



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 PM UTC

PDB ID : 1YUD / pdb_00001yud
Title : X-ray Crystal Structure of Protein SO0799 from Shewanella oneidensis. Northeast Structural Genomics Consortium Target SoR12.
Authors : Kuzin, A.P.; Vorobiev, S.; Chen, Y.; Forouhar, F.; Acton, T.; Ma, L.-C.; Xiao, R.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-02-14
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

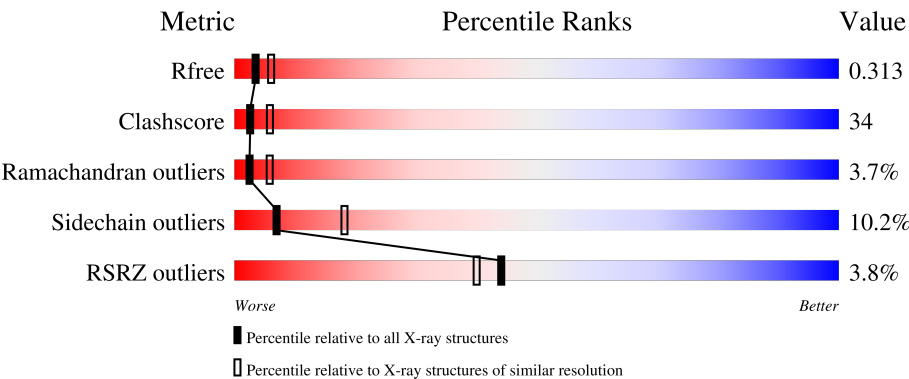
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	A	170	3% 45%39%7%7%
1	B	170	43%39%9%7%
1	C	170	2% 41%39%12%7%
1	D	170	2% 46%34%12%7%

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Mol	Chain	Length	Quality of chain
1	E	170	4% 45% 36% 11% 7%
1	F	170	5% 36% 45% 11% 7%
1	G	170	7% 40% 42% 9% 7%
1	H	170	% 40% 45% 7% 7%
1	I	170	8% 42% 42% 8% 7%
1	J	170	2% 47% 36% 9% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12762 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.

- Molecule 1 is a protein called hypothetical protein SO0799.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	B	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	C	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	D	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	E	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	F	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	G	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	H	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	I	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	J	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MSE	-	expression tag	UNP Q8EIN8
A	-8	GLY	-	expression tag	UNP Q8EIN8
A	-7	HIS	-	expression tag	UNP Q8EIN8
A	-6	HIS	-	expression tag	UNP Q8EIN8
A	-5	HIS	-	expression tag	UNP Q8EIN8
A	-4	HIS	-	expression tag	UNP Q8EIN8
A	-3	HIS	-	expression tag	UNP Q8EIN8
A	-2	HIS	-	expression tag	UNP Q8EIN8
A	-1	SER	-	expression tag	UNP Q8EIN8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q8EIN8
A	1	MSE	MET	modified residue	UNP Q8EIN8
A	62	MSE	MET	modified residue	UNP Q8EIN8
A	75	MSE	MET	modified residue	UNP Q8EIN8
A	111	MSE	MET	modified residue	UNP Q8EIN8
A	122	MSE	MET	modified residue	UNP Q8EIN8
A	143	MSE	MET	modified residue	UNP Q8EIN8
B	-9	MSE	-	expression tag	UNP Q8EIN8
B	-8	GLY	-	expression tag	UNP Q8EIN8
B	-7	HIS	-	expression tag	UNP Q8EIN8
B	-6	HIS	-	expression tag	UNP Q8EIN8
B	-5	HIS	-	expression tag	UNP Q8EIN8
B	-4	HIS	-	expression tag	UNP Q8EIN8
B	-3	HIS	-	expression tag	UNP Q8EIN8
B	-2	HIS	-	expression tag	UNP Q8EIN8
B	-1	SER	-	expression tag	UNP Q8EIN8
B	0	HIS	-	expression tag	UNP Q8EIN8
B	1	MSE	MET	modified residue	UNP Q8EIN8
B	62	MSE	MET	modified residue	UNP Q8EIN8
B	75	MSE	MET	modified residue	UNP Q8EIN8
B	111	MSE	MET	modified residue	UNP Q8EIN8
B	122	MSE	MET	modified residue	UNP Q8EIN8
B	143	MSE	MET	modified residue	UNP Q8EIN8
C	-9	MSE	-	expression tag	UNP Q8EIN8
C	-8	GLY	-	expression tag	UNP Q8EIN8
C	-7	HIS	-	expression tag	UNP Q8EIN8
C	-6	HIS	-	expression tag	UNP Q8EIN8
C	-5	HIS	-	expression tag	UNP Q8EIN8
C	-4	HIS	-	expression tag	UNP Q8EIN8
C	-3	HIS	-	expression tag	UNP Q8EIN8
C	-2	HIS	-	expression tag	UNP Q8EIN8
C	-1	SER	-	expression tag	UNP Q8EIN8
C	0	HIS	-	expression tag	UNP Q8EIN8
C	1	MSE	MET	modified residue	UNP Q8EIN8
C	62	MSE	MET	modified residue	UNP Q8EIN8
C	75	MSE	MET	modified residue	UNP Q8EIN8
C	111	MSE	MET	modified residue	UNP Q8EIN8
C	122	MSE	MET	modified residue	UNP Q8EIN8
C	143	MSE	MET	modified residue	UNP Q8EIN8
D	-9	MSE	-	expression tag	UNP Q8EIN8
D	-8	GLY	-	expression tag	UNP Q8EIN8
D	-7	HIS	-	expression tag	UNP Q8EIN8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	expression tag	UNP Q8EIN8
D	-5	HIS	-	expression tag	UNP Q8EIN8
D	-4	HIS	-	expression tag	UNP Q8EIN8
D	-3	HIS	-	expression tag	UNP Q8EIN8
D	-2	HIS	-	expression tag	UNP Q8EIN8
D	-1	SER	-	expression tag	UNP Q8EIN8
D	0	HIS	-	expression tag	UNP Q8EIN8
D	1	MSE	MET	modified residue	UNP Q8EIN8
D	62	MSE	MET	modified residue	UNP Q8EIN8
D	75	MSE	MET	modified residue	UNP Q8EIN8
D	111	MSE	MET	modified residue	UNP Q8EIN8
D	122	MSE	MET	modified residue	UNP Q8EIN8
D	143	MSE	MET	modified residue	UNP Q8EIN8
E	-9	MSE	-	expression tag	UNP Q8EIN8
E	-8	GLY	-	expression tag	UNP Q8EIN8
E	-7	HIS	-	expression tag	UNP Q8EIN8
E	-6	HIS	-	expression tag	UNP Q8EIN8
E	-5	HIS	-	expression tag	UNP Q8EIN8
E	-4	HIS	-	expression tag	UNP Q8EIN8
E	-3	HIS	-	expression tag	UNP Q8EIN8
E	-2	HIS	-	expression tag	UNP Q8EIN8
E	-1	SER	-	expression tag	UNP Q8EIN8
E	0	HIS	-	expression tag	UNP Q8EIN8
E	1	MSE	MET	modified residue	UNP Q8EIN8
E	62	MSE	MET	modified residue	UNP Q8EIN8
E	75	MSE	MET	modified residue	UNP Q8EIN8
E	111	MSE	MET	modified residue	UNP Q8EIN8
E	122	MSE	MET	modified residue	UNP Q8EIN8
E	143	MSE	MET	modified residue	UNP Q8EIN8
F	-9	MSE	-	expression tag	UNP Q8EIN8
F	-8	GLY	-	expression tag	UNP Q8EIN8
F	-7	HIS	-	expression tag	UNP Q8EIN8
F	-6	HIS	-	expression tag	UNP Q8EIN8
F	-5	HIS	-	expression tag	UNP Q8EIN8
F	-4	HIS	-	expression tag	UNP Q8EIN8
F	-3	HIS	-	expression tag	UNP Q8EIN8
F	-2	HIS	-	expression tag	UNP Q8EIN8
F	-1	SER	-	expression tag	UNP Q8EIN8
F	0	HIS	-	expression tag	UNP Q8EIN8
F	1	MSE	MET	modified residue	UNP Q8EIN8
F	62	MSE	MET	modified residue	UNP Q8EIN8
F	75	MSE	MET	modified residue	UNP Q8EIN8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	111	MSE	MET	modified residue	UNP Q8EIN8
F	122	MSE	MET	modified residue	UNP Q8EIN8
F	143	MSE	MET	modified residue	UNP Q8EIN8
G	-9	MSE	-	expression tag	UNP Q8EIN8
G	-8	GLY	-	expression tag	UNP Q8EIN8
G	-7	HIS	-	expression tag	UNP Q8EIN8
G	-6	HIS	-	expression tag	UNP Q8EIN8
G	-5	HIS	-	expression tag	UNP Q8EIN8
G	-4	HIS	-	expression tag	UNP Q8EIN8
G	-3	HIS	-	expression tag	UNP Q8EIN8
G	-2	HIS	-	expression tag	UNP Q8EIN8
G	-1	SER	-	expression tag	UNP Q8EIN8
G	0	HIS	-	expression tag	UNP Q8EIN8
G	1	MSE	MET	modified residue	UNP Q8EIN8
G	62	MSE	MET	modified residue	UNP Q8EIN8
G	75	MSE	MET	modified residue	UNP Q8EIN8
G	111	MSE	MET	modified residue	UNP Q8EIN8
G	122	MSE	MET	modified residue	UNP Q8EIN8
G	143	MSE	MET	modified residue	UNP Q8EIN8
H	-9	MSE	-	expression tag	UNP Q8EIN8
H	-8	GLY	-	expression tag	UNP Q8EIN8
H	-7	HIS	-	expression tag	UNP Q8EIN8
H	-6	HIS	-	expression tag	UNP Q8EIN8
H	-5	HIS	-	expression tag	UNP Q8EIN8
H	-4	HIS	-	expression tag	UNP Q8EIN8
H	-3	HIS	-	expression tag	UNP Q8EIN8
H	-2	HIS	-	expression tag	UNP Q8EIN8
H	-1	SER	-	expression tag	UNP Q8EIN8
H	0	HIS	-	expression tag	UNP Q8EIN8
H	1	MSE	MET	modified residue	UNP Q8EIN8
H	62	MSE	MET	modified residue	UNP Q8EIN8
H	75	MSE	MET	modified residue	UNP Q8EIN8
H	111	MSE	MET	modified residue	UNP Q8EIN8
H	122	MSE	MET	modified residue	UNP Q8EIN8
H	143	MSE	MET	modified residue	UNP Q8EIN8
I	-9	MSE	-	expression tag	UNP Q8EIN8
I	-8	GLY	-	expression tag	UNP Q8EIN8
I	-7	HIS	-	expression tag	UNP Q8EIN8
I	-6	HIS	-	expression tag	UNP Q8EIN8
I	-5	HIS	-	expression tag	UNP Q8EIN8
I	-4	HIS	-	expression tag	UNP Q8EIN8
I	-3	HIS	-	expression tag	UNP Q8EIN8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	HIS	-	expression tag	UNP Q8EIN8
I	-1	SER	-	expression tag	UNP Q8EIN8
I	0	HIS	-	expression tag	UNP Q8EIN8
I	1	MSE	MET	modified residue	UNP Q8EIN8
I	62	MSE	MET	modified residue	UNP Q8EIN8
I	75	MSE	MET	modified residue	UNP Q8EIN8
I	111	MSE	MET	modified residue	UNP Q8EIN8
I	122	MSE	MET	modified residue	UNP Q8EIN8
I	143	MSE	MET	modified residue	UNP Q8EIN8
J	-9	MSE	-	expression tag	UNP Q8EIN8
J	-8	GLY	-	expression tag	UNP Q8EIN8
J	-7	HIS	-	expression tag	UNP Q8EIN8
J	-6	HIS	-	expression tag	UNP Q8EIN8
J	-5	HIS	-	expression tag	UNP Q8EIN8
J	-4	HIS	-	expression tag	UNP Q8EIN8
J	-3	HIS	-	expression tag	UNP Q8EIN8
J	-2	HIS	-	expression tag	UNP Q8EIN8
J	-1	SER	-	expression tag	UNP Q8EIN8
J	0	HIS	-	expression tag	UNP Q8EIN8
J	1	MSE	MET	modified residue	UNP Q8EIN8
J	62	MSE	MET	modified residue	UNP Q8EIN8
J	75	MSE	MET	modified residue	UNP Q8EIN8
J	111	MSE	MET	modified residue	UNP Q8EIN8
J	122	MSE	MET	modified residue	UNP Q8EIN8
J	143	MSE	MET	modified residue	UNP Q8EIN8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	16	Total O 16 16	0	0
2	B	27	Total O 27 27	0	0
2	C	11	Total O 11 11	0	0
2	D	16	Total O 16 16	0	0
2	E	3	Total O 3 3	0	0
2	F	5	Total O 5 5	0	0
2	G	1	Total O 1 1	0	0

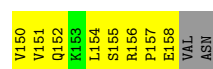
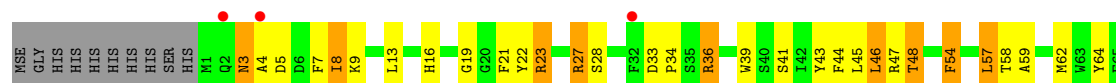
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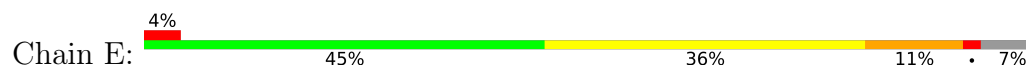
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	15	Total 15	O 15	0	0
2	I	6	Total 6	O 6	0	0
2	J	12	Total 12	O 12	0	0



