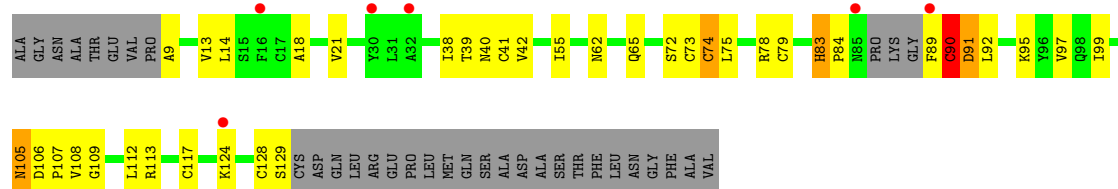
• Molecule 1: orf1a polypeptide

Chain W:



• Molecule 1: orf1a polypeptide

Chain X:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	159.74Å 322.70Å 162.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 45.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 98.6 (45.78-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.267 0.225 , 0.270	Depositor DCC
R_{free} test set	5553 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 222527 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/892	0.70	2/1211 (0.2%)
1	B	0.44	0/900	0.80	4/1222 (0.3%)
1	C	0.41	0/892	0.70	1/1211 (0.1%)
1	D	0.41	0/892	0.71	2/1211 (0.2%)
1	E	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	H	0.41	0/892	0.71	2/1211 (0.2%)
1	I	0.43	0/892	0.71	2/1211 (0.2%)
1	J	0.41	0/892	0.67	1/1211 (0.1%)
1	K	0.44	0/892	0.70	2/1211 (0.2%)
1	L	0.43	0/892	0.74	3/1211 (0.2%)
1	M	0.44	0/892	0.70	1/1211 (0.1%)
1	N	0.40	0/900	0.78	3/1222 (0.2%)
1	O	0.42	0/892	0.79	3/1211 (0.2%)
1	P	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	T	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	X	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:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	90	CYS	CA-CB-SG	9.60	131.27	114.00
1	B	117	CYS	CA-CB-SG	9.40	130.92	114.00
1	B	90	CYS	CA-CB-SG	9.18	130.52	114.00
1	N	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	O	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	O	90	CYS	CA-CB-SG	7.78	128.00	114.00
1	N	90	CYS	CA-CB-SG	7.75	127.94	114.00
1	I	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	P	90	CYS	CA-CB-SG	6.33	125.39	114.00
1	M	74	CYS	CA-CB-SG	6.18	125.12	114.00
1	C	74	CYS	CA-CB-SG	6.12	125.01	114.00
1	O	120	CYS	CA-CB-SG	6.07	124.92	114.00
1	K	74	CYS	CA-CB-SG	6.03	124.85	114.00
1	T	90	CYS	CA-CB-SG	5.91	124.64	114.00
1	B	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	A	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	I	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	N	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	E	74	CYS	CA-CB-SG	5.33	123.60	114.00
1	A	74	CYS	CA-CB-SG	5.32	123.57	114.00
1	H	74	CYS	CA-CB-SG	5.28	123.50	114.00
1	H	90	CYS	CA-CB-SG	5.21	123.38	114.00
1	P	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	T	74	CYS	CA-CB-SG	5.10	123.18	114.00
1	B	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(°)	Ideal(°)
1	X	74	CYS	CA-CB-SG	5.02	123.04	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	873	0	829	34	0
1	B	880	0	837	36	0
1	C	873	0	829	41	0
1	D	873	0	829	41	0
1	E	873	0	829	37	0
1	F	883	0	845	40	0
1	G	873	0	829	40	0
1	H	873	0	830	38	0
1	I	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	M	873	0	829	46	0
1	N	880	0	837	42	0
1	O	873	0	829	33	0
1	P	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	T	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	X	873	0	830	35	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	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	T	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	X	2	0	0	0	0
3	A	46	0	0	8	0
3	B	37	0	0	4	0
3	C	43	0	0	1	0
3	D	29	0	0	0	0
3	E	42	0	0	3	0
3	F	44	0	0	6	0
3	G	48	0	0	6	0
3	H	43	0	0	7	0
3	I	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	M	56	0	0	10	0
3	N	31	0	0	8	0
3	O	53	0	0	1	0
3	P	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	T	33	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	U	26	0	0	7	0
3	V	47	0	0	6	0
3	W	37	0	0	4	0
3	X	35	0	0	2	0
All	All	21977	0	19924	882	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (882) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:H	1:S:105:ASN:HD22	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:O:120:CYS:SG	1:O: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:N	1:M:105:ASN:HD22	1.76	0.83
1:I:90:CYS:HB3	1:I:93:LYS:HB2	1.63	0.81
1:V:90:CYS:C	1:V:92:LEU:H	1.83	0.81
1:B:120:CYS:SG	1:B:128:CYS:HA	2.21	0.81
1:H:105:ASN:H	1:H:105:ASN:HD22	1.26	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(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:I:74:CYS:HB2	1:I:92:LEU:HD12	1.70	0.74
1:A:90:CYS:C	1:A:92:LEU:H	1.89	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:X:39:THR:O	1:X:78:ARG:NH2	2.21	0.73
1:T:49:THR:OG1	1:T:63:MET:HE1	1.87	0.73
1:P:57:VAL:HG23	1:P:58:THR:HG23	1.69	0.73
1:E:113:ARG:HB2	1:E:113:ARG:HH11	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:N:90:CYS:HB3	1:N:93:LYS:N	2.02	0.70
1:S:105:ASN:N	1:S:105:ASN:HD22	1.88	0.70
1:L:74:CYS:HB2	1:L:92:LEU:HD12	1.73	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
1:T:41:CYS:HA	1:T:72:SER:OG	1.92	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HB2	1:W:113:ARG:HH11	1.57	0.69
1:K:113:ARG:HB2	1:K:113:ARG:HH11	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:W:51:THR:OG1	1:W:53:GLN:HG3	1.93	0.68
1:V:76:TYR:HB2	1:V:83:HIS:CD2	2.28	0.68
1:N:39:THR:O	1:N:40:ASN:HB2	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:U:9:ALA:O	1:U:13:VAL:HG23	1.95	0.67
1:E:83:HIS:ND1	1:E:83:HIS:N	2.42	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:Q:98:GLN:HE21	1:Q:98:GLN:N	1.92	0.67
1:P:83:HIS:CD2	1:P:90:CYS:N	2.63	0.67
1:O:47:THR:HG23	1:O:49:THR:H	1.58	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:ND2	1:M:105:ASN:H	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:Q:51:THR:OG1	1:Q:53:GLN:HG2	1.94	0.66
