Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 04:14 PM EDT

PDB ID	:	1YUD
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

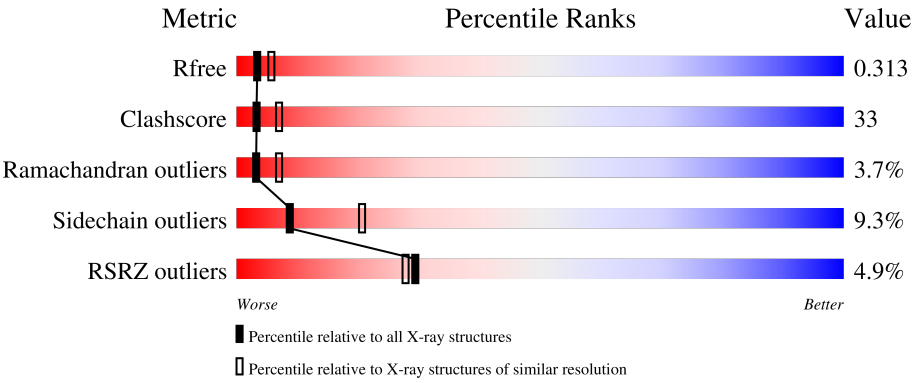
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	170	2% 49% 38% 5% • 7%
1	B	170	45% 39% 8% • 7%
1	C	170	% 42% 42% 7% • 7%
1	D	170	4% 47% 36% 9% • 7%

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Mol	Chain	Length	Quality of chain
1	E	170	6% 47% 35% 11% 7%
1	F	170	6% 38% 45% 10% 7%
1	G	170	10% 41% 44% 8% 7%
1	H	170	44% 43% 6% 7%
1	I	170	11% 46% 41% 6% 7%
1	J	170	3% 49% 38% 5% 7%

2 Entry composition (i)

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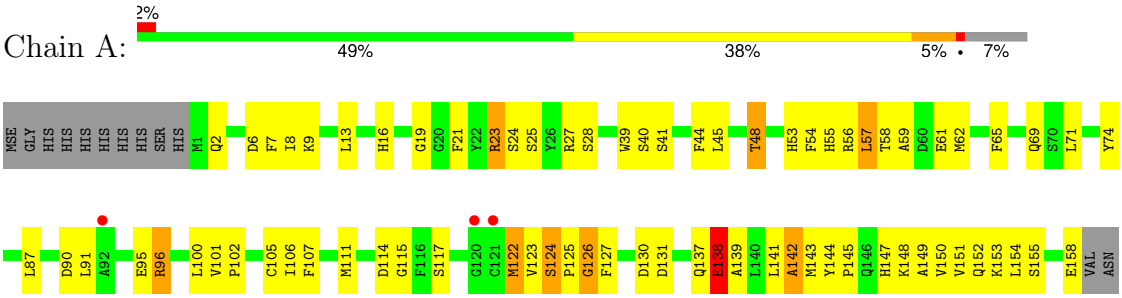
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	15	Total O 15 15	0	0
2	I	6	Total O 6 6	0	0
2	J	12	Total O 12 12	0	0

3 Residue-property plots (i)

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

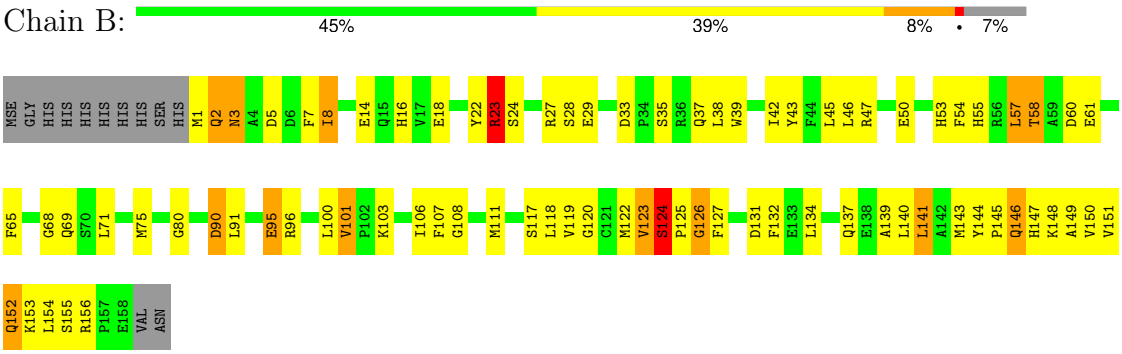
• Molecule 1: hypothetical protein SO0799

Chain A:



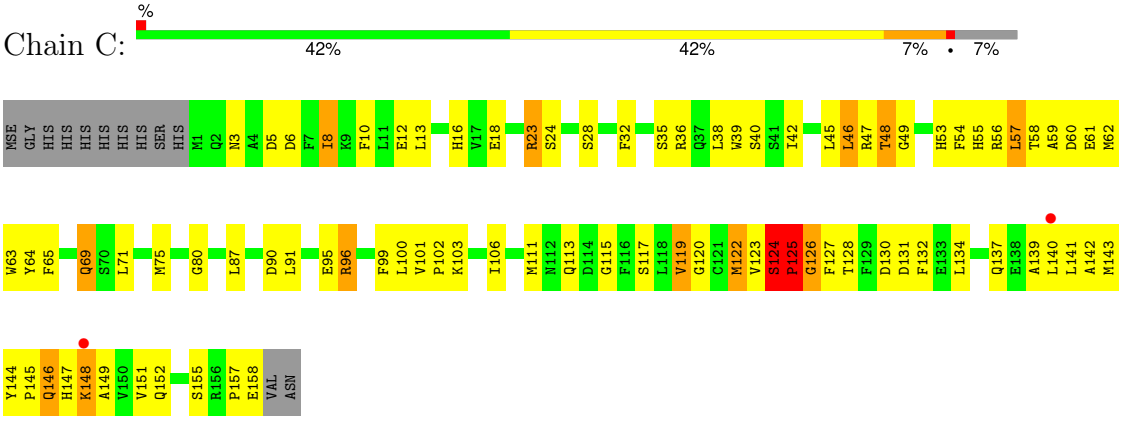
• Molecule 1: hypothetical protein SO0799

Chain B:



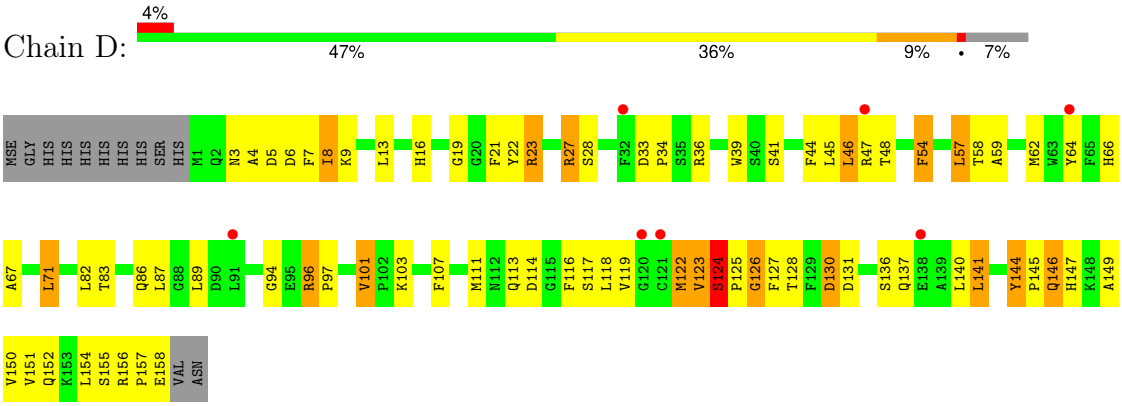
• Molecule 1: hypothetical protein SO0799

Chain C:



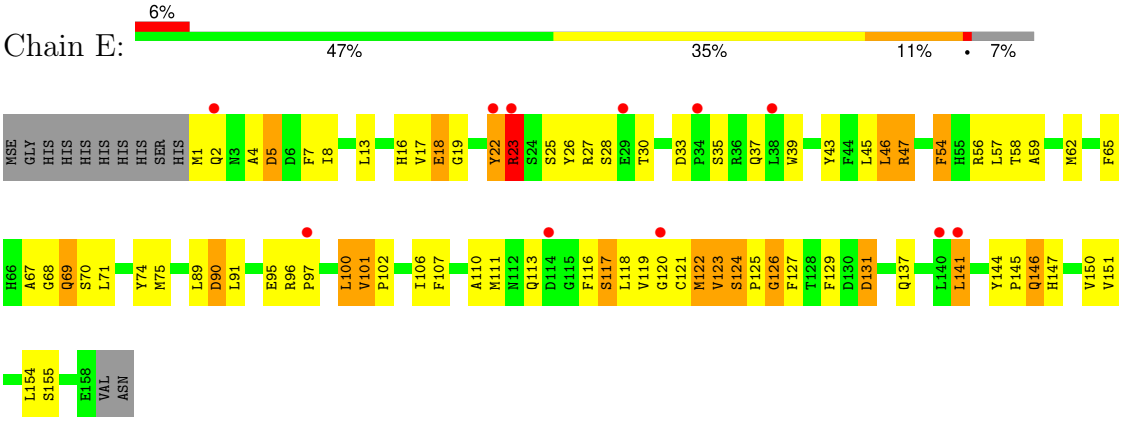
• Molecule 1: hypothetical protein SO0799