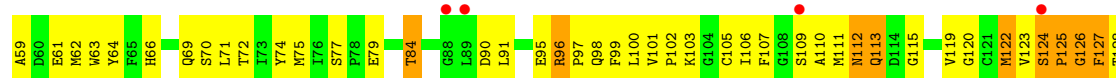
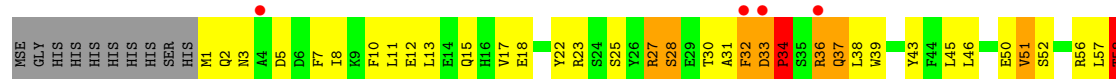
• Molecule 1: hypothetical protein SO0799



• Molecule 1: hypothetical protein SO0799

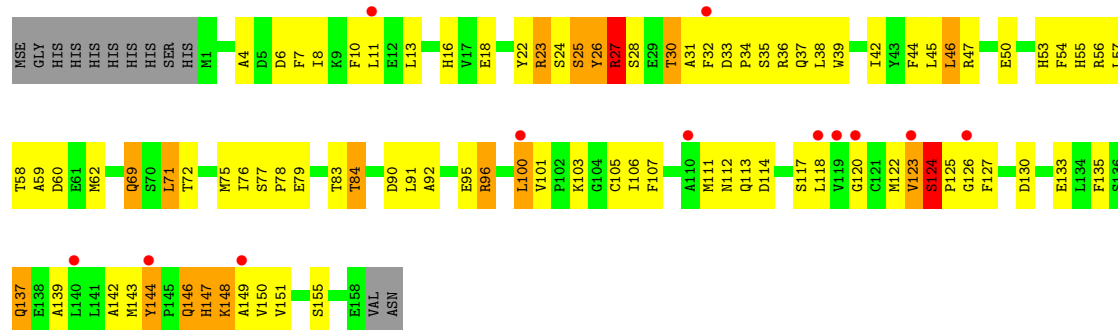


• Molecule 1: hypothetical protein SO0799

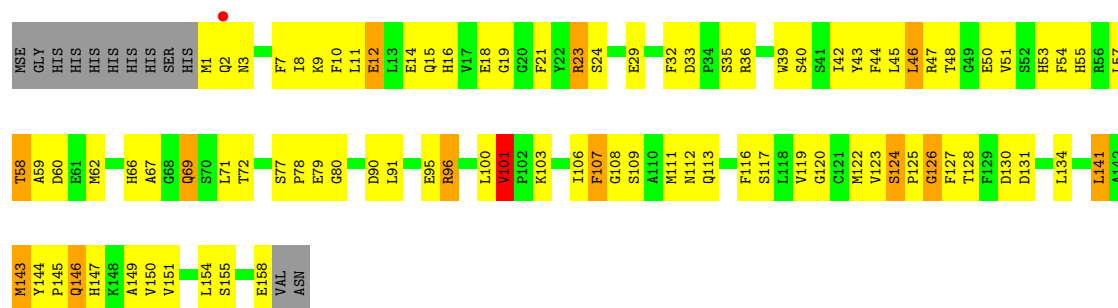
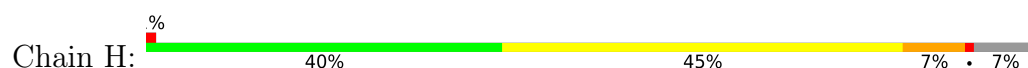


• Molecule 1: hypothetical protein SO0799

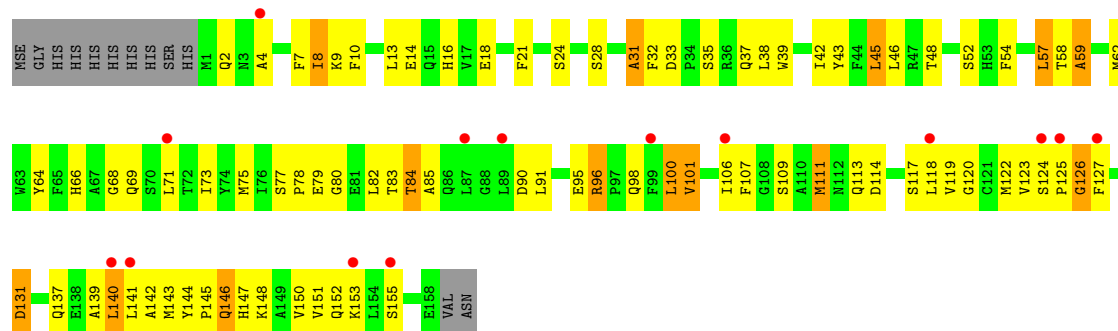
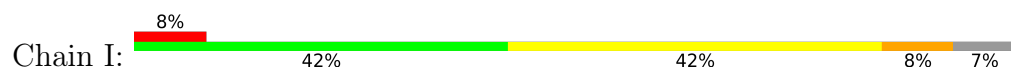




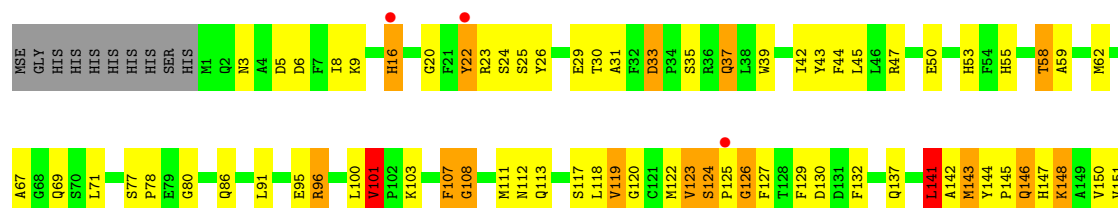
• Molecule 1: hypothetical protein SO0799



• Molecule 1: hypothetical protein SO0799



• Molecule 1: hypothetical protein SO0799



Q152	K153	L154	S155	R156	P157	E158	VAL	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.44Å 94.10Å 117.10Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	29.93 – 2.70 29.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.9 (29.93-2.70) 94.2 (29.93-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.292 0.256 , 0.313	Depositor DCC
R_{free} test set	5131 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12762	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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	0.47	0/1295	1.05	8/1742 (0.5%)
1	B	0.63	0/1295	1.21	8/1742 (0.5%)
1	C	0.50	0/1295	1.03	7/1742 (0.4%)
1	D	0.48	0/1295	1.04	8/1742 (0.5%)
1	E	0.45	0/1295	1.00	8/1742 (0.5%)
1	F	0.43	0/1295	0.95	7/1742 (0.4%)
1	G	0.39	0/1295	1.04	11/1742 (0.6%)
1	H	0.55	0/1295	1.16	12/1742 (0.7%)
1	I	0.41	0/1295	0.97	5/1742 (0.3%)
1	J	0.52	0/1295	1.11	15/1742 (0.9%)
All	All	0.49	0/12950	1.06	89/17420 (0.5%)