1:E:42:VAL:HG22	1:E:72:SER:OG	1.95	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:H	1:I:105:ASN:HD22	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:N:90:CYS:CB	1:N:93:LYS:HB2	2.27	0.65
1:H:89:PHE:O	1:H:90:CYS:C	2.34	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:Q:53:GLN:HB2	1:Q:56:THR:CG2	2.28	0.64
1:A:107:PRO:HB2	3:A:1016:HOH:O	1.97	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:G:74:CYS:HB2	1:G:92:LEU:HD12	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: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:O:74:CYS:HB2	1:O:92:LEU:HD12	1.79	0.63
1:N:57:VAL:HG23	1:N:58:THR:HG23	1.81	0.63
1:O:90:CYS:C	1:O:92:LEU:H	2.00	0.63
1:N:14:LEU:HD13	3:N:1022:HOH:O	1.98	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:O:89:PHE:O	1:O:90:CYS:C	2.37	0.63
1:D:48:HIS:HA	1:D:61:ALA:O	1.98	0.63
1:U:90:CYS:C	1:U:92:LEU:H	2.01	0.63
1:Q:40:ASN:HB3	1:X:21:VAL:HG11	1.79	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: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: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: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:J:45:LEU:HD11	1:M:47:THR:C	2.18	0.62
1:X:42:VAL:HG22	1:X:72:SER:OG	1.99	0.62
1:W:76:TYR:HB2	1:W:83:HIS:HD2	1.63	0.62
1:H:9:ALA:HB3	3:H:1015:HOH:O	1.99	0.62
1:Q:98:GLN:H	1:Q:98:GLN:HE21	1.47	0.62
1:M:108:VAL:HA	3:M:1035:HOH:O	1.99	0.62
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:68:PHE:HB3	3:F:1027:HOH:O	2.00	0.62
1:I:90:CYS:CB	1:I:93:LYS:HB2	2.28	0.62
1:E:50:GLY:HA3	1:E:60:GLU:HA	1.81	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:R:70:GLY:HA2	1:R:97:VAL:HG23	1.82	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: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:I:90:CYS:HB3	1:I:93:LYS:CB	2.30	0.61
1:A:73:CYS:HA	3:A:1016:HOH:O	2.01	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:N:90:CYS:C	1:N:92:LEU:N	2.53	0.61
1:L:44:MET:SD	3:L:1006:HOH:O	2.55	0.61
1:C:39:THR:O	1:C:40:ASN:HB2	2.00	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: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:G:14:LEU:HD21	1:G:38:ILE:HD13	1.84	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:P:105:ASN:ND2	1:P:105:ASN:H	1.95	0.59
1:K:89:PHE:O	1:K:90:CYS:C	2.40	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:Q:45:LEU:HB2	1:R:45:LEU:HB2	1.85	0.58
1:C:44:MET:CE	1:D:42:VAL:HG12	2.33	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:K:90:CYS:HB3	1:K:93:LYS:N	2.12	0.58
1:C:70:GLY:HA2	1:C:97:VAL:HG23	1.85	0.58
1:C:53:GLN:HA	1:C:122:MET:HG2	1.84	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:C:96:TYR:OH	1:D:42:VAL:HG21	2.03	0.58
1:R:39:THR:O	1:R:40:ASN:HB2	2.04	0.58
1:R:51:THR:HG23	1:R:60:GLU:OE1	2.04	0.58
1:M:84:PRO:HG2	1:M:85:ASN:H	1.67	0.58
1:F:92:LEU:HD22	1:F:97:VAL:CG2	2.33	0.58
1:W:98:GLN:HE21	1:W:98:GLN:H	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:T:39:THR:O	1:T:78:ARG:NH2	2.35	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: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:I:90:CYS:HB3	1:I:93:LYS:H	1.69	0.57
1:H:105:ASN:N	1:H:105:ASN:HD22	1.97	0.57
1:W:98:GLN:HE21	1:W:98:GLN:N	2.02	0.57
1:Q:46:CYS:SG	1:Q:61:ALA:HB3	2.43	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:X:105:ASN:H	1:X:105:ASN:ND2	2.01	0.57
1:X:89:PHE:O	1:X:91:ASP:N	2.37	0.57
1:J:28:LYS:HG2	3:J:1001:HOH:O	2.02	0.57
1:F:61:ALA:HB2	1:F:67:SER:OG	2.05	0.57
1:U:42:VAL:HG23	3:U:1006:HOH:O	2.05	0.57
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:D:89:PHE:O	1:D:90:CYS:C	2.42	0.57
1:M:46:CYS:SG	1:M:48:HIS:CD2	2.91	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:90:CYS:CB	1:K:93:LYS:HB2	2.35	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:Q:39:THR:O	1:Q:40:ASN:HB2	2.05	0.56
1:Q:13:VAL:O	1:Q:16:PHE:HB3	2.05	0.56
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:X:75:LEU:HD22	1:X:112:LEU:HD11	1.87	0.56
1:G:89:PHE:O	1:G:90:CYS:C	2.43	0.56
1:E:113:ARG:NH1	1:E:113:ARG:HB2	2.19	0.56
1:O:51:THR:OG1	1:O:53:GLN:HG3	2.05	0.56
1:J:51:THR:HG23	1:J:60:GLU:OE1	2.04	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:Q:96:TYR:OH	1:R:42:VAL:HG11	2.06	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:A:105:ASN:HD22	1:A:105:ASN:H	1.53	0.56
1:E:53:GLN:HB2	1:E:56:THR:CG2	2.35	0.56
1:O: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:K:39:THR:O	1:K:40:ASN:HB2	2.05	0.56
1:S:105:ASN:ND2	1:S:105:ASN:H	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:O:90:CYS:HB3	1:O:93:LYS:N	2.16	0.55
1:A:89:PHE:O	1:A:90:CYS:C	2.44	0.55
1:T:106:ASP:OD2	1:T:113:ARG:NH2	2.37	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:D:18:ALA:HB2	1:D:79:CYS:HB3	1.89	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:H:70:GLY:HA3	1:H:92:LEU:O	2.05	0.55
1:W:52:GLY:HA2	1:W:65:GLN:OE1	2.05	0.55
1:B:77:CYS:SG	1:B:83:HIS:NE2	2.78	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:10:ASN:ND2	1:R:40:ASN:HD22	2.04	0.55
1:K:57:VAL:HG23	1:K:58:THR:HG23	1.89	0.55
1:R:68:PHE:HD1	3:R:1017:HOH:O	1.89	0.55
1:D:90:CYS:C	1:D:92:LEU:N	2.58	0.55
1:C:44:MET:HG2	1:C:67:SER:O	2.06	0.55
1:A:13:VAL:HB	3:A:1020:HOH:O	2.07	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:HB2	1:U:113:ARG:NH1	2.22	0.55