Chain D:



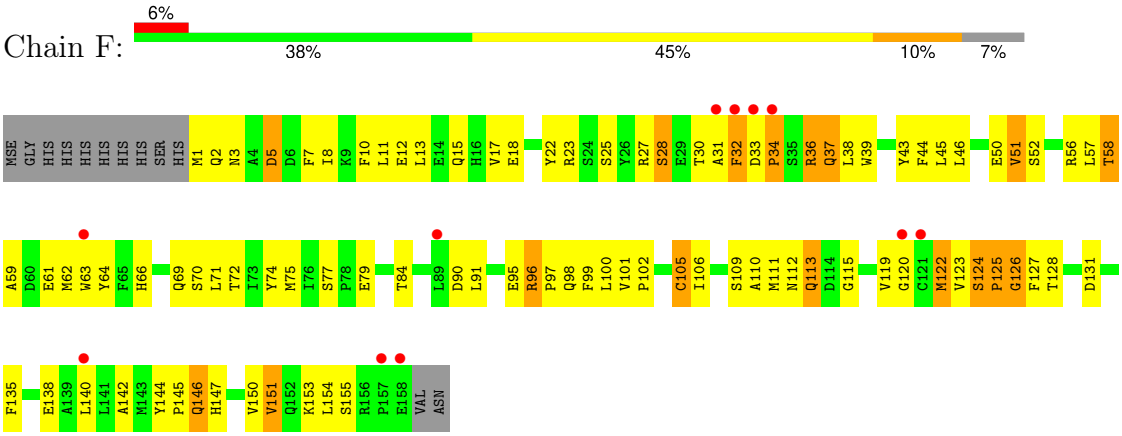
• Molecule 1: hypothetical protein SO0799

Chain E:



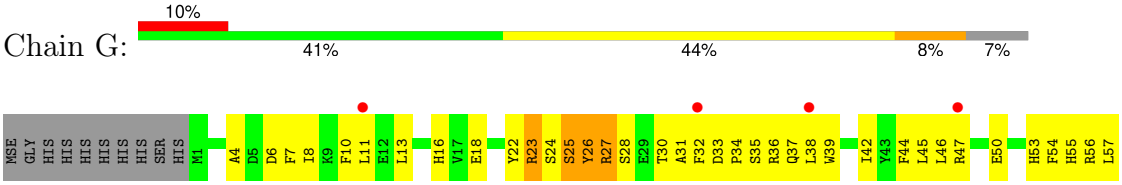
• Molecule 1: hypothetical protein SO0799

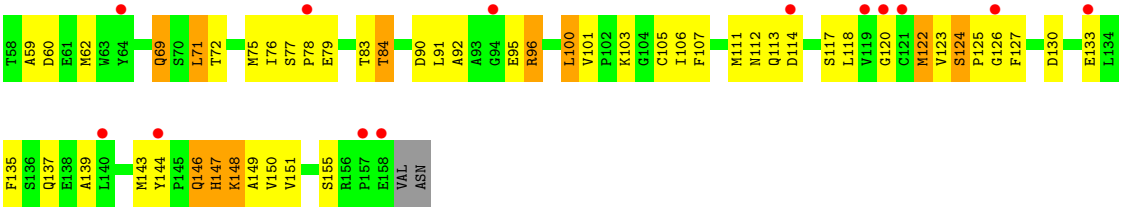
Chain F:



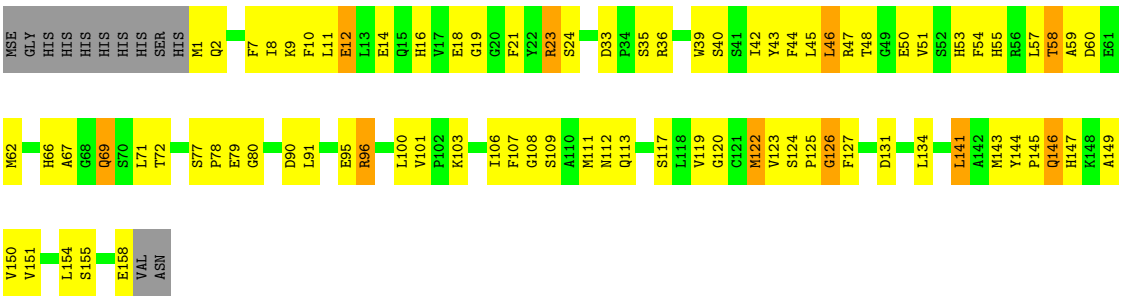
• Molecule 1: hypothetical protein SO0799