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	SER	CA-C-N	-12.64	105.32	119.98
1	B	124	SER	C-N-CA	-12.64	105.32	119.98
1	G	124	SER	CA-C-N	-11.02	109.61	120.52
1	G	124	SER	C-N-CA	-11.02	109.61	120.52
1	D	124	SER	CA-C-N	-9.48	108.00	119.84
1	D	124	SER	C-N-CA	-9.48	108.00	119.84
1	J	124	SER	CA-C-N	-8.83	108.80	119.84
1	J	124	SER	C-N-CA	-8.83	108.80	119.84
1	B	43	TYR	N-CA-C	-8.76	96.07	110.17
1	H	43	TYR	N-CA-C	-7.74	97.12	109.59
1	H	143	MSE	N-CA-C	-7.64	99.21	110.52
1	J	130	ASP	N-CA-C	-7.56	103.79	113.16
1	J	95	GLU	N-CA-C	7.43	121.17	110.24
1	C	43	TYR	N-CA-C	-7.34	99.65	110.52
1	A	43	TYR	N-CA-C	-7.29	100.02	110.59
1	A	124	SER	CA-C-N	-7.26	110.77	119.84
1	A	124	SER	C-N-CA	-7.26	110.77	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	130	ASP	N-CA-C	-7.09	103.63	111.36
1	I	43	TYR	N-CA-C	-6.96	98.89	109.95
1	H	124	SER	CA-C-N	-6.92	111.19	119.84
1	H	124	SER	C-N-CA	-6.92	111.19	119.84
1	E	124	SER	CA-C-N	-6.87	111.26	119.84
1	E	124	SER	C-N-CA	-6.87	111.26	119.84
1	C	128	THR	N-CA-C	-6.82	98.94	109.24
1	B	142	ALA	N-CA-C	-6.77	103.59	110.97
1	J	16	HIS	N-CA-C	-6.75	101.82	110.53
1	G	32	PHE	N-CA-C	-6.68	104.07	111.36
1	I	32	PHE	N-CA-C	-6.65	104.04	111.28
1	I	59	ALA	N-CA-C	6.45	118.34	109.18
1	H	128	THR	N-CA-C	-6.43	99.64	109.41
1	A	156	ARG	CA-C-N	6.42	126.37	120.21
1	A	156	ARG	C-N-CA	6.42	126.37	120.21
1	H	130	ASP	N-CA-C	-6.40	105.34	113.02
1	E	141	LEU	N-CA-C	-6.36	106.05	113.88
1	J	101	VAL	CA-C-N	6.34	126.36	119.89
1	J	101	VAL	C-N-CA	6.34	126.36	119.89
1	F	127	PHE	N-CA-C	6.26	119.11	110.35
1	H	32	PHE	N-CA-C	-6.21	101.58	111.02
1	J	142	ALA	N-CA-C	-6.20	104.06	111.69
1	B	112	ASN	N-CA-C	-6.12	105.98	113.50
1	G	58	THR	N-CA-C	-6.11	105.69	113.02
1	A	128	THR	N-CA-C	-6.11	101.48	110.52
1	B	32	PHE	N-CA-C	-6.08	103.28	112.04
1	E	32	PHE	N-CA-C	-6.08	106.40	113.88
1	C	135	PHE	N-CA-C	6.07	119.36	109.59
1	C	32	PHE	N-CA-C	-6.05	104.64	112.68
1	D	48	THR	N-CA-C	6.04	117.74	111.03
1	A	27	ARG	N-CA-C	-6.03	100.59	109.81
1	D	43	TYR	N-CA-C	-5.94	99.72	109.40
1	J	143	MSE	N-CA-C	-5.94	100.02	109.76
1	G	144	TYR	CA-C-N	5.89	125.10	118.97
1	G	144	TYR	C-N-CA	5.89	125.10	118.97
1	A	157	PRO	N-CA-C	5.88	119.44	111.22
1	G	123	VAL	N-CA-C	5.84	117.00	108.53
1	I	142	ALA	N-CA-C	-5.83	105.66	112.89
1	J	33	ASP	N-CA-C	-5.74	100.18	109.82
1	I	31	ALA	N-CA-C	5.71	118.09	107.99
1	J	141	LEU	N-CA-C	-5.70	106.20	114.12
1	E	43	TYR	N-CA-C	-5.67	101.78	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	143	MSE	N-CA-C	-5.66	102.10	110.48
1	J	108	GLY	N-CA-C	-5.66	106.00	112.79
1	J	29	GLU	N-CA-C	-5.65	105.97	112.92
1	F	33	ASP	N-CA-C	-5.64	101.21	109.50
1	D	130	ASP	N-CA-C	-5.60	106.13	114.64
1	C	143	MSE	N-CA-C	-5.59	102.21	110.48
1	H	101	VAL	CA-C-N	5.59	125.87	119.83
1	H	101	VAL	C-N-CA	5.59	125.87	119.83
1	J	58	THR	N-CA-C	-5.54	105.87	113.30
1	H	107	PHE	N-CA-C	5.54	118.59	109.72
1	B	67	ALA	N-CA-C	5.46	115.04	107.73
1	G	142	ALA	N-CA-C	-5.42	105.01	111.03
1	D	128	THR	N-CA-C	-5.38	100.94	108.96
1	G	130	ASP	N-CA-C	-5.32	105.65	111.82
1	H	29	GLU	N-CA-C	-5.31	106.03	112.88
1	F	58	THR	N-CA-C	-5.31	107.35	112.97
1	F	107	PHE	N-CA-C	5.29	117.90	109.81
1	F	84	THR	N-CA-C	5.22	116.84	107.80
1	E	75	MSE	N-CA-C	5.20	115.89	107.32
1	E	108	GLY	N-CA-C	-5.18	102.70	110.42
1	C	141	LEU	N-CA-C	-5.18	107.62	114.31
1	B	143	MSE	N-CA-C	-5.12	102.11	110.20
1	C	142	ALA	N-CA-C	-5.11	99.92	110.80
1	E	142	ALA	N-CA-C	-5.10	105.18	111.40
1	D	143	MSE	N-CA-C	-5.10	100.93	109.24
1	J	107	PHE	N-CA-C	5.07	117.75	109.59
1	G	27	ARG	N-CA-C	-5.07	101.38	109.23
1	G	30	THR	N-CA-C	-5.06	100.76	108.76
1	D	36	ARG	N-CA-C	5.06	117.37	110.24
1	H	15	GLN	N-CA-C	-5.02	103.42	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	A	1265	0	1204	82	0
1	B	1265	0	1204	86	0
1	C	1265	0	1204	98	0
1	D	1265	0	1204	82	0
1	E	1265	0	1204	93	0
1	F	1265	0	1204	93	0
1	G	1265	0	1204	94	0
1	H	1265	0	1204	97	0
1	I	1265	0	1204	94	0
1	J	1265	0	1204	77	0
2	A	16	0	0	2	0
2	B	27	0	0	4	0
2	C	11	0	0	1	0
2	D	16	0	0	2	0
2	E	3	0	0	0	0
2	F	5	0	0	1	0
2	G	1	0	0	0	0
2	H	15	0	0	1	0
2	I	6	0	0	1	0
2	J	12	0	0	2	0
All	All	12762	0	12040	844	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (844) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:TRP:HB2	1:A:122:MSE:HE3	1.29	1.14
1:A:124:SER:HB3	1:A:125:PRO:HD3	1.31	1.10
1:A:122:MSE:HE1	1:A:124:SER:HA	1.25	1.09
1:G:59:ALA:HB1	1:G:124:SER:HB3	1.35	1.08
1:B:146:GLN:H	1:B:146:GLN:NE2	1.55	1.03
1:F:123:VAL:HG21	1:F:127:PHE:HB2	1.37	1.01
1:G:56:ARG:HH21	1:G:106:ILE:HD11	1.29	0.95
1:A:123:VAL:HG11	1:A:127:PHE:HB2	1.48	0.95
1:C:59:ALA:HB1	1:C:124:SER:HB3	1.50	0.94
1:D:146:GLN:NE2	1:D:146:GLN:H	1.64	0.94
1:F:36:ARG:HE	1:F:128:THR:HG21	1.30	0.93
1:E:124:SER:HB3	1:E:125:PRO:HD3	1.49	0.93
1:J:146:GLN:H	1:J:146:GLN:NE2	1.64	0.93
1:H:146:GLN:H	1:H:146:GLN:NE2	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:SER:HB3	1:H:125:PRO:HD3	1.49	0.92
1:B:146:GLN:HE21	1:B:146:GLN:N	1.67	0.92
1:D:3:ASN:HD21	1:D:5:ASP:HB2	1.30	0.92
1:E:4:ALA:HB2	1:E:116:PHE:HB3	1.51	0.91
1:D:122:MSE:SE	1:J:122:MSE:HE3	2.21	0.91
1:D:146:GLN:H	1:D:146:GLN:HE21	0.90	0.90
1:E:122:MSE:HE1	1:E:124:SER:HA	1.53	0.89
1:F:124:SER:CB	1:F:125:PRO:HD3	2.03	0.88
1:C:75:MSE:HE3	1:C:102:PRO:HD2	1.54	0.88
1:H:146:GLN:H	1:H:146:GLN:HE21	1.22	0.88
1:D:122:MSE:HE1	1:D:124:SER:HA	1.57	0.87
1:D:146:GLN:HE21	1:D:146:GLN:N	1.73	0.86
1:D:39:TRP:HB2	1:D:122:MSE:HE3	1.58	0.85
1:A:124:SER:HB3	1:A:125:PRO:CD	2.07	0.85
1:B:146:GLN:H	1:B:146:GLN:HE21	0.85	0.85
1:A:122:MSE:SE	1:H:122:MSE:HE3	2.26	0.84
1:H:123:VAL:HG21	1:H:127:PHE:HB2	1.60	0.84
1:J:124:SER:HB3	1:J:125:PRO:HD3	1.58	0.84
1:E:146:GLN:H	1:E:146:GLN:NE2	1.75	0.84
1:J:146:GLN:H	1:J:146:GLN:HE21	1.20	0.84
1:E:39:TRP:HB2	1:E:122:MSE:HE3	1.59	0.83
1:D:13:LEU:HD23	1:D:23:ARG:HB2	1.59	0.83
1:H:39:TRP:HB2	1:H:122:MSE:HE2	1.61	0.83
1:H:45:LEU:HD23	1:H:46:LEU:N	1.93	0.83
1:H:119:VAL:HG12	1:H:120:GLY:H	1.44	0.83
1:H:39:TRP:CB	1:H:122:MSE:HE2	2.09	0.83
1:G:113:GLN:HG3	1:G:114:ASP:H	1.43	0.83
1:D:136:SER:HB2	1:D:158:GLU:HG2	1.61	0.82
1:I:39:TRP:HB2	1:I:122:MSE:HE2	1.61	0.82
1:F:150:VAL:HG13	1:F:151:VAL:H	1.42	0.82
1:D:124:SER:HB3	1:D:125:PRO:HD3	1.62	0.82
1:J:108:GLY:HA3	1:J:154:LEU:HD13	1.61	0.81
1:G:124:SER:OG	1:G:125:PRO:HD3	1.80	0.81
1:F:62:MSE:HB2	1:F:122:MSE:HB3	1.61	0.80
1:G:124:SER:CB	1:G:125:PRO:HD3	2.12	0.80
1:F:36:ARG:NE	1:F:128:THR:HG21	1.97	0.79
1:I:124:SER:HB3	1:I:125:PRO:HD3	1.63	0.79
1:D:36:ARG:HH22	1:D:130:ASP:HB3	1.47	0.79
1:D:39:TRP:HA	1:D:124:SER:O	1.82	0.79
1:I:39:TRP:CB	1:I:122:MSE:HE2	2.13	0.79
1:B:100:LEU:C	1:B:100:LEU:HD23	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD23	1:A:23:ARG:HB2	1.63	0.78
1:F:124:SER:HB3	1:F:125:PRO:HD3	1.64	0.78
1:J:39:TRP:HB2	1:J:122:MSE:HE2	1.65	0.77
1:J:86:GLN:HE22	1:J:112:ASN:ND2	1.81	0.77
1:B:1:MSE:HE3	1:B:2:GLN:H	1.50	0.77
1:D:59:ALA:HB1	1:D:125:PRO:HD2	1.66	0.77
1:C:58:THR:HB	2:C:163:HOH:O	1.84	0.76
1:D:39:TRP:HB2	1:D:122:MSE:CE	2.15	0.76
1:G:4:ALA:HB1	1:G:45:LEU:HD21	1.65	0.76
1:C:90:ASP:O	1:C:95:GLU:HB2	1.86	0.76
1:A:39:TRP:CB	1:A:122:MSE:HE3	2.14	0.76
1:C:35:SER:HB2	1:C:36:ARG:HH11	1.51	0.75
1:I:73:ILE:HB	1:I:85:ALA:HB3	1.68	0.75
1:G:8:ILE:HG13	1:G:13:LEU:HB2	1.68	0.75
1:I:146:GLN:NE2	1:I:146:GLN:H	1.83	0.75
1:B:91:LEU:HD13	1:C:10:PHE:HB2	1.67	0.75
1:B:23:ARG:HH11	1:H:23:ARG:HH11	1.34	0.74
1:F:45:LEU:HD23	1:F:46:LEU:N	2.02	0.74
1:E:91:LEU:HD11	1:F:7:PHE:HD2	1.51	0.74
1:F:27:ARG:HB3	1:F:27:ARG:HH11	1.50	0.74
1:F:146:GLN:H	1:F:146:GLN:NE2	1.85	0.74
1:C:53:HIS:O	1:C:55:HIS:HD2	1.70	0.74
1:D:3:ASN:ND2	1:D:5:ASP:HB2	2.03	0.73
1:B:16:HIS:HD2	1:B:18:GLU:H	1.35	0.73
1:C:59:ALA:HB1	1:C:124:SER:CB	2.19	0.73
1:A:39:TRP:HB2	1:A:122:MSE:CE	2.15	0.73
1:J:146:GLN:HE21	1:J:146:GLN:N	1.86	0.73
1:G:56:ARG:HB2	1:G:106:ILE:HG12	1.70	0.73
1:E:39:TRP:HA	1:E:124:SER:O	1.87	0.73
1:G:24:SER:HA	1:G:42:ILE:HG22	1.69	0.73
1:G:10:PHE:HB3	1:I:91:LEU:HD22	1.71	0.72
1:C:124:SER:O	1:C:125:PRO:C	2.32	0.72
1:J:39:TRP:HA	1:J:124:SER:O	1.89	0.72
1:C:124:SER:CB	1:C:125:PRO:HD2	2.19	0.72
1:F:75:MSE:HE1	1:F:102:PRO:HD2	1.69	0.72
1:I:13:LEU:HB3	1:I:21:PHE:HB3	1.71	0.72
1:I:28:SER:HB2	1:I:39:TRP:CD1	2.25	0.72
1:H:39:TRP:HA	1:H:124:SER:O	1.88	0.72
1:B:39:TRP:CB	1:B:122:MSE:HE2	2.20	0.72
1:J:86:GLN:HE22	1:J:112:ASN:HD21	1.38	0.71
1:B:23:ARG:HH11	1:H:23:ARG:NH1	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:VAL:HG12	1:H:120:GLY:N	2.03	0.71
1:A:39:TRP:HA	1:A:124:SER:O	1.90	0.71
1:E:146:GLN:H	1:E:146:GLN:HE21	1.35	0.71
1:D:45:LEU:HD23	1:D:46:LEU:N	2.06	0.71
1:G:27:ARG:HB2	1:G:27:ARG:HH11	1.56	0.71
1:B:124:SER:HB3	1:B:125:PRO:HD3	1.72	0.70
1:G:39:TRP:CB	1:G:122:MSE:HE3	2.21	0.70
1:C:146:GLN:H	1:C:146:GLN:NE2	1.89	0.70
1:C:36:ARG:H	1:C:36:ARG:HD2	1.57	0.70
1:D:8:ILE:HA	1:D:13:LEU:HD12	1.72	0.70
1:G:11:LEU:O	1:G:23:ARG:HD3	1.92	0.69
1:E:122:MSE:HE1	1:E:124:SER:CA	2.21	0.69
1:E:124:SER:HB3	1:E:125:PRO:CD	2.21	0.69
1:G:123:VAL:HG21	1:G:127:PHE:HB2	1.74	0.69
1:C:146:GLN:HG2	1:C:147:HIS:H	1.56	0.68
1:E:124:SER:CB	1:E:125:PRO:HD3	2.21	0.68
1:F:36:ARG:HE	1:F:128:THR:CG2	2.04	0.68
1:G:59:ALA:HB1	1:G:124:SER:CB	2.20	0.68
1:D:48:THR:HG23	1:D:114:ASP:OD1	1.94	0.68
1:B:3:ASN:HD21	1:B:5:ASP:HB2	1.57	0.68
1:H:33:ASP:C	1:H:35:SER:H	2.02	0.68
1:J:33:ASP:C	1:J:35:SER:H	2.01	0.68
1:D:58:THR:O	1:D:58:THR:HG22	1.93	0.68
1:E:91:LEU:HD13	1:F:10:PHE:HB2	1.76	0.68
1:H:48:THR:HA	1:H:111:MSE:HE1	1.75	0.67
1:H:146:GLN:HE21	1:H:146:GLN:N	1.90	0.67
1:G:27:ARG:HB2	1:G:27:ARG:NH1	2.10	0.67
1:G:124:SER:HB3	1:G:125:PRO:CD	2.24	0.67
1:C:122:MSE:HE2	1:C:123:VAL:C	2.19	0.67
1:F:13:LEU:HD23	1:F:23:ARG:HB2	1.77	0.67
1:H:16:HIS:CD2	1:H:18:GLU:H	2.13	0.67
1:A:58:THR:HB	1:A:131:ASP:HB3	1.76	0.67
1:B:23:ARG:HD2	1:H:23:ARG:HH12	1.60	0.67
1:J:22:TYR:H	1:J:22:TYR:HD2	1.41	0.67
1:F:31:ALA:HB2	1:F:37:GLN:NE2	2.10	0.66
1:H:124:SER:HB3	1:H:125:PRO:CD	2.22	0.66
1:B:39:TRP:HA	1:B:124:SER:O	1.95	0.66
1:G:37:GLN:HB2	1:G:126:GLY:HA3	1.78	0.66
1:C:127:PHE:HE1	1:C:132:PHE:HB2	1.60	0.66
1:D:137:GLN:NE2	1:D:152:GLN:HG2	2.10	0.66
1:F:39:TRP:HB2	1:F:122:MSE:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:HIS:O	1:H:55:HIS:HD2	1.77	0.66
1:I:153:LYS:HD2	1:I:153:LYS:N	2.11	0.66
2:B:169:HOH:O	1:C:96:ARG:HG2	1.94	0.66
1:G:122:MSE:HE2	1:G:123:VAL:O	1.96	0.66
1:E:91:LEU:HD11	1:F:7:PHE:CD2	2.31	0.66
1:B:39:TRP:HB2	1:B:122:MSE:HE2	1.78	0.66
1:C:137:GLN:HB2	1:C:155:SER:HB3	1.78	0.66
1:E:1:MSE:HE3	1:E:2:GLN:H	1.61	0.66
1:F:39:TRP:HB2	1:F:122:MSE:CE	2.26	0.66
1:I:8:ILE:HD12	1:I:13:LEU:HB2	1.77	0.65
1:E:8:ILE:HG13	1:E:13:LEU:HB2	1.79	0.65
1:F:3:ASN:HD22	1:F:5:ASP:HB2	1.60	0.65
1:C:111:MSE:HE1	1:C:115:GLY:H	1.61	0.65
1:B:100:LEU:C	1:B:100:LEU:CD2	2.70	0.65
1:C:39:TRP:HB2	1:C:122:MSE:HE3	1.77	0.65
1:J:39:TRP:CB	1:J:122:MSE:HE2	2.26	0.65
1:B:60:ASP:OD2	1:B:103:LYS:HG2	1.95	0.65
1:H:12:GLU:O	1:H:23:ARG:HG3	1.97	0.64
1:G:124:SER:CB	1:G:125:PRO:CD	2.73	0.64
1:I:58:THR:HB	1:I:131:ASP:HB3	1.78	0.64
1:G:69:GLN:HG2	1:G:113:GLN:HB3	1.78	0.64
1:G:124:SER:HB3	1:G:125:PRO:HD3	1.79	0.64
1:H:36:ARG:HG3	1:H:36:ARG:HH11	1.62	0.64
1:A:90:ASP:O	1:A:95:GLU:HB2	1.98	0.64
1:I:28:SER:HB2	1:I:39:TRP:NE1	2.12	0.64
1:C:148:LYS:O	1:C:152:GLN:HG3	1.97	0.64
1:G:39:TRP:HB2	1:G:122:MSE:HE3	1.78	0.64
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.63	0.63
1:F:64:TYR:O	1:F:119:VAL:HG13	1.98	0.63
1:D:124:SER:HB3	1:D:125:PRO:CD	2.27	0.63
1:H:8:ILE:HG13	1:H:9:LYS:N	2.11	0.63
1:B:122:MSE:HE3	1:C:122:MSE:SE	2.48	0.63
1:I:153:LYS:HD2	1:I:153:LYS:H	1.63	0.63
1:A:59:ALA:HB1	1:A:125:PRO:HD2	1.81	0.63
1:B:139:ALA:O	1:B:143:MSE:HG2	1.98	0.63
1:I:8:ILE:CD1	1:I:13:LEU:HB2	2.28	0.63
1:C:36:ARG:HD2	1:C:36:ARG:N	2.13	0.63
1:C:101:VAL:HG23	1:C:101:VAL:O	1.99	0.63
1:C:124:SER:OG	1:C:125:PRO:HD2	1.99	0.63
1:H:24:SER:HA	1:H:42:ILE:HG22	1.79	0.63
1:C:139:ALA:O	1:C:143:MSE:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:LEU:HA	1:I:96:ARG:NH2	2.14	0.62
1:B:16:HIS:CD2	1:B:18:GLU:H	2.17	0.62
1:A:8:ILE:HA	1:A:13:LEU:HD12	1.79	0.62
1:B:146:GLN:NE2	1:B:146:GLN:N	2.38	0.62
1:A:122:MSE:HE2	1:A:123:VAL:O	2.00	0.62
1:D:7:PHE:CD2	1:J:91:LEU:HD11	2.35	0.61
1:B:54:PHE:HD2	1:B:106:ILE:HG22	1.64	0.61
1:I:144:TYR:N	1:I:145:PRO:HD3	2.16	0.61
1:F:75:MSE:CE	1:F:102:PRO:HD2	2.30	0.61
1:B:39:TRP:HB3	1:B:122:MSE:HE2	1.82	0.61
1:A:152:GLN:C	1:A:153:LYS:HD2	2.24	0.61
1:G:56:ARG:NH2	1:G:106:ILE:HD11	2.11	0.61
1:E:146:GLN:HE21	1:E:146:GLN:N	1.98	0.60
1:D:71:LEU:HD11	1:D:117:SER:HB3	1.83	0.60
1:B:27:ARG:HD2	2:B:186:HOH:O	2.01	0.60
1:I:66:HIS:HB2	1:I:118:LEU:O	2.01	0.60
1:G:146:GLN:H	1:G:146:GLN:NE2	1.98	0.60
1:B:54:PHE:CD2	1:B:106:ILE:HG22	2.36	0.60
1:F:56:ARG:HB2	1:F:106:ILE:HG12	1.83	0.60
1:I:146:GLN:H	1:I:146:GLN:HE21	1.49	0.60
1:J:124:SER:O	1:J:126:GLY:N	2.34	0.60
1:F:50:GLU:O	1:F:51:VAL:HG13	2.01	0.60
1:B:54:PHE:HA	1:B:107:PHE:O	2.00	0.60
1:D:62:MSE:HB2	1:D:122:MSE:HB3	1.84	0.60
1:A:122:MSE:CE	1:A:124:SER:HA	2.16	0.59
1:F:77:SER:C	1:F:79:GLU:H	2.10	0.59
1:G:120:GLY:HA3	1:I:98:GLN:NE2	2.17	0.59
1:C:47:ARG:O	1:C:49:GLY:N	2.35	0.59
1:B:23:ARG:NH1	1:H:23:ARG:HH11	2.00	0.59
1:H:44:PHE:CE1	1:H:46:LEU:HD13	2.37	0.59
1:I:4:ALA:O	1:I:8:ILE:HG22	2.02	0.59
1:G:46:LEU:HD23	1:G:111:MSE:HG3	1.84	0.59
1:C:144:TYR:N	1:C:145:PRO:HD3	2.18	0.59
1:J:86:GLN:NE2	1:J:112:ASN:HD21	2.00	0.59
1:H:108:GLY:HA3	1:H:154:LEU:HD13	1.85	0.59
1:C:146:GLN:HG2	1:C:147:HIS:N	2.18	0.59
1:E:144:TYR:N	1:E:145:PRO:HD3	2.18	0.59
1:C:36:ARG:H	1:C:36:ARG:CD	2.16	0.59
1:C:62:MSE:SE	1:C:100:LEU:HB2	2.53	0.59