1:R:105:ASN:N	1:R:105:ASN:HD22	1.98	0.54
1:A:9:ALA:O	1:A:13:VAL:HG23	2.06	0.54
1:V:58:THR:O	1:V:60:GLU:HG2	2.07	0.54
1:I:101:THR:O	1:M:101:THR:CG2	2.55	0.54
1:C:122:MET:HE2	1:C:127:GLY:HA3	1.89	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:K:61:ALA:HB2	1:K:67:SER:OG	2.07	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:X:99:ILE:HD13	1:X:107:PRO:HA	1.89	0.54
1:H:41:CYS:HA	1:H:72:SER:OG	2.07	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:K:90:CYS:C	1:K:92:LEU:N	2.61	0.53
1:K:62:ASN:OD1	1:K:65:GLN:HG3	2.08	0.53
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:I:53:GLN:HB2	1:I:56:THR:CG2	2.38	0.53
1:H:9:ALA:HB1	3:H:1034:HOH:O	2.06	0.53
1:E:47:THR:HG22	1:E:48:HIS:N	2.23	0.53
1:T:58:THR:O	1:T:60:GLU:HG2	2.08	0.53
1:O:90:CYS:CB	1:O:93:LYS:HB2	2.38	0.53
1:C:9:ALA:HB3	3:C:1008:HOH:O	2.07	0.53
1:U:89:PHE:HB3	3:U:1008:HOH:O	2.09	0.53
1:T:28:LYS:HE3	3:T:1013:HOH:O	2.08	0.53
1:U:98:GLN:NE2	1:U:98:GLN:N	2.57	0.53
1:O:27:TYR:O	1:O:30:TYR:HB3	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:90:CYS:CB	1:B:93:LYS:HB2	2.36	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:I:117:CYS:HB3	1:I:120:CYS:HB2	1.91	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:T:48:HIS:CG	1:T:49:THR:H	2.27	0.53
1:R:83:HIS:ND1	1:R:89:PHE:HA	2.24	0.53
1:W:110:PHE:HA	1:W:113:ARG:HH12	1.74	0.53
1:M:92:LEU:HD22	1:M:97:VAL:CG2	2.38	0.53
1:Q:44:MET:HE3	1:R:44:MET:SD	2.49	0.53
1:P:10:ASN:HB2	3:P:1045:HOH:O	2.09	0.53
1:O:99:ILE:HD13	1:O:107:PRO:HA	1.90	0.53
1:T:84:PRO:HA	3:T:1015:HOH:O	2.09	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:K:53:GLN:HA	1:K:122:MET:HG2	1.91	0.53
1:P:11:SER:HB2	3:P:1031:HOH:O	2.08	0.53
1:M:113:ARG:NE	3:M:1003:HOH:O	2.41	0.53
1:U:74:CYS:HB2	1:U:92:LEU:HD12	1.91	0.53
1:R:92:LEU:HD22	1:R:97:VAL:CG2	2.38	0.52
1:K:52:GLY:HA2	1:K:65:GLN:OE1	2.09	0.52
1:W:47:THR:O	1:W:49:THR:HG23	2.09	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:S:50:GLY:HA3	1:S:60:GLU:OE1	2.09	0.52
1:G:84:PRO:HG2	1:G:85:ASN:N	2.23	0.52
1:T:10:ASN:ND2	1:T:40:ASN:HD22	2.08	0.52
1:C:44:MET:HE2	1:D:42:VAL:CG1	2.39	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:S:9:ALA:HB3	3:S:1003:HOH:O	2.10	0.52
1:J:10:ASN:ND2	1:J:40:ASN:HD22	2.07	0.52
1:A:90:CYS:O	1:A:92:LEU:N	2.42	0.52
1:F:113:ARG:NH1	1:F:113:ARG:HB2	2.25	0.52
1:G:56:THR:HG21	1:G:60:GLU:HG3	1.92	0.52
1:F:43:LYS:HE2	1:F:66:GLU:OE1	2.10	0.52
1:J:92:LEU:HD22	1:J:97:VAL:HG22	1.92	0.52
1:D:52:GLY:O	1:D:122:MET:HG2	2.09	0.52
1:R:43:LYS:HE2	1:R:66:GLU:OE1	2.10	0.52
1:M:120:CYS:HB3	3:M:1022:HOH:O	2.09	0.52
1:W:113:ARG:NE	3:W:1021:HOH:O	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:10:ASN:HD21	1:R:40:ASN:HD22	1.58	0.52
1:D:74:CYS:CB	1:D:92:LEU:HD12	2.36	0.52
1:R:42:VAL:HG22	1:R:72:SER:OG	2.09	0.52
1:P:84:PRO:HG2	1:P:85:ASN:H	1.75	0.52
1:W:42:VAL:HG22	1:W:72:SER:OG	2.10	0.52
1:B:47:THR:HG23	1:B:49:THR:H	1.76	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:R:47:THR:HB	1:R:49:THR:OG1	2.10	0.51
1:Q:44:MET:HG3	1:Q:96:TYR:HD2	1.74	0.51
1:O:10:ASN:ND2	1:O:40:ASN:ND2	2.57	0.51
1:A:97:VAL:HB	3:A:1029:HOH:O	2.11	0.51
1:V:97:VAL:HB	3:V:1035:HOH:O	2.10	0.51
1:N:83:HIS:HB3	3:N:1016:HOH:O	2.10	0.51
1:K:9:ALA:N	3:K:1027:HOH:O	2.43	0.51
1:Q:61:ALA:HB2	1:Q:67:SER:OG	2.11	0.51
1:O:10:ASN:ND2	1:O:40:ASN:HD22	2.09	0.51
1:E:39:THR:O	1:E:40:ASN:HB2	2.10	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: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:L:105:ASN:H	1:L:105:ASN:HD22	1.58	0.51
1:P:106:ASP:OD2	1:P:113:ARG:NH2	2.44	0.51
1:J:52:GLY:HA2	1:J:65:GLN:OE1	2.10	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:G:47:THR:OG1	1:G:48:HIS:CD2	2.64	0.51
1:L:39:THR:O	1:L:40:ASN:HB2	2.11	0.51
1:E:47:THR:O	1:E:48:HIS:HB2	2.09	0.51
1:B:39:THR:O	1:B:40:ASN:HB2	2.10	0.51
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: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:G:69:GLY:O	1:G:72:SER:HB3	2.12	0.50
1:Q:47:THR:O	1:Q:49:THR:N	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:45:LEU:HD23	1:D:43:LYS:HD3	1.92	0.50
1:N:47:THR:O	1:N:49:THR:HG23	2.10	0.50
1:M:48:HIS:HE1	1:M:66:GLU:OE2	1.95	0.50
1:S:105:ASN:ND2	1:S:105:ASN:N	2.57	0.50
1:S:106:ASP:OD2	1:S: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:B:89:PHE:O	1:F:87:LYS:HD3	2.12	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:F:9:ALA:O	1:F:13:VAL:HG23	2.11	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:M:47:THR:O	1:M:47:THR:OG1	2.29	0.50
1:Q:44:MET:HG3	1:Q:96:TYR:CD2	2.47	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: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:V:90:CYS:HB3	1:V:93:LYS:HB2	1.93	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: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:I:98:GLN:N	1:I:98:GLN:NE2	2.59	0.49
1:H:108:VAL:HA	3:H:1027:HOH:O	2.12	0.49
1:E:90:CYS:C	1:E:92:LEU:H	2.15	0.49
1:E:14:LEU:HD21	1:E:38:ILE:HD13	1.94	0.49
1:P:83:HIS:CD2	1:P:90:CYS:H	2.30	0.49
1:B:113:ARG:HB2	1:B:113:ARG:NH1	2.28	0.49
1:A:120:CYS:SG	1:A:128:CYS:HA	2.52	0.49
1:W:10:ASN:ND2	1:W:40:ASN:ND2	2.61	0.49
1:L:13:VAL:HG22	1:L:30:TYR:CZ	2.47	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:X:38:ILE:HG22	1:X:78:ARG:NH2	2.28	0.49
1:V:39:THR:O	1:V:40:ASN:HB2	2.13	0.49
1:D:51:THR:HG23	1:D:60:GLU:OE1	2.11	0.49