1:D:144:TYR:N	1:D:145:PRO:HD3	2.18	0.58
1:J:37:GLN:HE21	1:J:37:GLN:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:SER:HB3	1:C:126:GLY:HA2	1.83	0.58
1:E:75:MSE:HE1	1:E:102:PRO:HD2	1.84	0.58
1:H:39:TRP:HB3	1:H:122:MSE:HE2	1.84	0.58
1:J:5:ASP:HA	1:J:8:ILE:CG1	2.33	0.58
1:F:28:SER:OG	1:F:38:LEU:HB3	2.04	0.58
1:G:76:ILE:HG22	1:G:106:ILE:O	2.03	0.58
1:I:123:VAL:HG23	1:I:123:VAL:O	2.04	0.58
1:A:91:LEU:HD13	1:H:10:PHE:HB2	1.84	0.58
1:E:75:MSE:HB3	1:E:107:PHE:HB3	1.85	0.58
1:I:14:GLU:O	1:I:21:PHE:HA	2.03	0.58
1:I:148:LYS:O	1:I:152:GLN:HG3	2.03	0.58
1:E:16:HIS:HB3	1:E:18:GLU:HG3	1.84	0.58
1:E:65:PHE:HZ	1:E:68:GLY:O	1.87	0.58
1:B:38:LEU:HD21	1:C:125:PRO:HD3	1.85	0.58
1:G:6:ASP:O	1:G:10:PHE:HB2	2.04	0.58
1:H:151:VAL:HG12	1:H:151:VAL:O	2.04	0.58
1:G:45:LEU:HD12	1:G:117:SER:O	2.04	0.58
1:I:73:ILE:N	1:I:73:ILE:HD12	2.19	0.58
1:D:87:LEU:HD12	1:D:96:ARG:O	2.05	0.57
1:E:45:LEU:HD23	1:E:46:LEU:N	2.19	0.57
1:J:59:ALA:HB1	1:J:125:PRO:HD2	1.86	0.57
1:C:128:THR:HA	1:F:15:GLN:HE22	1.70	0.57
1:D:111:MSE:HE3	1:D:113:GLN:O	2.04	0.57
1:H:151:VAL:O	1:H:155:SER:HB2	2.04	0.57
1:I:147:HIS:O	1:I:151:VAL:HG23	2.03	0.57
1:E:90:ASP:O	1:E:95:GLU:HB2	2.04	0.57
1:J:148:LYS:O	1:J:152:GLN:HG3	2.03	0.57
1:D:124:SER:O	1:D:126:GLY:N	2.38	0.57
1:D:122:MSE:HE1	1:D:124:SER:CA	2.32	0.57
1:G:146:GLN:HG2	1:G:147:HIS:H	1.69	0.57
1:G:151:VAL:O	1:G:155:SER:HB3	2.05	0.57
1:B:33:ASP:C	1:B:35:SER:H	2.13	0.57
1:E:125:PRO:O	1:E:126:GLY:C	2.47	0.56
1:A:122:MSE:HE1	1:A:124:SER:CA	2.16	0.56
1:B:28:SER:HB2	1:B:39:TRP:CD1	2.39	0.56
1:C:45:LEU:HD23	1:C:46:LEU:N	2.19	0.56
1:G:39:TRP:HB3	1:G:122:MSE:HE3	1.87	0.56
1:G:123:VAL:CG2	1:G:127:PHE:HB2	2.35	0.56
1:H:16:HIS:HD2	1:H:18:GLU:H	1.52	0.56
1:I:75:MSE:HB2	1:I:83:THR:HB	1.87	0.56
1:J:145:PRO:HD2	1:J:146:GLN:HE22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:LEU:C	1:E:100:LEU:HD23	2.30	0.56
1:F:111:MSE:HE3	1:F:113:GLN:O	2.06	0.56
1:F:119:VAL:HG12	1:F:120:GLY:N	2.21	0.56
1:H:54:PHE:CD2	1:H:106:ILE:HG22	2.40	0.56
1:A:147:HIS:O	1:A:151:VAL:HG23	2.05	0.56
1:B:58:THR:HG22	1:B:131:ASP:HB3	1.86	0.56
1:E:71:LEU:HD11	1:E:117:SER:HB2	1.87	0.56
1:G:122:MSE:SE	1:I:122:MSE:HE3	2.55	0.56
1:J:71:LEU:HD23	1:J:111:MSE:HA	1.88	0.56
1:E:70:SER:C	1:E:71:LEU:HD12	2.30	0.56
1:F:61:GLU:HB3	1:F:101:VAL:CG2	2.35	0.56
1:G:90:ASP:O	1:G:95:GLU:HB2	2.05	0.56
1:A:122:MSE:HE2	1:A:123:VAL:C	2.31	0.56
1:C:124:SER:HB3	1:C:125:PRO:HD2	1.88	0.56
1:D:71:LEU:N	1:D:71:LEU:HD12	2.20	0.56
1:I:119:VAL:HG12	1:I:120:GLY:N	2.20	0.56
1:G:96:ARG:HH21	1:I:10:PHE:HB3	1.70	0.56
1:I:8:ILE:HA	1:I:13:LEU:HD12	1.87	0.56
1:E:91:LEU:HD13	1:F:10:PHE:CB	2.35	0.55
1:F:124:SER:OG	1:F:125:PRO:HD3	2.06	0.55
1:B:150:VAL:HG13	1:B:151:VAL:N	2.21	0.55
1:C:65:PHE:HB2	1:C:87:LEU:CD2	2.36	0.55
1:F:145:PRO:HD2	1:F:146:GLN:HE22	1.71	0.55
1:A:137:GLN:O	1:A:141:LEU:HD23	2.06	0.55
1:B:80:GLY:O	1:B:147:HIS:HE1	1.89	0.55
1:G:75:MSE:HG2	1:G:107:PHE:HB3	1.88	0.55
1:C:12:GLU:O	1:C:23:ARG:HG3	2.06	0.55
1:H:16:HIS:HB3	1:H:19:GLY:O	2.06	0.55
1:A:139:ALA:O	1:A:143:MSE:HG2	2.07	0.55
1:D:16:HIS:HA	2:D:167:HOH:O	2.06	0.55
1:E:110:ALA:HB2	1:E:154:LEU:HD21	1.88	0.55
1:H:45:LEU:HD23	1:H:45:LEU:C	2.31	0.55
1:C:3:ASN:ND2	1:C:5:ASP:H	2.04	0.55
1:F:150:VAL:HG13	1:F:151:VAL:N	2.15	0.55
1:G:10:PHE:HB2	1:I:91:LEU:HD13	1.87	0.55
1:G:137:GLN:HG3	1:G:155:SER:C	2.31	0.55
1:H:59:ALA:HB1	1:H:125:PRO:HD2	1.87	0.55
1:E:59:ALA:HB1	1:E:125:PRO:HD2	1.88	0.55
1:H:149:ALA:HB1	1:J:146:GLN:CD	2.32	0.55
1:I:39:TRP:HB3	1:I:122:MSE:HE2	1.89	0.55
1:J:5:ASP:HA	1:J:8:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:GLN:CB	1:G:126:GLY:HA3	2.36	0.55
1:G:137:GLN:HG3	1:G:155:SER:O	2.07	0.55
1:C:54:PHE:CD2	1:C:106:ILE:HG22	2.42	0.55
1:E:100:LEU:C	1:E:100:LEU:CD2	2.80	0.55
1:I:33:ASP:C	1:I:35:SER:H	2.14	0.55
1:C:28:SER:HB2	1:C:39:TRP:CD1	2.41	0.55
1:D:124:SER:CB	1:D:125:PRO:HD3	2.34	0.55
1:A:7:PHE:CE2	1:H:91:LEU:HD11	2.42	0.54
1:B:151:VAL:O	1:B:155:SER:HB2	2.06	0.54
1:F:74:TYR:HA	1:F:84:THR:HG22	1.89	0.54
1:H:1:MSE:HE3	1:H:2:GLN:H	1.72	0.54
1:A:2:GLN:OE1	1:H:91:LEU:HD12	2.08	0.54
1:B:145:PRO:HD2	1:B:146:GLN:HE22	1.71	0.54
1:J:147:HIS:O	1:J:151:VAL:HG23	2.08	0.54
1:I:147:HIS:O	1:I:150:VAL:HG12	2.08	0.54
1:J:101:VAL:HG21	1:J:107:PHE:CD2	2.43	0.54
1:J:124:SER:HB3	1:J:125:PRO:CD	2.35	0.54
1:B:127:PHE:CE1	1:B:132:PHE:HB2	2.43	0.54
1:D:4:ALA:HB2	1:D:116:PHE:HB3	1.90	0.54
1:D:146:GLN:NE2	1:D:146:GLN:N	2.45	0.54
1:H:55:HIS:HB3	1:H:134:LEU:HD12	1.90	0.54
1:A:91:LEU:HD11	1:H:7:PHE:CD2	2.42	0.54
1:F:100:LEU:HD23	1:F:101:VAL:N	2.23	0.54
1:E:147:HIS:HB3	1:E:150:VAL:HG12	1.90	0.54
1:I:16:HIS:HD2	1:I:18:GLU:HG2	1.73	0.54
1:D:64:TYR:O	1:D:119:VAL:HG22	2.08	0.54
1:F:27:ARG:HD2	2:F:161:HOH:O	2.07	0.54
1:I:137:GLN:HG3	1:I:151:VAL:HG12	1.89	0.53
1:E:68:GLY:HA3	1:E:117:SER:HA	1.90	0.53
1:G:113:GLN:CG	1:G:114:ASP:H	2.14	0.53
1:J:22:TYR:HA	1:J:43:TYR:O	2.08	0.53
1:J:26:TYR:HA	2:J:162:HOH:O	2.08	0.53
1:B:124:SER:O	1:B:126:GLY:N	2.41	0.53
1:F:144:TYR:N	1:F:145:PRO:HD3	2.22	0.53
1:G:91:LEU:HD11	1:I:7:PHE:CD2	2.42	0.53
1:H:72:THR:OG1	1:H:112:ASN:ND2	2.41	0.53
1:J:100:LEU:C	1:J:100:LEU:HD23	2.34	0.53
1:D:147:HIS:O	1:D:151:VAL:HG23	2.07	0.53
1:C:8:ILE:HD12	1:C:8:ILE:O	2.09	0.53
1:H:7:PHE:O	1:H:11:LEU:HB2	2.08	0.53
1:C:24:SER:HA	1:C:42:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:SER:CB	1:C:125:PRO:CD	2.85	0.53
1:E:7:PHE:CD2	1:E:118:LEU:HD22	2.44	0.53
1:J:137:GLN:NE2	1:J:152:GLN:HA	2.24	0.53
1:E:150:VAL:HG13	1:E:151:VAL:N	2.24	0.53
1:B:124:SER:O	1:B:125:PRO:C	2.44	0.52
1:F:5:ASP:HA	1:F:8:ILE:HG22	1.89	0.52
1:I:101:VAL:HG21	1:I:107:PHE:CD2	2.44	0.52
1:E:17:VAL:C	1:E:19:GLY:H	2.17	0.52
1:J:45:LEU:HA	1:J:117:SER:O	2.09	0.52
1:B:53:HIS:CE1	1:B:156:ARG:HH11	2.27	0.52
1:E:69:GLN:HG2	1:E:113:GLN:HB3	1.90	0.52
1:H:50:GLU:O	1:H:51:VAL:HG13	2.10	0.52
1:I:7:PHE:CD2	1:I:118:LEU:HD22	2.44	0.52
1:E:56:ARG:C	1:E:57:LEU:HD12	2.33	0.52
1:F:27:ARG:HB3	1:F:27:ARG:NH1	2.23	0.52
1:J:53:HIS:HB3	2:J:169:HOH:O	2.08	0.52
1:B:124:SER:HB3	1:B:125:PRO:CD	2.39	0.52
1:D:27:ARG:HH11	1:D:27:ARG:CB	2.22	0.52
1:H:59:ALA:C	1:H:103:LYS:HB3	2.35	0.52
1:A:125:PRO:O	1:A:126:GLY:C	2.53	0.52
1:D:82:LEU:HD13	1:D:150:VAL:HG11	1.91	0.52
1:H:77:SER:C	1:H:79:GLU:H	2.18	0.52
1:I:137:GLN:O	1:I:141:LEU:HB2	2.09	0.52
1:C:71:LEU:HD21	1:C:117:SER:HB3	1.92	0.52
2:D:172:HOH:O	1:J:96:ARG:HG2	2.08	0.52
1:E:54:PHE:HA	1:E:107:PHE:O	2.10	0.52
1:I:38:LEU:O	1:I:124:SER:O	2.28	0.52
1:E:27:ARG:HE	1:E:37:GLN:HG3	1.74	0.52
1:G:16:HIS:HD2	1:G:18:GLU:H	1.56	0.52
1:A:8:ILE:HD12	1:A:9:LYS:N	2.25	0.52
1:B:90:ASP:O	1:B:95:GLU:HB2	2.09	0.52
1:D:141:LEU:O	1:D:145:PRO:HG3	2.11	0.52
1:F:37:GLN:O	1:F:126:GLY:N	2.43	0.52
1:J:143:MSE:HG3	1:J:144:TYR:CD2	2.45	0.51
1:B:119:VAL:HG12	1:B:120:GLY:N	2.25	0.51
1:H:58:THR:HG22	1:H:131:ASP:HB3	1.92	0.51
1:I:137:GLN:HE21	1:I:152:GLN:HA	1.73	0.51
1:H:122:MSE:SE	1:H:122:MSE:C	3.03	0.51
1:C:28:SER:HB2	1:C:39:TRP:CE2	2.46	0.51
1:C:71:LEU:HD21	1:C:117:SER:CB	2.41	0.51
1:D:28:SER:HB2	1:D:39:TRP:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:SER:O	1:H:126:GLY:N	2.44	0.51
1:A:100:LEU:C	1:A:100:LEU:HD13	2.35	0.51
1:A:101:VAL:HG21	1:A:107:PHE:CD2	2.46	0.51
1:E:28:SER:C	1:E:30:THR:H	2.18	0.51
1:G:75:MSE:HB3	1:G:105:CYS:SG	2.51	0.51
1:A:8:ILE:HD11	2:A:170:HOH:O	2.09	0.51
1:E:62:MSE:O	1:E:121:CYS:HA	2.10	0.51
1:F:17:VAL:HG13	1:F:18:GLU:N	2.26	0.51
1:H:147:HIS:HB3	1:H:150:VAL:CG1	2.41	0.51
1:B:71:LEU:HD23	1:B:111:MSE:HA	1.92	0.51
1:I:45:LEU:HA	1:I:117:SER:O	2.11	0.51
1:E:13:LEU:HA	1:E:23:ARG:HB2	1.93	0.51
1:E:124:SER:CB	1:E:125:PRO:CD	2.83	0.51
1:F:59:ALA:HB1	1:F:125:PRO:HD2	1.93	0.51
1:I:24:SER:HA	1:I:42:ILE:HG22	1.93	0.51
1:B:137:GLN:HA	1:B:155:SER:HB3	1.93	0.51
1:C:65:PHE:HB2	1:C:87:LEU:HD21	1.92	0.51
1:E:123:VAL:HG11	1:E:127:PHE:HB2	1.93	0.51
1:H:71:LEU:HD21	1:H:117:SER:OG	2.10	0.51
1:H:72:THR:N	1:H:112:ASN:HD21	2.09	0.51
1:I:146:GLN:HG2	1:I:147:HIS:ND1	2.26	0.51
1:B:53:HIS:O	1:B:55:HIS:HD2	1.95	0.50
1:G:16:HIS:CD2	1:G:18:GLU:HG2	2.46	0.50
1:A:151:VAL:O	1:A:155:SER:HB3	2.11	0.50
1:C:100:LEU:HD13	1:C:100:LEU:C	2.37	0.50
1:D:124:SER:O	1:D:125:PRO:C	2.50	0.50
1:G:53:HIS:CD2	1:G:155:SER:HA	2.46	0.50
1:H:33:ASP:C	1:H:35:SER:N	2.61	0.50
1:I:66:HIS:HD2	1:I:119:VAL:C	2.20	0.50
1:A:16:HIS:HB3	1:A:19:GLY:O	2.11	0.50
1:A:54:PHE:CE1	1:A:154:LEU:HB2	2.47	0.50
1:I:91:LEU:HD23	1:I:96:ARG:HH21	1.76	0.50
1:J:86:GLN:HE22	1:J:112:ASN:CG	2.18	0.50
1:A:27:ARG:HE	1:A:40:SER:HB3	1.76	0.50
1:C:39:TRP:CB	1:C:122:MSE:HE3	2.42	0.50
1:E:89:LEU:HD23	1:E:97:PRO:HG3	1.93	0.50
1:F:124:SER:CB	1:F:125:PRO:CD	2.80	0.50
1:H:36:ARG:HG3	1:H:36:ARG:NH1	2.26	0.50
1:A:39:TRP:CD1	1:H:124:SER:HB2	2.46	0.50
1:E:123:VAL:CG1	1:E:127:PHE:HB2	2.42	0.50
1:F:13:LEU:HA	1:F:22:TYR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:GLN:HG2	1:G:147:HIS:N	2.26	0.50
1:H:125:PRO:O	1:H:126:GLY:C	2.55	0.50
1:C:47:ARG:C	1:C:49:GLY:H	2.20	0.50
1:C:147:HIS:O	1:C:151:VAL:HG23	2.12	0.49
1:E:122:MSE:HE2	1:E:123:VAL:C	2.36	0.49
1:J:80:GLY:HA2	1:J:144:TYR:CE1	2.46	0.49
1:J:144:TYR:N	1:J:145:PRO:HD3	2.27	0.49
1:D:86:GLN:HB2	1:D:94:GLY:O	2.12	0.49
1:H:80:GLY:O	1:H:147:HIS:HE1	1.95	0.49
1:B:119:VAL:CG1	1:B:120:GLY:N	2.75	0.49
1:H:69:GLN:CG	1:H:113:GLN:HB3	2.43	0.49
1:B:23:ARG:HD2	1:H:23:ARG:NH1	2.25	0.49
1:C:75:MSE:CE	1:C:102:PRO:HD2	2.34	0.49
1:G:56:ARG:HG2	1:G:57:LEU:N	2.27	0.49
1:J:3:ASN:HD22	1:J:5:ASP:HB2	1.78	0.49
1:E:122:MSE:HE1	1:E:124:SER:N	2.27	0.49
1:F:1:MSE:HE3	1:F:2:GLN:HB3	1.93	0.49
1:G:59:ALA:C	1:G:103:LYS:HB3	2.37	0.49
1:J:33:ASP:C	1:J:35:SER:N	2.69	0.49
1:A:48:THR:O	1:A:48:THR:HG22	2.12	0.49
1:B:149:ALA:HB3	2:B:168:HOH:O	2.13	0.49
1:F:122:MSE:HE2	1:F:123:VAL:N	2.28	0.49
1:A:45:LEU:HA	1:A:117:SER:O	2.11	0.49
1:C:80:GLY:O	1:C:147:HIS:HE1	1.95	0.49
1:G:60:ASP:H	1:G:124:SER:HB2	1.77	0.49
1:I:123:VAL:HG21	1:I:127:PHE:HB2	1.95	0.49
1:J:122:MSE:SE	1:J:122:MSE:C	3.06	0.49
1:J:145:PRO:HD2	1:J:146:GLN:NE2	2.28	0.49
1:C:61:GLU:HB2	1:C:123:VAL:HG22	1.94	0.49
1:E:27:ARG:HH11	1:E:27:ARG:HB3	1.77	0.49
1:I:69:GLN:NE2	1:I:69:GLN:H	2.11	0.49
1:B:65:PHE:HZ	1:B:68:GLY:O	1.95	0.49
1:G:56:ARG:C	1:G:57:LEU:HD12	2.38	0.49
1:F:5:ASP:HA	1:F:8:ILE:CG2	2.43	0.48
1:H:66:HIS:O	1:H:67:ALA:HB2	2.13	0.48
1:H:144:TYR:N	1:H:145:PRO:HD3	2.28	0.48
1:B:7:PHE:CE2	1:B:118:LEU:HD22	2.49	0.48
1:B:7:PHE:CD2	1:C:91:LEU:HD11	2.48	0.48
1:B:100:LEU:CD2	1:B:100:LEU:O	2.62	0.48
1:C:35:SER:HB2	1:C:36:ARG:HD2	1.94	0.48
1:D:16:HIS:HB3	1:D:19:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:SER:CB	1:J:62:MSE:HE2	2.42	0.48
1:F:30:THR:HB	1:F:38:LEU:HD22	1.94	0.48
1:G:96:ARG:HG2	2:I:162:HOH:O	2.14	0.48
1:A:48:THR:HG23	1:A:114:ASP:OD1	2.13	0.48
1:D:101:VAL:HG21	1:D:107:PHE:CE2	2.48	0.48
1:I:137:GLN:NE2	1:I:152:GLN:HA	2.28	0.48
1:C:61:GLU:HG2	1:C:63:TRP:CD1	2.48	0.48
1:G:33:ASP:C	1:G:35:SER:H	2.22	0.48
1:I:62:MSE:HB3	1:I:64:TYR:CE2	2.48	0.48
1:J:77:SER:HB2	1:J:78:PRO:HD2	1.94	0.48
1:I:91:LEU:HA	1:I:96:ARG:HH21	1.79	0.48
1:C:35:SER:CB	1:C:36:ARG:HH11	2.24	0.48
1:D:54:PHE:HE1	1:D:151:VAL:HA	1.78	0.48
1:D:59:ALA:C	1:D:103:LYS:HB3	2.39	0.48
1:F:145:PRO:HD2	1:F:146:GLN:NE2	2.27	0.48
1:I:106:ILE:HG21	1:I:140:LEU:HD11	1.95	0.48
1:C:147:HIS:O	1:C:148:LYS:C	2.57	0.48
1:D:54:PHE:CZ	1:D:154:LEU:HD12	2.49	0.48
1:E:27:ARG:HB3	1:E:27:ARG:NH1	2.29	0.48
1:A:27:ARG:HE	1:A:40:SER:CB	2.27	0.48
1:B:14:GLU:OE1	1:H:24:SER:HB2	2.14	0.48
1:B:61:GLU:HG3	1:B:123:VAL:HG12	1.95	0.48
1:E:1:MSE:CE	1:E:2:GLN:H	2.24	0.48
1:E:123:VAL:HG22	1:E:123:VAL:O	2.14	0.48
1:F:58:THR:N	1:F:131:ASP:OD1	2.42	0.48
1:H:48:THR:HA	1:H:111:MSE:CE	2.41	0.48
1:F:110:ALA:HB2	1:F:154:LEU:HD21	1.96	0.47
1:A:65:PHE:O	1:H:66:HIS:HA	2.14	0.47
1:B:37:GLN:HA	1:B:37:GLN:NE2	2.28	0.47
1:F:61:GLU:OE1	1:F:63:TRP:NE1	2.47	0.47
1:G:77:SER:HB2	1:G:78:PRO:HD2	1.95	0.47
1:I:124:SER:O	1:I:126:GLY:N	2.47	0.47
1:A:148:LYS:HE2	1:A:152:GLN:NE2	2.29	0.47
1:C:124:SER:OG	1:C:125:PRO:CD	2.62	0.47
1:F:96:ARG:HG3	1:F:97:PRO:CD	2.44	0.47
1:F:124:SER:OG	1:F:125:PRO:CD	2.61	0.47
1:G:16:HIS:CD2	1:G:18:GLU:H	2.30	0.47
1:H:90:ASP:O	1:H:95:GLU:HB2	2.14	0.47
1:B:24:SER:HA	1:B:42:ILE:HG22	1.96	0.47
1:E:5:ASP:HA	1:E:8:ILE:HG22	1.96	0.47
1:E:58:THR:HG22	1:E:131:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:THR:OG1	1:F:112:ASN:ND2	2.46	0.47
1:F:101:VAL:O	1:F:101:VAL:HG23	2.13	0.47
1:H:36:ARG:NE	1:H:131:ASP:OD2	2.47	0.47
1:H:69:GLN:HG2	1:H:113:GLN:HB3	1.94	0.47
1:A:21:PHE:O	1:A:44:PHE:HA	2.13	0.47
1:A:59:ALA:CB	1:A:125:PRO:HD2	2.45	0.47
1:C:101:VAL:O	1:C:101:VAL:CG2	2.62	0.47
1:C:140:LEU:O	1:C:151:VAL:HG11	2.14	0.47
1:B:3:ASN:ND2	1:B:5:ASP:HB2	2.27	0.47
1:B:55:HIS:HB3	1:B:134:LEU:HD12	1.96	0.47
1:B:57:LEU:HA	1:B:131:ASP:O	2.15	0.47
1:C:28:SER:HB2	1:C:39:TRP:NE1	2.29	0.47
1:F:111:MSE:HE1	1:F:115:GLY:O	2.13	0.47
1:G:38:LEU:O	1:G:125:PRO:HA	2.14	0.47
1:A:48:THR:HA	1:A:111:MSE:HE2	1.97	0.47
1:B:124:SER:HB2	1:C:39:TRP:CD1	2.50	0.47
1:C:64:TYR:O	1:C:120:GLY:N	2.46	0.47
1:F:45:LEU:HD23	1:F:45:LEU:C	2.40	0.47
1:H:91:LEU:HD23	1:H:96:ARG:HH21	1.79	0.47
1:H:112:ASN:ND2	1:H:112:ASN:N	2.62	0.47
1:H:151:VAL:O	1:H:151:VAL:CG1	2.63	0.47
1:J:33:ASP:O	1:J:35:SER:N	2.48	0.47
1:J:147:HIS:HB3	1:J:150:VAL:CG1	2.45	0.47
1:B:47:ARG:O	1:B:50:GLU:HB2	2.14	0.47
1:E:33:ASP:C	1:E:35:SER:N	2.72	0.47
1:I:77:SER:HB2	1:I:78:PRO:HD2	1.96	0.47
1:I:123:VAL:O	1:I:123:VAL:CG2	2.62	0.47
1:D:5:ASP:HA	1:D:8:ILE:HG23	1.97	0.47
1:E:119:VAL:CG1	1:E:120:GLY:N	2.76	0.47
1:G:72:THR:OG1	1:G:112:ASN:ND2	2.48	0.47
1:H:112:ASN:N	1:H:112:ASN:HD22	2.13	0.47
1:I:73:ILE:HG22	1:I:75:MSE:HG3	1.95	0.47
1:J:125:PRO:O	1:J:126:GLY:C	2.57	0.47
1:E:39:TRP:HB2	1:E:122:MSE:CE	2.37	0.46
1:I:151:VAL:O	1:I:155:SER:HB3	2.14	0.46
1:B:147:HIS:HB3	1:B:150:VAL:CG1	2.45	0.46
1:C:111:MSE:HE3	1:C:113:GLN:O	2.15	0.46
1:D:103:LYS:O	1:D:103:LYS:HG3	2.16	0.46
1:D:124:SER:CB	1:D:125:PRO:CD	2.92	0.46
1:H:80:GLY:HA2	1:H:144:TYR:CD1	2.50	0.46
1:C:5:ASP:O	1:C:8:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:HD13	1:C:100:LEU:O	2.15	0.46
1:G:123:VAL:O	1:G:124:SER:C	2.58	0.46
1:I:58:THR:CB	1:I:131:ASP:HB3	2.44	0.46
1:B:149:ALA:O	1:B:153:LYS:HD3	2.16	0.46
1:G:30:THR:OG1	1:G:38:LEU:HD22	2.16	0.46
1:G:46:LEU:HD22	1:G:71:LEU:HD22	1.97	0.46
1:G:57:LEU:N	1:G:57:LEU:HD12	2.31	0.46
1:I:37:GLN:OE1	1:I:37:GLN:HA	2.16	0.46
1:B:45:LEU:HB2	1:B:118:LEU:HD12	1.98	0.46
1:B:125:PRO:O	1:B:126:GLY:C	2.59	0.46
1:B:127:PHE:HE1	1:B:132:PHE:HB2	1.80	0.46
1:D:7:PHE:CE2	1:J:91:LEU:HD11	2.50	0.46
1:A:53:HIS:O	1:A:54:PHE:C	2.59	0.46
1:E:8:ILE:HA	1:E:13:LEU:HG	1.98	0.46
1:F:90:ASP:O	1:F:95:GLU:HB2	2.16	0.46
1:F:98:GLN:O	1:F:99:PHE:HB2	2.15	0.46
1:I:52:SER:HB3	1:I:109:SER:H	1.80	0.46
1:D:8:ILE:HG13	1:D:9:LYS:N	2.30	0.45
1:G:96:ARG:NH2	1:I:10:PHE:HB3	2.31	0.45
1:B:45:LEU:HA	1:B:117:SER:O	2.16	0.45
1:B:148:LYS:O	1:B:152:GLN:HB2	2.16	0.45
1:C:8:ILE:HA	1:C:13:LEU:HG	1.99	0.45
1:E:25:SER:C	1:E:26:TYR:CD1	2.94	0.45
1:E:27:ARG:NE	1:E:37:GLN:HG3	2.30	0.45
1:F:28:SER:CB	1:F:39:TRP:H	2.30	0.45
1:F:77:SER:C	1:F:79:GLU:N	2.74	0.45
1:B:29:GLU:HG3	2:B:167:HOH:O	2.16	0.45
1:B:147:HIS:HB3	1:B:150:VAL:HG12	1.99	0.45
1:D:66:HIS:O	1:D:67:ALA:HB2	2.16	0.45
1:G:25:SER:H	1:G:42:ILE:HA	1.82	0.45
1:I:71:LEU:HD23	1:I:111:MSE:HA	1.99	0.45
1:I:146:GLN:HE21	1:I:146:GLN:N	2.15	0.45
1:D:89:LEU:HD23	1:D:97:PRO:HG3	1.99	0.45
1:D:127:PHE:CD2	1:D:128:THR:N	2.84	0.45
1:G:83:THR:O	1:G:84:THR:HG23	2.17	0.45
1:C:59:ALA:C	1:C:103:LYS:HB3	2.41	0.45
1:D:8:ILE:O	1:D:8:ILE:HD12	2.16	0.45
1:F:30:THR:HG22	1:F:31:ALA:N	2.31	0.45
1:J:158:GLU:O	1:J:158:GLU:HG3	2.16	0.45
1:A:91:LEU:HB2	2:A:169:HOH:O	2.17	0.45
1:B:22:TYR:CG	1:B:23:ARG:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:SER:HB2	1:J:39:TRP:CD1	2.52	0.45
1:J:8:ILE:HD12	1:J:9:LYS:N	2.32	0.45
1:J:100:LEU:HD23	1:J:101:VAL:N	2.31	0.45
1:J:127:PHE:CE1	1:J:132:PHE:HB2	2.52	0.45
1:A:23:ARG:HD3	1:A:24:SER:N	2.31	0.45
1:E:57:LEU:HD12	1:E:57:LEU:N	2.32	0.45
1:F:146:GLN:H	1:F:146:GLN:HE21	1.60	0.45
1:G:7:PHE:O	1:G:11:LEU:HB2	2.17	0.45
1:G:47:ARG:HB3	1:G:50:GLU:HG2	1.99	0.45
1:H:21:PHE:HZ	1:H:47:ARG:HH11	1.65	0.45
1:A:54:PHE:CZ	1:A:154:LEU:HD12	2.52	0.44
1:E:56:ARG:HG2	1:E:57:LEU:N	2.32	0.44
1:E:137:GLN:HB2	1:E:155:SER:HB3	1.98	0.44
1:F:71:LEU:HD11	1:F:119:VAL:HG21	1.99	0.44
1:F:135:PHE:HB2	1:F:140:LEU:HD21	2.00	0.44
1:G:30:THR:O	1:G:38:LEU:HB2	2.16	0.44
1:G:78:PRO:HG2	1:G:79:GLU:OE2	2.17	0.44
1:I:147:HIS:HB3	1:I:150:VAL:HG12	1.98	0.44
1:G:54:PHE:HA	1:G:107:PHE:O	2.17	0.44
1:I:71:LEU:HD21	1:I:117:SER:OG	2.17	0.44
1:B:53:HIS:CD2	1:B:156:ARG:HG3	2.53	0.44
1:C:125:PRO:O	1:C:126:GLY:C	2.60	0.44
1:E:65:PHE:O	1:F:66:HIS:HA	2.17	0.44
1:E:122:MSE:CE	1:E:123:VAL:C	2.90	0.44
1:I:33:ASP:C	1:I:35:SER:N	2.76	0.44
1:A:124:SER:CB	1:A:125:PRO:HD3	2.23	0.44
1:C:16:HIS:CD2	1:C:18:GLU:H	2.36	0.44
1:F:38:LEU:O	1:F:125:PRO:HA	2.17	0.44
1:H:124:SER:O	1:H:125:PRO:C	2.58	0.44
1:I:59:ALA:HB1	1:I:125:PRO:HD2	1.99	0.44
1:A:100:LEU:HD13	1:A:100:LEU:O	2.18	0.44
1:A:101:VAL:HA	1:A:102:PRO:HD2	1.83	0.44
1:A:111:MSE:HE1	1:A:115:GLY:O	2.16	0.44
1:C:60:ASP:HB3	1:C:100:LEU:HD21	2.00	0.44
1:D:89:LEU:CD1	1:J:67:ALA:HB2	2.48	0.44
1:E:67:ALA:O	1:E:117:SER:HA	2.18	0.44
1:G:62:MSE:SE	1:G:100:LEU:HB2	2.67	0.44
1:G:71:LEU:HD23	1:G:111:MSE:HG2	1.98	0.44
1:F:28:SER:HB2	1:F:39:TRP:CD1	2.53	0.44
1:G:26:TYR:CE2	1:I:100:LEU:HB3	2.53	0.44
1:J:37:GLN:HA	1:J:37:GLN:NE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:LYS:O	1:G:150:VAL:N	2.51	0.44
1:H:16:HIS:CD2	1:H:18:GLU:HG2	2.53	0.44
1:I:62:MSE:SE	1:I:100:LEU:HB2	2.67	0.44
1:J:119:VAL:CG1	1:J:120:GLY:N	2.81	0.44
1:G:44:PHE:O	1:G:118:LEU:HD12	2.17	0.44
1:C:8:ILE:CD1	1:C:13:LEU:HB2	2.47	0.44
1:E:47:ARG:HB2	1:E:47:ARG:CZ	2.47	0.44
1:J:123:VAL:O	1:J:123:VAL:CG2	2.64	0.44
1:B:8:ILE:HD12	1:B:8:ILE:O	2.18	0.43
1:C:12:GLU:O	1:C:23:ARG:NH1	2.51	0.43
1:C:123:VAL:O	1:C:124:SER:O	2.36	0.43
1:D:128:THR:OG1	1:D:130:ASP:HB2	2.18	0.43
1:D:140:LEU:HD12	1:D:155:SER:OG	2.17	0.43
1:F:142:ALA:O	1:F:145:PRO:HG3	2.18	0.43
1:H:33:ASP:O	1:H:35:SER:N	2.51	0.43
1:I:31:ALA:HB1	1:I:33:ASP:O	2.18	0.43
1:A:23:ARG:HD3	1:A:23:ARG:C	2.43	0.43
1:C:146:GLN:H	1:C:146:GLN:HE21	1.64	0.43
1:F:103:LYS:C	1:F:105:CYS:H	2.25	0.43
1:F:105:CYS:SG	1:F:106:ILE:N	2.92	0.43
1:G:10:PHE:CG	1:I:91:LEU:HB3	2.53	0.43
1:I:101:VAL:HG21	1:I:107:PHE:CG	2.53	0.43
1:D:44:PHE:CE1	1:D:46:LEU:HD13	2.53	0.43
1:E:147:HIS:HB3	1:E:150:VAL:CG1	2.48	0.43
1:G:91:LEU:CD1	1:I:7:PHE:HA	2.48	0.43
1:G:101:VAL:HG13	1:G:101:VAL:O	2.18	0.43
1:A:59:ALA:C	1:A:103:LYS:HB3	2.42	0.43
1:B:145:PRO:HD2	1:B:146:GLN:NE2	2.32	0.43
1:H:54:PHE:CD1	1:H:154:LEU:HB2	2.54	0.43
1:A:69:GLN:O	1:A:70:SER:C	2.62	0.43
1:A:143:MSE:HE2	1:A:144:TYR:CZ	2.54	0.43
1:B:54:PHE:CD1	1:B:154:LEU:HB2	2.53	0.43
1:C:3:ASN:HB3	1:C:6:ASP:OD2	2.19	0.43
1:D:122:MSE:HE1	1:D:124:SER:N	2.33	0.43
1:G:139:ALA:O	1:G:143:MSE:HG2	2.18	0.43
1:I:90:ASP:O	1:I:95:GLU:HB2	2.19	0.43
1:I:131:ASP:OD1	1:I:131:ASP:N	2.50	0.43
1:A:65:PHE:H	1:H:66:HIS:CE1	2.37	0.43
1:C:33:ASP:C	1:C:35:SER:N	2.76	0.43
1:D:39:TRP:CD1	1:J:124:SER:HB2	2.53	0.43
1:A:149:ALA:O	1:A:153:LYS:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HG21	1:D:107:PHE:CD2	2.54	0.43
1:E:74:TYR:CD1	1:E:74:TYR:N	2.86	0.43
1:A:87:LEU:HD12	1:A:96:ARG:O	2.19	0.43
1:C:16:HIS:HD2	1:C:18:GLU:H	1.67	0.43
1:D:27:ARG:HH11	1:D:27:ARG:HB3	1.83	0.43
1:J:141:LEU:CD1	1:J:151:VAL:HG11	2.49	0.43
1:A:122:MSE:CE	1:A:123:VAL:C	2.91	0.43
1:A:143:MSE:HE2	1:A:144:TYR:OH	2.19	0.43
1:B:145:PRO:CD	1:B:146:GLN:HE22	2.32	0.43
1:F:153:LYS:HD2	1:F:153:LYS:N	2.34	0.43
1:B:23:ARG:HG2	1:H:14:GLU:OE2	2.19	0.43
1:C:47:ARG:C	1:C:49:GLY:N	2.76	0.43
1:E:47:ARG:HH21	1:E:47:ARG:HG2	1.84	0.43
1:F:33:ASP:O	1:F:34:PRO:C	2.62	0.43
1:F:146:GLN:HG2	1:F:147:HIS:N	2.33	0.43
1:I:2:GLN:HE21	1:I:2:GLN:HB2	1.63	0.43
1:I:68:GLY:O	1:I:69:GLN:C	2.62	0.43
1:D:141:LEU:HD12	1:D:141:LEU:HA	1.77	0.42
1:E:13:LEU:HD23	1:E:23:ARG:CB	2.49	0.42
1:G:22:TYR:O	1:G:23:ARG:HB2	2.18	0.42
1:J:103:LYS:O	1:J:103:LYS:HG3	2.19	0.42
1:B:33:ASP:C	1:B:35:SER:N	2.77	0.42
1:B:143:MSE:HE2	1:B:144:TYR:CE2	2.54	0.42
1:H:146:GLN:NE2	1:H:146:GLN:N	2.49	0.42
1:F:150:VAL:CG1	1:F:151:VAL:H	2.24	0.42
1:G:55:HIS:O	1:G:106:ILE:HA	2.18	0.42
1:I:124:SER:HB3	1:I:125:PRO:CD	2.41	0.42
1:I:125:PRO:O	1:I:126:GLY:C	2.62	0.42
1:I:119:VAL:HG12	1:I:120:GLY:H	1.85	0.42
1:A:71:LEU:HD21	1:A:117:SER:CB	2.49	0.42
1:B:45:LEU:C	1:B:45:LEU:HD23	2.44	0.42
1:C:69:GLN:O	1:C:71:LEU:HD23	2.20	0.42
1:C:119:VAL:HG13	1:C:120:GLY:N	2.34	0.42
1:E:16:HIS:NE2	1:E:22:TYR:CE2	2.87	0.42
1:C:99:PHE:CD2	1:C:100:LEU:N	2.88	0.42
1:D:57:LEU:HA	1:D:131:ASP:O	2.20	0.42
1:E:106:ILE:HD12	1:E:144:TYR:HE2	1.85	0.42
1:E:145:PRO:HD2	1:E:146:GLN:HE22	1.85	0.42
1:F:52:SER:HB3	1:F:109:SER:H	1.85	0.42
1:F:119:VAL:CG1	1:F:120:GLY:N	2.83	0.42
1:C:56:ARG:HG2	1:C:57:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ASP:HB3	1:D:34:PRO:CD	2.49	0.42
1:G:30:THR:HG1	1:G:38:LEU:HD22	1.85	0.42
1:H:71:LEU:HD11	1:H:119:VAL:HG21	2.01	0.42
1:I:91:LEU:HD23	1:I:96:ARG:NH2	2.35	0.42
1:A:57:LEU:HA	1:A:131:ASP:O	2.19	0.42
1:A:142:ALA:O	1:A:145:PRO:HG3	2.19	0.42
1:B:91:LEU:HD13	1:C:10:PHE:CB	2.42	0.42
1:C:157:PRO:HB2	1:C:158:GLU:OE1	2.20	0.42
1:F:11:LEU:O	1:F:12:GLU:HB2	2.20	0.42
1:G:133:GLU:HG2	1:G:135:PHE:CZ	2.55	0.42
1:H:45:LEU:HD23	1:H:46:LEU:C	2.45	0.42
1:H:77:SER:HB2	1:H:78:PRO:HD2	2.01	0.42
1:H:116:PHE:CD2	1:H:116:PHE:C	2.98	0.42
1:I:139:ALA:O	1:I:143:MSE:HG2	2.19	0.42
1:J:5:ASP:HA	1:J:8:ILE:HG13	2.01	0.42
1:C:8:ILE:HA	1:C:13:LEU:CG	2.50	0.42
1:E:25:SER:HB3	1:E:43:TYR:CE2	2.55	0.42
1:I:45:LEU:HD23	1:I:46:LEU:N	2.35	0.42
1:A:62:MSE:SE	1:A:100:LEU:HB2	2.70	0.41
1:E:33:ASP:C	1:E:35:SER:H	2.27	0.41
1:F:151:VAL:O	1:F:155:SER:HB3	2.19	0.41
1:H:48:THR:N	2:H:171:HOH:O	2.52	0.41
1:H:143:MSE:HE2	1:H:144:TYR:CZ	2.55	0.41
1:J:137:GLN:HE21	1:J:152:GLN:HA	1.85	0.41
1:B:37:GLN:HA	1:B:37:GLN:HE21	1.85	0.41
1:E:5:ASP:HA	1:E:8:ILE:CG2	2.51	0.41
1:I:77:SER:C	1:I:79:GLU:H	2.28	0.41
1:A:54:PHE:CD1	1:A:154:LEU:HB2	2.55	0.41
1:A:144:TYR:N	1:A:145:PRO:HD3	2.36	0.41
1:C:5:ASP:HA	1:C:8:ILE:CG2	2.49	0.41
1:C:13:LEU:HD23	1:C:23:ARG:HB2	2.02	0.41
1:C:32:PHE:HB2	1:C:38:LEU:HA	2.02	0.41
1:D:122:MSE:HE2	1:D:123:VAL:N	2.35	0.41
1:E:17:VAL:C	1:E:19:GLY:N	2.78	0.41
1:E:141:LEU:HD12	1:E:141:LEU:HA	1.82	0.41
1:G:10:PHE:CB	1:I:91:LEU:HD13	2.51	0.41
1:J:45:LEU:HD23	1:J:45:LEU:C	2.45	0.41
1:A:124:SER:CB	1:A:125:PRO:CD	2.87	0.41
1:B:140:LEU:HD12	1:B:155:SER:OG	2.21	0.41
1:C:145:PRO:HD2	1:C:146:GLN:HE22	1.85	0.41
1:D:28:SER:HB2	1:D:39:TRP:NE1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:GLU:O	1:F:101:VAL:HG22	2.20	0.41
1:A:41:SER:CB	1:H:62:MSE:HE2	2.49	0.41
1:B:101:VAL:HG21	1:B:107:PHE:CG	2.56	0.41
1:F:32:PHE:HB3	1:F:33:ASP:H	1.72	0.41
1:H:147:HIS:HB3	1:H:150:VAL:HG12	2.02	0.41
1:I:7:PHE:C	1:I:9:LYS:N	2.77	0.41
1:I:82:LEU:HD12	1:I:83:THR:H	1.86	0.41
1:J:59:ALA:C	1:J:103:LYS:HB3	2.45	0.41
1:J:101:VAL:HG21	1:J:107:PHE:CG	2.55	0.41
1:A:53:HIS:O	1:A:55:HIS:HD2	2.03	0.41
1:A:57:LEU:HD22	1:A:107:PHE:HZ	1.86	0.41
1:C:54:PHE:O	1:C:134:LEU:HD12	2.20	0.41
1:C:136:SER:O	1:C:137:GLN:C	2.63	0.41
1:E:75:MSE:HA	1:E:107:PHE:HA	2.02	0.41
1:G:39:TRP:CD1	1:I:124:SER:HB2	2.55	0.41
1:G:90:ASP:OD2	1:G:92:ALA:HB3	2.21	0.41
1:H:16:HIS:HD2	1:H:18:GLU:HG2	1.85	0.41
1:H:108:GLY:O	1:H:109:SER:HB2	2.20	0.41
1:J:53:HIS:O	1:J:55:HIS:CD2	2.74	0.41
1:C:151:VAL:O	1:C:151:VAL:HG12	2.21	0.41
1:D:8:ILE:HA	1:D:13:LEU:CD1	2.47	0.41
1:D:66:HIS:HB2	1:D:118:LEU:O	2.20	0.41
1:D:151:VAL:O	1:D:151:VAL:HG12	2.18	0.41
1:E:46:LEU:HB3	1:E:111:MSE:SE	2.71	0.41
1:F:39:TRP:HB2	1:F:122:MSE:HE1	2.01	0.41
1:F:147:HIS:O	1:F:151:VAL:HG23	2.21	0.41
1:G:36:ARG:HG3	1:G:36:ARG:HH11	1.85	0.41
1:H:101:VAL:HG21	1:H:107:PHE:CD1	2.55	0.41
1:A:28:SER:HB2	1:A:39:TRP:CD1	2.56	0.41
1:D:58:THR:O	1:D:58:THR:CG2	2.63	0.41
1:D:145:PRO:C	1:D:147:HIS:H	2.28	0.41
1:E:151:VAL:O	1:E:155:SER:HB2	2.21	0.41
1:I:57:LEU:N	1:I:57:LEU:HD22	2.36	0.41
1:J:24:SER:HA	1:J:42:ILE:HG22	2.02	0.41
1:J:37:GLN:HE21	1:J:37:GLN:CA	2.28	0.41
1:A:137:GLN:HG2	1:A:141:LEU:HD23	2.02	0.41
1:B:108:GLY:HA3	1:B:154:LEU:HD13	2.02	0.41
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.90	0.41
1:C:142:ALA:O	1:C:145:PRO:HG3	2.21	0.41
1:D:21:PHE:HZ	1:D:47:ARG:HH11	1.69	0.41
1:D:122:MSE:CE	1:D:123:VAL:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:VAL:O	1:D:150:VAL:HG22	2.19	0.41
1:E:89:LEU:O	1:E:91:LEU:N	2.54	0.41
1:E:122:MSE:HE2	1:E:123:VAL:N	2.36	0.41
1:F:25:SER:HB3	1:F:43:TYR:CE2	2.55	0.41
1:F:56:ARG:C	1:F:57:LEU:HD12	2.46	0.41
1:I:48:THR:HA	1:I:111:MSE:CE	2.51	0.41
1:I:69:GLN:HG2	1:I:113:GLN:HB2	2.03	0.41
1:J:25:SER:HB2	1:J:26:TYR:CD1	2.56	0.41
1:J:118:LEU:HD12	1:J:118:LEU:HA	1.77	0.41
1:J:137:GLN:HB2	1:J:155:SER:HB3	2.02	0.41
1:A:61:GLU:HB3	1:A:101:VAL:HG13	2.02	0.41
1:A:137:GLN:HB2	1:A:156:ARG:C	2.46	0.41
1:C:125:PRO:O	1:C:126:GLY:O	2.39	0.41
1:D:13:LEU:CD2	1:D:23:ARG:HB2	2.40	0.41
1:E:39:TRP:HE1	1:F:124:SER:HB2	1.86	0.41
1:E:59:ALA:C	1:E:103:LYS:HB3	2.46	0.41
1:G:31:ALA:HB1	1:G:36:ARG:O	2.20	0.41
1:H:60:ASP:HB3	1:H:100:LEU:HD11	2.02	0.41
1:H:141:LEU:HD12	1:H:141:LEU:HA	1.91	0.41
1:I:77:SER:C	1:I:79:GLU:N	2.79	0.41
1:J:47:ARG:O	1:J:50:GLU:HB2	2.21	0.41
1:A:101:VAL:HG21	1:A:107:PHE:CE2	2.56	0.40
1:G:56:ARG:HE	1:G:106:ILE:CG1	2.34	0.40
1:G:77:SER:C	1:G:79:GLU:H	2.28	0.40
1:G:113:GLN:CG	1:G:114:ASP:N	2.82	0.40
1:J:143:MSE:HG3	1:J:144:TYR:CE2	2.55	0.40
1:E:7:PHE:CD2	1:F:91:LEU:HD11	2.56	0.40
1:F:32:PHE:CE2	1:F:125:PRO:HB3	2.56	0.40
1:I:54:PHE:HB3	1:I:106:ILE:CG2	2.51	0.40
1:J:30:THR:HG22	1:J:31:ALA:N	2.37	0.40
1:A:138:GLU:OE2	1:A:158:GLU:N	2.47	0.40
1:E:23:ARG:C	1:E:23:ARG:HD3	2.47	0.40
1:E:122:MSE:CE	1:E:124:SER:N	2.84	0.40
1:G:71:LEU:CD2	1:G:111:MSE:HG2	2.52	0.40
1:A:74:TYR:CD2	1:A:150:VAL:HG21	2.57	0.40
1:C:23:ARG:CG	1:C:23:ARG:HH11	2.35	0.40
1:D:22:TYR:CD1	1:D:23:ARG:N	2.89	0.40
1:D:27:ARG:HB3	1:D:27:ARG:NH1	2.37	0.40
1:E:23:ARG:HD3	1:E:23:ARG:O	2.22	0.40
1:E:43:TYR:HE1	1:F:97:PRO:HB2	1.86	0.40
1:F:56:ARG:HG2	1:F:57:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:ILE:CG1	1:H:9:LYS:N	2.82	0.40
1:H:119:VAL:CG1	1:H:120:GLY:H	2.21	0.40
1:J:86:GLN:NE2	1:J:112:ASN:ND2	2.57	0.40
1:A:7:PHE:CD2	1:H:91:LEU:HD11	2.57	0.40
1:A:56:ARG:HH21	1:A:106:ILE:HD11	1.87	0.40
1:E:101:VAL:HA	1:E:102:PRO:HD2	1.92	0.40
1:F:70:SER:O	1:F:112:ASN:HB2	2.22	0.40
1:G:31:ALA:HB2	1:G:37:GLN:OE1	2.21	0.40
1:J:3:ASN:HB3	1:J:6:ASP:OD1	2.22	0.40
1:J:20:GLY:HA3	1:J:44:PHE:CE2	2.57	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	156/170 (92%)	134 (86%)	17 (11%)	5 (3%)	3	7
1	B	156/170 (92%)	139 (89%)	11 (7%)	6 (4%)	2	5
1	C	156/170 (92%)	136 (87%)	14 (9%)	6 (4%)	2	5
1	D	156/170 (92%)	132 (85%)	18 (12%)	6 (4%)	2	5
1	E	156/170 (92%)	134 (86%)	15 (10%)	7 (4%)	2	4
1	F	156/170 (92%)	123 (79%)	24 (15%)	9 (6%)	1	2
1	G	156/170 (92%)	117 (75%)	30 (19%)	9 (6%)	1	2
1	H	156/170 (92%)	137 (88%)	18 (12%)	1 (1%)	21	44
1	I	156/170 (92%)	129 (83%)	22 (14%)	5 (3%)	3	7
1	J	156/170 (92%)	140 (90%)	12 (8%)	4 (3%)	4	11
All	All	1560/1700 (92%)	1321 (85%)	181 (12%)	58 (4%)	2	6