1:M:52:GLY:HA2	1:M:65:GLN:OE1	2.12	0.49
1:H:109:GLY:HA3	3:H:1019:HOH:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:117:CYS:HB2	1:C:124:LYS:HD2	1.95	0.49
1:M:83:HIS:ND1	1:M:89:PHE:HB3	2.27	0.49
1:V:31:LEU:HD13	3:V:1016:HOH:O	2.13	0.49
1:O:44:MET:CE	1:P:42:VAL:HG13	2.42	0.49
1:H:92:LEU:HD22	1:H:97:VAL:CG2	2.43	0.49
1:W:110:PHE:HA	1:W:113:ARG:NH1	2.28	0.49
1:M:83:HIS:CE1	1:M:89:PHE:HB3	2.47	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:CD2	1:P:89:PHE:N	2.81	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:E:113:ARG:CB	1:E:113:ARG:HH11	2.24	0.49
1:K:113:ARG:HB2	1:K:113:ARG:NH1	2.25	0.49
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
3:M:1042:HOH:O	1:T:25:LYS:HE2	2.11	0.48
1:J:43:LYS:HG2	1:J:68:PHE:CE2	2.48	0.48
1:X:91:ASP:HB2	3:X:1011:HOH:O	2.12	0.48
1:W:13:VAL:HG22	1:W:30:TYR:CZ	2.49	0.48
1:D:42:VAL:HG23	1:D:72:SER:OG	2.12	0.48
1:C:103:CYS:O	1:C:105:ASN:N	2.46	0.48
1:Q:62:ASN:HB3	1:Q:65:GLN:CG	2.42	0.48
1:L:58:THR:O	1:L:60:GLU:HG2	2.13	0.48
1:Q:47:THR:O	1:Q:49:THR:HG23	2.13	0.48
1:W:103:CYS:C	1:W:105:ASN:H	2.17	0.48
1:P:75:LEU:HD22	1:P:112:LEU:HD11	1.96	0.48
1:Q:100:PRO:HG2	1:Q:126:TYR:CD2	2.49	0.48
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:O:119:VAL:HG22	1:V:124:LYS:HD3	1.95	0.48
1:C:91:ASP:N	1:C:91:ASP:OD2	2.47	0.48
1:N:74:CYS:CB	1:N:92:LEU:HD12	2.42	0.48
1:X:91:ASP:OD2	1:X:91:ASP:N	2.46	0.48
1:J:90:CYS:O	1:J:92:LEU:N	2.45	0.48
1:V:66:GLU:HG2	1:V:101:THR:CG2	2.44	0.48
1:K:55:ILE:HG22	1:K:95:LYS:HD3	1.96	0.48
1:W:96:TYR:OH	1:X:42:VAL:HG21	2.14	0.48
1:I:105:ASN:H	1:I:105:ASN:ND2	2.11	0.48
1:A:51:THR:HG23	1:A:60:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:91:ASP:N	1:D:91:ASP:OD2	2.47	0.48
1:F:83:HIS:CD2	1:F:83:HIS:N	2.80	0.48
1:V:90:CYS:HB3	1:V:93:LYS:CB	2.44	0.48
1:T:112:LEU:HD13	3:T:1013:HOH:O	2.14	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:T:44:MET:HG3	1:T:96:TYR:HD2	1.78	0.48
1:M:44:MET:SD	3:M:1015:HOH:O	2.61	0.48
1:A:110:PHE:HE2	1:A:123:TRP:CE2	2.31	0.48
1:B:90:CYS:CB	1:B:93:LYS:H	2.16	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: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:T:41:CYS:HA	1:T:72:SER:HG	1.78	0.47
1:N:44:MET:SD	3:N:1003:HOH:O	2.61	0.47
1:L:62:ASN:OD1	1:L:65:GLN:HG3	2.14	0.47
1:O:11:SER:O	1:O:15:SER:HB2	2.13	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:V:66:GLU:HG2	1:V:101:THR:HG22	1.95	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: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:U:10:ASN:ND2	1:U:40:ASN:HD22	2.12	0.47
1:E:14:LEU:HD11	1:E:78:ARG:NH1	2.30	0.47
1:X:90:CYS:O	1:X:92:LEU:N	2.46	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:R:83:HIS:HB2	3:R:1022:HOH:O	2.14	0.47
1:B:39:THR:O	1:B:78:ARG:NH2	2.37	0.47
1:P:70:GLY:HA3	1:P:92:LEU:O	2.14	0.47
1:O:13:VAL:HG13	1:O:14:LEU:N	2.29	0.47
1:F:42:VAL:O	1:F:42:VAL:HG23	2.13	0.47
1:O:75:LEU:HD22	1:O:112:LEU:HD11	1.97	0.47
1:X:128:CYS:O	1:X:129:SER:HB2	2.15	0.47
1:O:106:ASP:OD2	1:O:113:ARG:NH2	2.47	0.47
1:Q:45:LEU:HB2	1:R:45:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:58:THR:O	1:K:60:GLU:HG2	2.14	0.47
1:F:32:ALA:C	1:F:34:GLY:H	2.17	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:I:48:HIS:HA	1:I:61:ALA:O	2.14	0.47
1:O:55:ILE:HG22	1:O:95:LYS:HD2	1.97	0.47
1:A:42:VAL:O	1:A:42:VAL:HG23	2.14	0.47
1:Q:90:CYS:O	1:Q:90:CYS:SG	2.72	0.47
1:N:110:PHE:HE2	1:N:123:TRP:CE2	2.33	0.47
1:S:47:THR:HG23	1:S:48:HIS:N	2.18	0.46
1:H:76:TYR:HB2	1:H:83:HIS:CD2	2.50	0.46
1:U:9:ALA:HB3	3:U:1011:HOH:O	2.14	0.46
1:P:48:HIS:HA	1:P:61:ALA:O	2.15	0.46
1:D:105:ASN:HD22	1:D:105:ASN:H	1.63	0.46
1:B:129:SER:HA	3:B:1036:HOH:O	2.15	0.46
1:S:117:CYS:HB3	1:S:120:CYS:HB3	1.96	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:D:76:TYR:HB2	1:D:83:HIS:CD2	2.51	0.46
1:U:90:CYS:O	1:U:92:LEU:N	2.39	0.46
1:S:117:CYS:HB2	1:S:124:LYS:HD2	1.97	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:K:90:CYS:HB2	1:K:93:LYS:HB2	1.97	0.46
1:T:48:HIS:CG	1:T:49:THR:N	2.84	0.46
1:O:44:MET:HE1	1:P:42:VAL:CG1	2.46	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:R:84:PRO:HG2	1:R:85:ASN:H	1.80	0.46
1:V:76:TYR:CB	1:V:83:HIS:CD2	2.97	0.46
1:G:40:ASN:HB2	3:G:1046:HOH:O	2.15	0.46
1:W:79:CYS:O	1:W:80:HIS:HB2	2.15	0.46
1:D:39:THR:O	1:D:40:ASN:HB2	2.15	0.46
1:I:108:VAL:HA	3:I:1020:HOH:O	2.16	0.46
1:C:110:PHE:HE2	1:C:123:TRP:CE2	2.32	0.46
1:A:99:ILE:HD13	1:A:107:PRO:HA	1.98	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:F:120:CYS:SG	1:F:128:CYS:HA	2.56	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:90:CYS:SG	1:C:93:LYS:HB2	2.56	0.46
1:C:39:THR:O	1:C:78:ARG:NH2	2.42	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:S:92:LEU:HD22	1:S:97:VAL:CG2	2.46	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:K:43:LYS:HG3	1:K:68:PHE:CE2	2.51	0.46
1:C:38:ILE:HD12	1:C:108:VAL:HG11	1.96	0.46
1:Q:51:THR:HG23	1:Q:60:GLU:OE1	2.16	0.45
1:K:113:ARG:HH11	1:K:113:ARG:CB	2.25	0.45
1:N:82:ASP:C	1:N:83:HIS:ND1	2.69	0.45
1:N:52:GLY:O	1:N:122:MET:HE2	2.15	0.45
1:F:14:LEU:HD21	1:F:38:ILE:HD13	1.97	0.45
1:H:90:CYS:CB	1:H:93:LYS:HB2	2.42	0.45
1:A:92:LEU:HD22	1:A:97:VAL:CG2	2.46	0.45
1:E:54:ALA:HB1	1:E:123:TRP:CE2	2.50	0.45
1:C:109:GLY:HA3	1:C:113:ARG:HH21	1.81	0.45
1:A:56:THR:O	1:A:95:LYS:HB3	2.16	0.45
1:G:76:TYR:HB2	1:G:83:HIS:CD2	2.52	0.45
1:F:89:PHE:CD2	1:F:89:PHE:N	2.82	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:E:113:ARG:NH2	3:E:1006:HOH:O	2.48	0.45
1:I:61:ALA:HB2	1:I:67:SER:OG	2.16	0.45
1:V:68:PHE:HB2	3:V:1035:HOH:O	2.16	0.45
1:P:9:ALA:O	1:P:13:VAL:HG23	2.17	0.45
1:G:92:LEU:HD22	1:G:97:VAL:CG2	2.47	0.45
1:F:58:THR:O	1:F:60:GLU:HG2	2.16	0.45
1:U:69:GLY:N	3:U:1006:HOH:O	2.49	0.45
1:U:113:ARG:HH11	1:U:113:ARG:CB	2.29	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:S:32:ALA:O	1:S:34:GLY:N	2.50	0.45
1:V:61:ALA:HB2	1:V:67:SER:OG	2.17	0.45
1:R:99:ILE:HD13	1:R:107:PRO:HA	1.97	0.45
1:C:99:ILE:HD13	1:C:107:PRO:HA	1.99	0.45
1:C:13:VAL:HG13	1:C:14:LEU:N	2.32	0.45
1:J:91:ASP:N	1:J:91:ASP:OD2	2.50	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:A:21:VAL:HG23	1:A:22:ASP:N	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:92:LEU:HD22	1:X:97:VAL:CG2	2.46	0.45
1:S:69:GLY:O	1:S:72:SER:HB3	2.17	0.45
1:M:53:GLN:HE21	1:M:53:GLN:HA	1.80	0.45
1:A:51:THR:OG1	1:A:53:GLN:HG3	2.16	0.45
1:S:14:LEU:HD21	1:S:38:ILE:HD13	1.99	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:P:55:ILE:HG22	1:P:95:LYS:HD2	1.98	0.45
1:X:55:ILE:HG22	1:X:95:LYS:HD2	1.99	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:G:62:ASN:OD1	1:G:65:GLN:HG3	2.17	0.45
1:O:30:TYR:HE2	1:O:36:GLN:O	2.00	0.45
1:N:84:PRO:O	1:N:85:ASN:C	2.54	0.45
1:E:44:MET:HG2	1:E:67:SER:O	2.17	0.45
1:B:14:LEU:HD22	1:B:79:CYS:SG	2.57	0.45
1:I:66:GLU:HB2	1:I:68:PHE:CE1	2.53	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:N:90:CYS:HB2	1:N:93:LYS:CB	2.42	0.44
1:G:90:CYS:HB3	1:G:93:LYS:HB2	1.96	0.44
1:B:90:CYS:HB2	1:B:93:LYS:CB	2.39	0.44
1:W:58:THR:O	1:W:60:GLU:HG2	2.17	0.44
1:I:120:CYS:HB3	1:I:122:MET:H	1.82	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:I:106:ASP:N	1:I:107:PRO:HD3	2.31	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:C:103:CYS:C	1:C:105:ASN:N	2.70	0.44
1:W:42:VAL:HG23	3:W:1030:HOH:O	2.17	0.44
1:S:42:VAL:O	1:S:42:VAL:HG23	2.17	0.44
1:A:73:CYS:O	1:A:108:VAL:HG22	2.17	0.44
1:L:43:LYS:HE2	1:L:68:PHE:CZ	2.52	0.44
1:E:10:ASN:ND2	1:E:40:ASN:HD22	2.15	0.44
1:B:115:THR:HG22	1:B:116:VAL:N	2.32	0.44
1:S:120:CYS:SG	1:S:128:CYS:HA	2.57	0.44
1:F:39:THR:O	1:F:40:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:84:PRO:CG	1:H:85:ASN:H	2.27	0.44
1:T:41:CYS:CA	1:T:72:SER:OG	2.64	0.44
1:R:70:GLY:HA3	1:R:92:LEU:O	2.17	0.44
1:G:58:THR:O	1:G:60:GLU:HG2	2.18	0.44
1:R:58:THR:O	1:R:60:GLU:HG2	2.18	0.44
1:M:40:ASN:CB	1:R:21:VAL:HG11	2.47	0.44
1:F:13:VAL:HG22	1:F:30:TYR:CZ	2.53	0.44
1:N:103:CYS:C	1:N:105:ASN:H	2.20	0.44
1:L:42:VAL:HG22	1:L:72:SER:OG	2.17	0.44
1:J:10:ASN:ND2	1:J:40:ASN:ND2	2.66	0.44
1:I:129:SER:HA	3:I:1023:HOH:O	2.18	0.44
1:T:55:ILE:HD13	1:T:92:LEU:CD2	2.48	0.44
3:O:1039:HOH:O	1:Q:57:VAL:HG11	2.17	0.44
1:E:70:GLY:HA3	1:E:92:LEU:O	2.18	0.44
1:M:45:LEU:HB2	1:N:45:LEU:HD13	1.99	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:P:61:ALA:HB2	1:P:67:SER:OG	2.18	0.44
1:J:54:ALA:HB1	1:J:123:TRP:CE2	2.53	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:Q:62:ASN:CG	1:Q:63:MET:H	2.20	0.44
1:I:51:THR:OG1	1:I:53:GLN:CG	2.66	0.44
1:G:92:LEU:HD22	1:G:97:VAL:HG22	2.00	0.43
1:F:70:GLY:HA3	1:F:92:LEU:O	2.18	0.43
1:I:42:VAL:HG22	1:I:72:SER:OG	2.18	0.43
1:E:47:THR:CG2	1:E:48:HIS:N	2.81	0.43
1:B:62:ASN:OD1	1:B:65:GLN:HG3	2.17	0.43
1:S:44:MET:SD	1:T:44:MET:HE1	2.58	0.43
1:O:76:TYR:CZ	1:O:84:PRO:HG3	2.53	0.43
1:H:39:THR:O	1:H:40:ASN:HB2	2.17	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:M:45:LEU:HA	1:N:45:LEU:HD13	2.00	0.43
1:J:92:LEU:HD22	1:J:97:VAL:CG2	2.48	0.43
1:U:113:ARG:HH11	1:U:113:ARG:HB2	1.82	0.43
1:K:76:TYR:HB2	1:K:83:HIS:CD2	2.53	0.43
1:C:30:TYR:HE2	1:C:36:GLN:O	2.01	0.43
1:T:89:PHE:O	1:T:90:CYS:C	2.57	0.43
1:Q:45:LEU:HB2	1:R:45:LEU:CB	2.46	0.43
1:P:76:TYR:CE2	1:P:84:PRO:HD3	2.53	0.43
1:N:99:ILE:HD13	1:N:107:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:84:PRO:O	1:F:85:ASN:C	2.57	0.43
1:J:83:HIS:HE1	3:J:1010:HOH:O	2.00	0.43
1:E:44:MET:HE3	1:F:44:MET:SD	2.59	0.43
1:K:106:ASP:N	1:K:107:PRO:HD3	2.33	0.43
1:H:28:LYS:HG2	3:H:1028:HOH:O	2.17	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:M:63:MET:HA	3:M:1021:HOH:O	2.17	0.43
1:H:83:HIS:HB3	1:H:84:PRO:HD2	2.00	0.43
1:F:54:ALA:HB1	1:F:123:TRP:CE2	2.54	0.43
1:I:39:THR:O	1:I:40:ASN:HB2	2.19	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:M:48:HIS:HB3	3:M:1021:HOH:O	2.17	0.43
1:X:105:ASN:N	1:X:105:ASN:HD22	2.08	0.43
1:F:80:HIS:N	3:F:1036:HOH:O	2.50	0.43
1:U:92:LEU:HD22	1:U:97:VAL:CG2	2.49	0.43
1:R:89:PHE:O	1:R:90:CYS:C	2.56	0.43
1:I:98:GLN:N	1:I:98:GLN:HE21	2.14	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:N:100:PRO:HG2	1:N:126:TYR:CD2	2.53	0.43
1:U:47:THR:O	1:U:49:THR:HG23	2.19	0.43
1:W:27:TYR:CE2	1:W:31:LEU:HD11	2.54	0.43
1:V:91:ASP:OD2	1:V:91:ASP:N	2.51	0.43
1:K:92:LEU:HD22	1:K:97:VAL:HG22	2.00	0.43
1:Q:92:LEU:HD22	1:Q:97:VAL:CG2	2.48	0.43
1:G:53:GLN:O	1:G:98:GLN:NE2	2.45	0.43
1:F:47:THR:HG22	1:F:49:THR:HG23	2.00	0.43
1:J:51:THR:OG1	1:J:53:GLN:HG3	2.19	0.43
1:S:51:THR:OG1	1:S:53:GLN:HG3	2.19	0.43
1:O:45:LEU:HD23	1:P:43:LYS:HE2	2.00	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:M:113:ARG:NH1	3:M:1001:HOH:O	2.50	0.43
1:A:58:THR:O	1:A:59:PRO:C	2.57	0.43
1:R:62:ASN:O	1:R:64:ASP:N	2.52	0.43
1:U:98:GLN:HE21	1:U:98:GLN:N	2.14	0.42