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	THR
1	C	125	PRO
1	C	126	GLY
1	D	124	SER
1	E	124	SER
1	F	28	SER
1	F	34	PRO
1	F	37	GLN
1	F	138	GLU
1	G	71	LEU
1	G	124	SER
1	G	148	LYS
1	J	23	ARG
1	A	48	THR
1	A	126	GLY
1	B	23	ARG
1	B	90	ASP
1	C	148	LYS
1	D	126	GLY
1	E	54	PHE
1	E	90	ASP
1	E	117	SER
1	E	126	GLY
1	E	129	PHE
1	F	124	SER
1	F	126	GLY
1	F	151	VAL
1	G	23	ARG
1	G	28	SER
1	G	149	ALA
1	I	114	ASP
1	I	126	GLY
1	J	126	GLY
1	J	129	PHE
1	A	142	ALA
1	B	95	GLU
1	C	124	SER
1	E	23	ARG
1	F	32	PHE
1	H	126	GLY
1	A	124	SER
1	D	54	PHE

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Mol	Chain	Res	Type
1	D	149	ALA
1	I	84	THR
1	A	138	GLU
1	B	2	GLN
1	C	149	ALA
1	D	144	TYR
1	G	25	SER
1	J	157	PRO
1	B	124	SER
1	D	157	PRO
1	F	125	PRO
1	G	34	PRO
1	G	147	HIS
1	I	111	MSE
1	I	80	GLY
1	B	126	GLY

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	135/139 (97%)	122 (90%)	13 (10%)	8	20
1	B	135/139 (97%)	119 (88%)	16 (12%)	5	13
1	C	135/139 (97%)	117 (87%)	18 (13%)	4	10
1	D	135/139 (97%)	117 (87%)	18 (13%)	4	10
1	E	135/139 (97%)	120 (89%)	15 (11%)	6	15
1	F	135/139 (97%)	124 (92%)	11 (8%)	11	27
1	G	135/139 (97%)	125 (93%)	10 (7%)	13	32
1	H	135/139 (97%)	122 (90%)	13 (10%)	8	20
1	I	135/139 (97%)	125 (93%)	10 (7%)	13	32
1	J	135/139 (97%)	121 (90%)	14 (10%)	7	17
All	All	1350/1390 (97%)	1212 (90%)	138 (10%)	7	18

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	23	ARG
1	A	25	SER
1	A	46	LEU
1	A	57	LEU
1	A	69	GLN
1	A	96	ARG
1	A	101	VAL
1	A	105	CYS
1	A	119	VAL
1	A	122	MSE
1	A	123	VAL
1	A	138	GLU
1	B	3	ASN
1	B	8	ILE
1	B	23	ARG
1	B	45	LEU
1	B	46	LEU
1	B	47	ARG
1	B	57	LEU
1	B	58	THR
1	B	69	GLN
1	B	75	MSE
1	B	96	ARG
1	B	100	LEU
1	B	101	VAL
1	B	123	VAL
1	B	141	LEU
1	B	146	GLN
1	C	8	ILE
1	C	23	ARG
1	C	46	LEU
1	C	48	THR
1	C	57	LEU
1	C	58	THR
1	C	69	GLN
1	C	71	LEU
1	C	75	MSE
1	C	96	ARG
1	C	100	LEU
1	C	119	VAL
1	C	122	MSE