1:M:113:ARG:HB2	1:M:113:ARG:HH11	1.84	0.42
1:K:48:HIS:CB	1:K:63:MET:HE1	2.48	0.42
1:J:99:ILE:HD13	1:J:107:PRO:HA	2.00	0.42
1:Q:27:TYR:CE2	1:Q:31:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:13:VAL:HG22	1:P:30:TYR:CZ	2.54	0.42
1:I:106:ASP:OD2	1:I:113:ARG:NH2	2.52	0.42
1:W:73:CYS:HB3	3:W:1023:HOH:O	2.19	0.42
1:O:91:ASP:N	1:O:91:ASP:OD2	2.52	0.42
1:I:52:GLY:HA2	1:I:65:GLN:OE1	2.18	0.42
1:H:79:CYS:O	1:H:81:ILE:HG23	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:V:13:VAL:O	1:V:16:PHE:HB3	2.19	0.42
1:Q:106:ASP:N	1:Q:107:PRO:HD3	2.35	0.42
1:L:106:ASP:N	1:L:107:PRO:HD3	2.34	0.42
1:M:48:HIS:C	1:M:49:THR:HG23	2.40	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:G:84:PRO:CG	1:G:85:ASN:H	2.18	0.42
1:L:84:PRO:CG	1:L:85:ASN:H	2.31	0.42
1:I:39:THR:O	1:I:78:ARG:NH2	2.45	0.42
1:Q:58:THR:O	1:Q:60:GLU:HG2	2.20	0.42
1:J:47:THR:O	1:J:48:HIS:HB2	2.20	0.42
1:G:10:ASN:ND2	3:G:1046:HOH:O	2.53	0.42
1:F:79:CYS:O	1:F:80:HIS:HB2	2.20	0.42
1:L:117:CYS:HB2	1:L:124:LYS:HD2	2.00	0.42
1:A:83:HIS:N	1:A:83:HIS:ND1	2.67	0.42
1:C:56:THR:HG21	1:C:60:GLU:HB2	2.01	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: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:S:97:VAL:HG11	1:S:99:ILE:HD11	2.02	0.42
1:W:69:GLY:N	3:W:1030:HOH:O	2.52	0.42
1:R:16:PHE:CE2	1:R:26:ALA:HB1	2.55	0.42
1:P:62:ASN:OD1	1:P:65:GLN:HG3	2.20	0.42
1:V:79:CYS:O	1:V:80:HIS:HB2	2.20	0.42
1:U:62:ASN:OD1	1:U:65:GLN:HG3	2.19	0.42
1:O:90:CYS:HB3	1:O:93:LYS:HB2	2.01	0.42
1:F:90:CYS:C	1:F:92:LEU:H	2.16	0.42
1:V:25:LYS:HB2	1:V:25:LYS:HE3	1.86	0.42
1:S:32:ALA:C	1:S:34:GLY:N	2.71	0.42
1:Q:54:ALA:HB1	1:Q:123:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:LEU:HD23	1:B:43:LYS:HD2	2.01	0.42
1:W:113:ARG:CB	1:W:113:ARG:HH11	2.29	0.41
1:O:60:GLU:OE2	1:V:25:LYS:NZ	2.52	0.41
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:S:39:THR:O	1:S:40:ASN:HB2	2.20	0.41
1:R:22:ASP:C	1:R:22:ASP:OD1	2.58	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:I:89:PHE:N	3:I:1032:HOH:O	2.53	0.41
1:M:51:THR:OG1	1:M:53:GLN:HG2	2.20	0.41
1:G:72:SER:HB2	3:G:1001:HOH:O	2.20	0.41
1:N:84:PRO:HD2	3:N:1016:HOH:O	2.18	0.41
1:M:9:ALA:O	1:M:13:VAL:HG23	2.21	0.41
1:L:82:ASP:HA	3:L:1018:HOH:O	2.18	0.41
1:D:25:LYS:HE3	1:D:25:LYS:HB2	1.93	0.41
1:H:82:ASP:HA	3:H:1020:HOH:O	2.21	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:G:85:ASN:HB2	3:G:1025:HOH:O	2.19	0.41
1:A:108:VAL:HG23	3:A:1016:HOH:O	2.20	0.41
1:Q:69:GLY:O	1:Q:70:GLY:C	2.57	0.41
1:P:106:ASP:CG	1:P:113:ARG:HH22	2.23	0.41
1:J:98:GLN:N	1:J:98:GLN:NE2	2.69	0.41
1:G:89:PHE:N	3:G:1017:HOH:O	2.54	0.41
1:V:90:CYS:O	1:V:92:LEU:N	2.54	0.41
1:R:105:ASN:N	1:R:105:ASN:ND2	2.65	0.41
1:U:83:HIS:N	1:U:83:HIS:ND1	2.67	0.41
1:L:113:ARG:NH1	1:L:113:ARG:HB2	2.32	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:F:87:LYS:HA	1:F:87:LYS:HD2	1.65	0.41
1:O:90:CYS:HB3	1:O:93:LYS:CB	2.50	0.41
1:N:83:HIS:N	1:N:83:HIS:ND1	2.69	0.41
1:C:51:THR:HG23	1:C:60:GLU:OE1	2.21	0.41
1:V:74:CYS:CB	1:V:92:LEU:HD12	2.48	0.41
1:T:49:THR:HG23	1:T:63:MET:HE3	2.02	0.41
1:W:58:THR:O	1:W:59:PRO:C	2.58	0.41
1:K:62:ASN:OD1	1:K:64:ASP:N	2.48	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:22:ASP:C	1:S:22:ASP:OD1	2.59	0.41
1:U:13:VAL:HG22	1:U:30:TYR:CZ	2.56	0.41
1:O:47:THR:HG23	1:O:49:THR:N	2.30	0.41
1:U:69:GLY:O	1:U:72:SER:OG	2.36	0.41
1:B:113:ARG:HH11	1:B:113:ARG:CB	2.30	0.41
1:U:10:ASN:HD21	1:U:40:ASN:HD22	1.69	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:T:84:PRO:O	1:T:85:ASN:C	2.59	0.41
1:E:10:ASN:HD21	1:E:40:ASN:HD22	1.68	0.41
1:S:128:CYS:O	1:S:129:SER:C	2.59	0.41
1:G:36:GLN:HA	1:G:37:PRO:HD3	2.00	0.41
1:E:105:ASN:ND2	1:E:105:ASN:H	2.19	0.41
1:U:91:ASP:OD2	1:U:91:ASP:N	2.54	0.41
1:E:106:ASP:N	1:E:107:PRO:HD3	2.35	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: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:D:32:ALA:C	1:D:34:GLY:H	2.25	0.41
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:B:9:ALA:HA	3:B:1024:HOH:O	2.19	0.40
1:E:57:VAL:HG23	1:E:58:THR:HG23	2.02	0.40
1:A:62:ASN:OD1	1:A:64:ASP:N	2.51	0.40
1:N:39:THR:O	1:N:78:ARG:NH2	2.41	0.40
1:D:47:THR:O	1:D:48:HIS:HB2	2.21	0.40
1:M:45:LEU:HD12	1:M:45:LEU:C	2.42	0.40
1:W:90:CYS:C	1:W:92:LEU:N	2.74	0.40
1:E:36:GLN:HA	1:E:37:PRO:HD3	1.94	0.40
1:K:92:LEU:HD22	1:K:97:VAL:CG2	2.51	0.40
1:H:90:CYS:O	1:H:92:LEU:N	2.53	0.40
1:X:105:ASN:N	1:X:105:ASN:ND2	2.69	0.40
1:N:14:LEU:HD21	1:N:38:ILE:HD13	2.04	0.40
1:R:9:ALA:O	1:R:13:VAL:HG23	2.22	0.40
1:E:25:LYS:HE3	1:E:25:LYS:HB2	1.95	0.40
1:N:98:GLN:NE2	1:N:98:GLN:N	2.70	0.40
1:C:90:CYS:HB3	1:C:93:LYS:CB	2.51	0.40
1:X:14:LEU:HD21	1:X:38:ILE:HD13	2.04	0.40
1:U:98:GLN:H	1:U:98:GLN:NE2	2.15	0.40
1:K:103:CYS:C	1:K:105:ASN:H	2.24	0.40
1:H:25:LYS:HG2	1:H:29:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:53:GLN:HA	1:R:122:MET:HG2	2.03	0.40
1:G:109:GLY:HA3	3:G:1009:HOH:O	2.22	0.40
1:B:25:LYS:HE3	1:B:25:LYS:HB2	1.91	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:T:50:GLY:HA3	1:T:60:GLU:C	2.41	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:U:91:ASP:HA	3:U:1013:HOH:O	2.20	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	114/152 (75%)	100 (88%)	9 (8%)	5 (4%)	4	8
1	B	115/152 (76%)	103 (90%)	8 (7%)	4 (4%)	6	12
1	C	114/152 (75%)	100 (88%)	12 (10%)	2 (2%)	13	31
1	D	114/152 (75%)	100 (88%)	12 (10%)	2 (2%)	13	31