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Mol	Chain	Res	Type
1	C	124	SER
1	C	125	PRO
1	C	131	ASP
1	C	141	LEU
1	C	146	GLN
1	D	3	ASN
1	D	8	ILE
1	D	23	ARG
1	D	27	ARG
1	D	46	LEU
1	D	57	LEU
1	D	69	GLN
1	D	71	LEU
1	D	83	THR
1	D	96	ARG
1	D	101	VAL
1	D	119	VAL
1	D	122	MSE
1	D	123	VAL
1	D	130	ASP
1	D	141	LEU
1	D	146	GLN
1	D	156	ARG
1	E	5	ASP
1	E	16	HIS
1	E	18	GLU
1	E	23	ARG
1	E	46	LEU
1	E	47	ARG
1	E	69	GLN
1	E	96	ARG
1	E	100	LEU
1	E	101	VAL
1	E	119	VAL
1	E	122	MSE
1	E	123	VAL
1	E	141	LEU
1	E	146	GLN
1	F	27	ARG
1	F	34	PRO
1	F	36	ARG
1	F	51	VAL

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Mol	Chain	Res	Type
1	F	58	THR
1	F	69	GLN
1	F	96	ARG
1	F	112	ASN
1	F	113	GLN
1	F	122	MSE
1	F	146	GLN
1	G	26	TYR
1	G	27	ARG
1	G	46	LEU
1	G	69	GLN
1	G	84	THR
1	G	96	ARG
1	G	100	LEU
1	G	137	GLN
1	G	144	TYR
1	G	146	GLN
1	H	3	ASN
1	H	12	GLU
1	H	23	ARG
1	H	40	SER
1	H	46	LEU
1	H	57	LEU
1	H	58	THR
1	H	69	GLN
1	H	96	ARG
1	H	101	VAL
1	H	141	LEU
1	H	146	GLN
1	H	158	GLU
1	I	8	ILE
1	I	45	LEU
1	I	57	LEU
1	I	84	THR
1	I	96	ARG
1	I	100	LEU
1	I	101	VAL
1	I	131	ASP
1	I	140	LEU
1	I	146	GLN
1	J	16	HIS
1	J	22	TYR

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Mol	Chain	Res	Type
1	J	37	GLN
1	J	58	THR
1	J	69	GLN
1	J	96	ARG
1	J	101	VAL
1	J	113	GLN
1	J	119	VAL
1	J	123	VAL
1	J	141	LEU
1	J	146	GLN
1	J	148	LYS
1	J	153	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	55	HIS
1	A	69	GLN
1	A	86	GLN
1	A	112	ASN
1	B	15	GLN
1	B	16	HIS
1	B	55	HIS
1	B	69	GLN
1	B	86	GLN
1	B	112	ASN
1	B	146	GLN
1	C	2	GLN
1	C	3	ASN
1	C	16	HIS
1	C	55	HIS
1	C	69	GLN
1	C	86	GLN
1	C	112	ASN
1	C	146	GLN
1	C	147	HIS
1	D	3	ASN
1	D	15	GLN
1	D	55	HIS
1	D	112	ASN
1	D	113	GLN

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Mol	Chain	Res	Type
1	D	137	GLN
1	D	146	GLN
1	D	147	HIS
1	D	152	GLN
1	E	2	GLN
1	E	15	GLN
1	E	55	HIS
1	E	69	GLN
1	E	112	ASN
1	E	113	GLN
1	E	137	GLN
1	E	146	GLN
1	E	147	HIS
1	F	2	GLN
1	F	3	ASN
1	F	15	GLN
1	F	16	HIS
1	F	69	GLN
1	F	86	GLN
1	F	112	ASN
1	F	113	GLN
1	F	146	GLN
1	F	147	HIS
1	F	152	GLN
1	G	2	GLN
1	G	16	HIS
1	G	53	HIS
1	G	55	HIS
1	G	69	GLN
1	G	86	GLN
1	G	146	GLN
1	H	16	HIS
1	H	55	HIS
1	H	69	GLN
1	H	86	GLN
1	H	112	ASN
1	H	146	GLN
1	H	152	GLN
1	I	69	GLN
1	I	86	GLN
1	I	137	GLN
1	I	146	GLN

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Mol	Chain	Res	Type
1	J	3	ASN
1	J	37	GLN
1	J	55	HIS
1	J	86	GLN
1	J	112	ASN
1	J	137	GLN
1	J	146	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	152/170 (89%)	0.27	5 (3%) 49 45	24, 62, 87, 120	0
1	B	152/170 (89%)	-0.24	0 100 100	16, 39, 72, 110	0
1	C	152/170 (89%)	0.09	4 (2%) 57 54	27, 55, 86, 118	0
1	D	152/170 (89%)	0.35	3 (1%) 65 62	36, 60, 84, 115	0
1	E	152/170 (89%)	0.69	7 (4%) 37 34	39, 72, 98, 122	0
1	F	152/170 (89%)	0.69	9 (5%) 28 25	43, 77, 112, 132	0
1	G	152/170 (89%)	0.90	12 (7%) 18 16	65, 89, 115, 137	0
1	H	152/170 (89%)	-0.01	1 (0%) 84 83	23, 47, 79, 115	0
1	I	152/170 (89%)	0.86	14 (9%) 14 12	53, 86, 116, 132	0
1	J	152/170 (89%)	0.22	3 (1%) 65 62	33, 59, 85, 127	0
All	All	1520/1700 (89%)	0.38	58 (3%) 44 40	16, 66, 106, 137	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	140	LEU	5.1
1	F	4	ALA	3.7
1	E	22	TYR	3.6
1	G	126	GLY	3.4
1	I	4	ALA	3.3
1	G	110	ALA	3.1
1	F	124	SER	3.0
1	A	154	LEU	2.9
1	F	88	GLY	2.9
1	C	48	THR	2.8
1	G	140	LEU	2.8
1	A	4	ALA	2.8
1	F	32	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	4	ALA	2.7
1	A	125	PRO	2.7
1	I	153	LYS	2.7
1	G	11	LEU	2.6
1	J	22	TYR	2.6
1	I	89	LEU	2.5
1	I	140	LEU	2.5
1	I	124	SER	2.5
1	G	149	ALA	2.5
1	I	99	PHE	2.4
1	E	71	LEU	2.4
1	F	89	LEU	2.4
1	F	33	ASP	2.4
1	G	123	VAL	2.4
1	I	106	ILE	2.4
1	C	155	SER	2.3
1	H	2	GLN	2.3
1	G	144	TYR	2.3
1	I	155	SER	2.3
1	E	97	PRO	2.2
1	G	32	PHE	2.2
1	I	127	PHE	2.2
1	C	4	ALA	2.2
1	F	36	ARG	2.2
1	I	71	LEU	2.2
1	I	141	LEU	2.2
1	D	2	GLN	2.2
1	E	54	PHE	2.2
1	J	16	HIS	2.2
1	I	118	LEU	2.2
1	E	109	SER	2.2
1	J	125	PRO	2.1
1	G	120	GLY	2.1
1	A	106	ILE	2.1
1	A	127	PHE	2.1
1	E	124	SER	2.1
1	F	109	SER	2.1
1	G	100	LEU	2.1
1	I	125	PRO	2.1
1	G	118	LEU	2.1
1	D	32	PHE	2.1
1	C	125	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	87	LEU	2.0
1	G	119	VAL	2.0
1	F	154	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.