1	E	114/152 (75%)	100 (88%)	12 (10%)	2 (2%)	13	31
1	F	116/152 (76%)	99 (85%)	14 (12%)	3 (3%)	8	20
1	G	114/152 (75%)	104 (91%)	7 (6%)	3 (3%)	8	20
1	H	114/152 (75%)	96 (84%)	13 (11%)	5 (4%)	4	8
1	I	114/152 (75%)	101 (89%)	12 (10%)	1 (1%)	25	55
1	J	114/152 (75%)	103 (90%)	8 (7%)	3 (3%)	8	20
1	K	114/152 (75%)	104 (91%)	7 (6%)	3 (3%)	8	20
1	L	114/152 (75%)	106 (93%)	7 (6%)	1 (1%)	25	55
1	M	114/152 (75%)	104 (91%)	6 (5%)	4 (4%)	6	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	115/152 (76%)	100 (87%)	12 (10%)	3 (3%)	8	20
1	O	114/152 (75%)	101 (89%)	10 (9%)	3 (3%)	8	20
1	P	114/152 (75%)	106 (93%)	7 (6%)	1 (1%)	25	55
1	Q	114/152 (75%)	96 (84%)	11 (10%)	7 (6%)	2	3
1	R	111/152 (73%)	99 (89%)	10 (9%)	2 (2%)	13	31
1	S	114/152 (75%)	99 (87%)	11 (10%)	4 (4%)	6	12
1	T	114/152 (75%)	99 (87%)	10 (9%)	5 (4%)	4	8
1	U	114/152 (75%)	105 (92%)	7 (6%)	2 (2%)	13	31
1	V	114/152 (75%)	103 (90%)	8 (7%)	3 (3%)	8	20
1	W	114/152 (75%)	95 (83%)	15 (13%)	4 (4%)	6	12
1	X	114/152 (75%)	102 (90%)	9 (8%)	3 (3%)	8	20
All	All	2737/3648 (75%)	2425 (89%)	237 (9%)	75 (3%)	8	19

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	CYS
1	D	84	PRO
1	F	91	ASP
1	G	84	PRO
1	I	90	CYS
1	J	91	ASP
1	M	48	HIS
1	M	84	PRO
1	M	90	CYS
1	Q	48	HIS
1	S	47	THR
1	S	48	HIS
1	S	84	PRO
1	W	84	PRO
1	X	91	ASP
1	A	91	ASP
1	C	104	ALA
1	E	91	ASP
1	F	86	PRO
1	F	87	LYS
1	H	49	THR
1	H	84	PRO

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Mol	Chain	Res	Type
1	H	90	CYS
1	J	84	PRO
1	K	84	PRO
1	K	104	ALA
1	Q	71	ALA
1	Q	91	ASP
1	R	63	MET
1	S	33	SER
1	T	40	ASN
1	T	48	HIS
1	T	90	CYS
1	U	91	ASP
1	V	84	PRO
1	V	90	CYS
1	W	51	THR
1	W	104	ALA
1	X	84	PRO
1	X	90	CYS
1	C	91	ASP
1	E	72	SER
1	J	82	ASP
1	M	91	ASP
1	N	40	ASN
1	O	90	CYS
1	P	104	ALA
1	Q	40	ASN
1	Q	50	GLY
1	Q	90	CYS
1	T	84	PRO
1	W	74	CYS
1	A	82	ASP
1	B	84	PRO
1	H	91	ASP
1	K	90	CYS
1	N	84	PRO
1	O	84	PRO
1	O	104	ALA
1	R	40	ASN
1	U	40	ASN
1	A	104	ALA
1	B	54	ALA
1	B	128	CYS

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Mol	Chain	Res	Type
1	G	90	CYS
1	N	90	CYS
1	T	50	GLY
1	V	91	ASP
1	H	70	GLY
1	L	84	PRO
1	G	70	GLY
1	Q	70	GLY
1	B	70	GLY
1	D	127	GLY
1	A	84	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/123 (79%)	94 (97%)	3 (3%)	52	83
1	B	98/123 (80%)	95 (97%)	3 (3%)	52	83
1	C	97/123 (79%)	95 (98%)	2 (2%)	66	91
1	D	97/123 (79%)	93 (96%)	4 (4%)	41	74
1	E	97/123 (79%)	95 (98%)	2 (2%)	66	91
1	F	98/123 (80%)	93 (95%)	5 (5%)	33	64
1	G	97/123 (79%)	93 (96%)	4 (4%)	41	74
1	H	97/123 (79%)	90 (93%)	7 (7%)	21	45
1	I	97/123 (79%)	90 (93%)	7 (7%)	21	45
1	J	97/123 (79%)	92 (95%)	5 (5%)	32	63
1	K	97/123 (79%)	93 (96%)	4 (4%)	41	74
1	L	97/123 (79%)	95 (98%)	2 (2%)	66	91
1	M	97/123 (79%)	90 (93%)	7 (7%)	21	45
1	N	98/123 (80%)	93 (95%)	5 (5%)	33	64
1	O	97/123 (79%)	94 (97%)	3 (3%)	52	83
1	P	97/123 (79%)	93 (96%)	4 (4%)	41	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	97/123 (79%)	92 (95%)	5 (5%)	32	63
1	R	96/123 (78%)	89 (93%)	7 (7%)	20	44
1	S	97/123 (79%)	91 (94%)	6 (6%)	26	54
1	T	97/123 (79%)	95 (98%)	2 (2%)	66	91
1	U	97/123 (79%)	92 (95%)	5 (5%)	32	63
1	V	97/123 (79%)	89 (92%)	8 (8%)	17	36
1	W	97/123 (79%)	93 (96%)	4 (4%)	41	74
1	X	97/123 (79%)	93 (96%)	4 (4%)	41	74
All	All	2330/2952 (79%)	2222 (95%)	108 (5%)	37	70

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

Mol	Chain	Res	Type
1	A	74	CYS
1	A	90	CYS
1	A	105	ASN
1	B	74	CYS
1	B	84	PRO
1	B	129	SER
1	C	74	CYS
1	C	90	CYS
1	D	74	CYS
1	D	90	CYS
1	D	91	ASP
1	D	105	ASN
1	E	83	HIS
1	E	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	H	16	PHE
1	H	44	MET
1	H	74	CYS

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Mol	Chain	Res	Type
1	H	90	CYS
1	H	91	ASP
1	H	105	ASN
1	H	120	CYS
1	I	53	GLN
1	I	74	CYS
1	I	84	PRO
1	I	89	PHE
1	I	90	CYS
1	I	98	GLN
1	I	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
1	M	45	LEU
1	M	47	THR
1	M	53	GLN
1	M	74	CYS
1	M	83	HIS
1	M	90	CYS
1	M	105	ASN
1	N	74	CYS
1	N	90	CYS
1	N	98	GLN
1	N	105	ASN
1	N	129	SER
1	O	47	THR
1	O	74	CYS
1	O	90	CYS
1	P	74	CYS
1	P	83	HIS
1	P	101	THR
1	P	105	ASN
1	Q	74	CYS

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Mol	Chain	Res	Type
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
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	X	74	CYS
1	X	83	HIS
1	X	90	CYS
1	X	105	ASN

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

Mol	Chain	Res	Type
1	A	40	ASN
1	A	85	ASN
1	A	105	ASN
1	B	40	ASN
1	B	48	HIS
1	B	53	GLN
1	B	85	ASN
1	C	40	ASN
1	C	53	GLN
1	D	40	ASN
1	D	53	GLN
1	D	105	ASN
1	D	114	ASN
1	E	40	ASN
1	E	53	GLN
1	E	62	ASN
1	E	105	ASN
1	F	40	ASN
1	F	53	GLN
1	F	83	HIS
1	F	85	ASN
1	F	114	ASN
1	G	48	HIS
1	G	105	ASN
1	H	53	GLN
1	H	62	ASN
1	H	105	ASN
1	I	40	ASN
1	I	48	HIS
1	I	53	GLN
1	I	105	ASN
1	I	114	ASN
1	J	40	ASN
1	J	48	HIS
1	J	53	GLN
1	K	40	ASN
1	K	53	GLN
1	L	40	ASN
1	L	53	GLN
1	L	105	ASN
1	M	48	HIS
1	M	53	GLN
1	M	105	ASN

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Mol	Chain	Res	Type
1	M	114	ASN
1	N	40	ASN
1	N	48	HIS
1	N	53	GLN
1	O	40	ASN
1	P	105	ASN
1	P	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
1	S	53	GLN
1	S	105	ASN
1	S	114	ASN
1	T	40	ASN
1	T	48	HIS
1	T	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	X	40	ASN
1	X	105	ASN
1	X	114	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	A	118/152 (77%)	-0.12	0 100 100	22, 32, 52, 67	0
1	B	119/152 (78%)	0.05	3 (2%) 54 61	21, 36, 53, 82	0
1	C	118/152 (77%)	0.08	6 (5%) 27 30	24, 36, 53, 73	0
1	D	118/152 (77%)	0.13	5 (4%) 35 39	25, 36, 54, 77	0
1	E	118/152 (77%)	0.11	4 (3%) 43 48	23, 34, 56, 79	0
1	F	120/152 (78%)	0.12	6 (5%) 28 30	19, 35, 59, 75	0
1	G	118/152 (77%)	0.12	4 (3%) 43 48	24, 33, 53, 70	0
1	H	118/152 (77%)	0.15	4 (3%) 43 48	22, 36, 58, 76	0
1	I	118/152 (77%)	0.05	3 (2%) 54 61	23, 34, 53, 66	0
1	J	118/152 (77%)	0.04	4 (3%) 43 48	22, 35, 54, 76	0
1	K	118/152 (77%)	0.14	5 (4%) 35 39	21, 33, 55, 75	0
1	L	118/152 (77%)	-0.02	3 (2%) 54 61	19, 31, 48, 61	0
1	M	118/152 (77%)	0.16	6 (5%) 27 30	18, 32, 55, 81	0
1	N	119/152 (78%)	0.16	3 (2%) 54 61	23, 38, 57, 81	0
1	O	118/152 (77%)	0.08	7 (5%) 22 23	17, 31, 49, 71	0
1	P	118/152 (77%)	-0.02	5 (4%) 35 39	18, 29, 47, 67	0
1	Q	118/152 (77%)	0.39	6 (5%) 27 30	30, 42, 69, 97	0
1	R	117/152 (76%)	0.05	4 (3%) 43 48	20, 33, 56, 74	0
1	S	118/152 (77%)	0.09	6 (5%) 27 30	18, 32, 62, 83	0
1	T	118/152 (77%)	0.33	9 (7%) 14 14	24, 38, 62, 75	0
1	U	118/152 (77%)	0.14	1 (0%) 83 87	24, 39, 53, 69	0
1	V	118/152 (77%)	0.08	3 (2%) 54 61	22, 32, 55, 73	0
1	W	118/152 (77%)	0.23	4 (3%) 43 48	29, 42, 60, 75	0
1	X	118/152 (77%)	0.27	6 (5%) 27 30	25, 40, 56, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	2835/3648 (77%)	0.12	107 (3%)	39	43	17, 35, 57, 97	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	48	HIS	12.0
1	N	8	PRO	6.6
1	W	89	PHE	5.9
1	S	85	ASN	5.8
1	E	89	PHE	5.8
1	T	85	ASN	5.6
1	R	89	PHE	5.6
1	Q	48	HIS	5.3
1	J	89	PHE	5.3
1	N	89	PHE	5.2
1	S	48	HIS	5.1
1	O	89	PHE	5.1
1	D	85	ASN	4.9
1	M	47	THR	4.3
1	S	47	THR	4.2
1	F	87	LYS	4.1
1	B	8	PRO	4.0
1	K	89	PHE	4.0
1	L	85	ASN	4.0
1	V	85	ASN	3.9
1	B	89	PHE	3.9
1	G	89	PHE	3.9
1	F	88	GLY	3.8
1	K	90	CYS	3.8
1	E	85	ASN	3.7
1	O	129	SER	3.7
1	D	89	PHE	3.7
1	C	85	ASN	3.6
1	H	49	THR	3.6
1	Q	85	ASN	3.5
1	U	89	PHE	3.5
1	S	90	CYS	3.4
1	X	85	ASN	3.4
1	V	89	PHE	3.3
1	D	90	CYS	3.3
1	P	89	PHE	3.2
1	R	85	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	85	ASN	3.2
1	T	48	HIS	3.2
1	G	85	ASN	3.1
1	M	85	ASN	3.1
1	W	85	ASN	3.1
1	C	34	GLY	3.1
1	T	33	SER	3.0
1	O	34	GLY	3.0
1	O	90	CYS	2.9
1	J	34	GLY	2.9
1	D	129	SER	2.9
1	M	49	THR	2.9
1	B	85	ASN	2.9
1	E	84	PRO	2.8
1	T	16	PHE	2.8
1	I	34	GLY	2.8
1	X	16	PHE	2.8
1	T	49	THR	2.7
1	T	63	MET	2.7
1	G	32	ALA	2.7
1	J	32	ALA	2.7
1	Q	126	TYR	2.6
1	I	129	SER	2.6
1	L	33	SER	2.6
1	P	85	ASN	2.6
1	X	89	PHE	2.6
1	Q	33	SER	2.6
1	C	89	PHE	2.6
1	F	86	PRO	2.6
1	Q	89	PHE	2.6
1	T	126	TYR	2.6
1	X	32	ALA	2.5
1	H	48	HIS	2.5
1	C	32	ALA	2.5
1	P	90	CYS	2.5
1	S	89	PHE	2.5
1	D	32	ALA	2.4
1	F	33	SER	2.3
1	O	85	ASN	2.3
1	X	30	TYR	2.3
1	C	33	SER	2.3
1	R	32	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	124	LYS	2.3
1	C	90	CYS	2.2
1	O	126	TYR	2.2
1	Q	91	ASP	2.2
1	I	84	PRO	2.2
1	L	129	SER	2.2
1	N	129	SER	2.2
1	M	90	CYS	2.2
1	P	32	ALA	2.2
1	H	84	PRO	2.2
1	T	125	GLY	2.2
1	K	34	GLY	2.2
1	G	90	CYS	2.2
1	J	90	CYS	2.2
1	H	16	PHE	2.2
1	M	129	SER	2.2
1	W	34	GLY	2.1
1	V	46	CYS	2.1
1	T	34	GLY	2.1
1	W	84	PRO	2.1
1	K	124	LYS	2.1
1	S	32	ALA	2.1
1	F	90	CYS	2.1
1	O	124	LYS	2.0
1	P	33	SER	2.0
1	E	34	GLY	2.0
1	F	89	PHE	2.0
1	R	84	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	F	998	1/1	0.18	-0.67	73,73,73,73	0
2	ZN	T	998	1/1	0.16	-0.68	78,78,78,78	0
2	ZN	N	998	1/1	0.15	-0.68	62,62,62,62	0
2	ZN	L	998	1/1	0.16	-0.71	74,74,74,74	0
2	ZN	O	998	1/1	0.13	-0.86	55,55,55,55	0
2	ZN	J	998	1/1	0.12	-0.88	85,85,85,85	0
2	ZN	X	998	1/1	0.15	-0.89	72,72,72,72	0
2	ZN	W	998	1/1	0.10	-0.93	80,80,80,80	0
2	ZN	E	998	1/1	0.11	-0.96	73,73,73,73	0
2	ZN	D	998	1/1	0.13	-0.96	75,75,75,75	0
2	ZN	M	999	1/1	0.10	-0.98	42,42,42,42	0
2	ZN	R	998	1/1	0.11	-0.99	64,64,64,64	0
2	ZN	G	998	1/1	0.11	-1.11	51,51,51,51	0
2	ZN	I	998	1/1	0.14	-1.13	67,67,67,67	0
2	ZN	V	998	1/1	0.12	-1.18	83,83,83,83	0
2	ZN	U	998	1/1	0.12	-1.22	84,84,84,84	0
2	ZN	M	998	1/1	0.14	-1.22	62,62,62,62	0
2	ZN	Q	999	1/1	0.07	-1.22	49,49,49,49	0
2	ZN	P	998	1/1	0.12	-1.23	76,76,76,76	0
2	ZN	C	998	1/1	0.12	-1.23	84,84,84,84	0
2	ZN	S	998	1/1	0.12	-1.23	49,49,49,49	0
2	ZN	E	999	1/1	0.10	-1.24	44,44,44,44	0
2	ZN	K	998	1/1	0.11	-1.26	66,66,66,66	0
2	ZN	B	998	1/1	0.10	-1.30	67,67,67,67	0
2	ZN	D	999	1/1	0.10	-1.32	63,63,63,63	0
2	ZN	N	999	1/1	0.09	-1.32	79,79,79,79	0
2	ZN	O	999	1/1	0.10	-1.34	67,67,67,67	0
2	ZN	P	999	1/1	0.10	-1.34	40,40,40,40	0
2	ZN	R	999	1/1	0.07	-1.49	46,46,46,46	0
2	ZN	L	999	1/1	0.07	-1.53	40,40,40,40	0
2	ZN	K	999	1/1	0.08	-1.55	46,46,46,46	0
2	ZN	J	999	1/1	0.07	-1.59	40,40,40,40	0
2	ZN	S	999	1/1	0.07	-1.60	39,39,39,39	0
2	ZN	B	999	1/1	0.10	-1.61	74,74,74,74	0
2	ZN	Q	998	1/1	0.10	-1.61	76,76,76,76	0
2	ZN	G	999	1/1	0.07	-1.63	46,46,46,46	0
2	ZN	A	999	1/1	0.08	-1.66	43,43,43,43	0
2	ZN	H	998	1/1	0.13	-1.67	78,78,78,78	0
2	ZN	I	999	1/1	0.08	-1.72	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	H	999	1/1	0.09	-1.78	41,41,41,41	0
2	ZN	W	999	1/1	0.07	-1.81	48,48,48,48	0
2	ZN	V	999	1/1	0.07	-1.91	42,42,42,42	0
2	ZN	A	998	1/1	0.09	-2.01	72,72,72,72	0
2	ZN	C	999	1/1	0.05	-2.11	45,45,45,45	0
2	ZN	U	999	1/1	0.07	-2.13	50,50,50,50	0
2	ZN	F	999	1/1	0.08	-2.22	42,42,42,42	0
2	ZN	T	999	1/1	0.06	-3.04	35,35,35,35	0
2	ZN	X	999	1/1	0.09	-3.59	54,54,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.