Chain G:

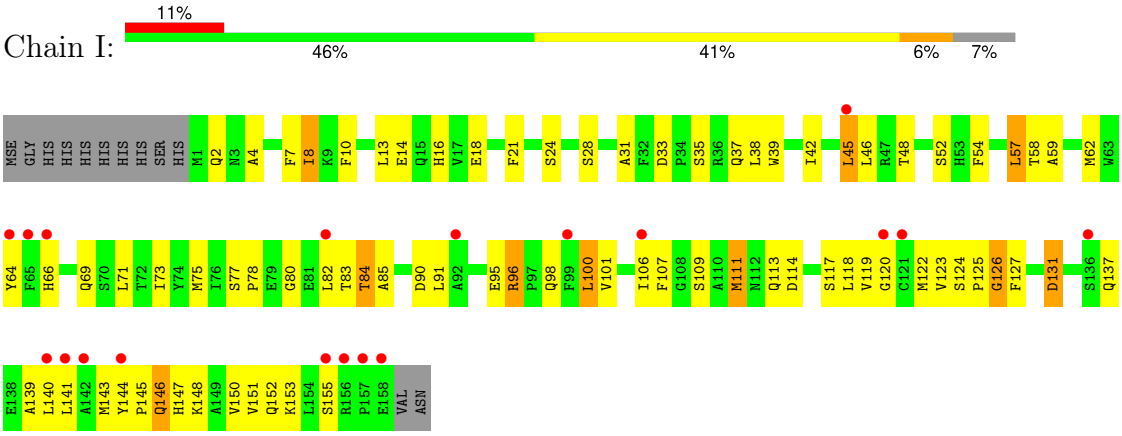




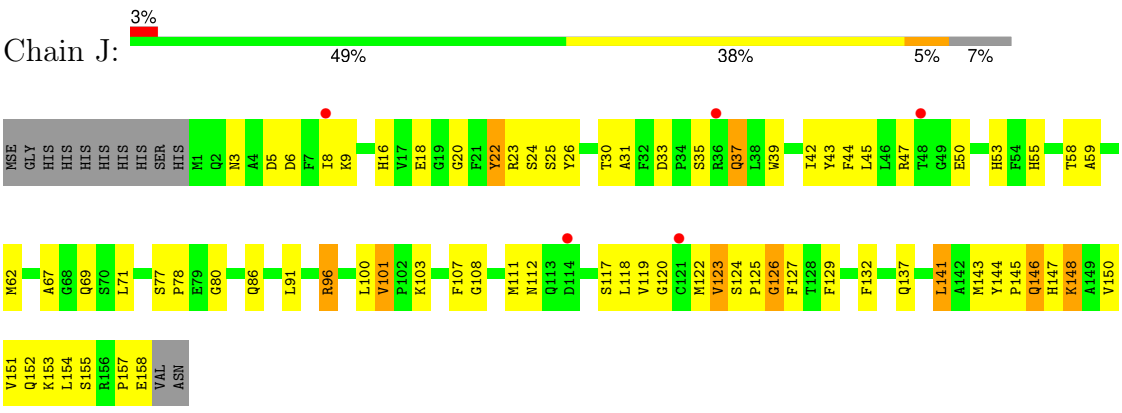
• Molecule 1: hypothetical protein SO0799



• Molecule 1: hypothetical protein SO0799



• Molecule 1: hypothetical protein SO0799



4 Data and refinement statistics (i)

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) 97.6 (29.93-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.29 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.42	0/1295	0.66	0/1742
1	B	0.53	0/1295	0.76	2/1742 (0.1%)
1	C	0.43	0/1295	0.73	0/1742
1	D	0.42	0/1295	0.68	1/1742 (0.1%)
1	E	0.41	0/1295	0.63	0/1742
1	F	0.40	0/1295	0.63	0/1742
1	G	0.37	0/1295	0.63	0/1742
1	H	0.48	0/1295	0.74	1/1742 (0.1%)
1	I	0.37	0/1295	0.63	0/1742
1	J	0.45	0/1295	0.72	0/1742
All	All	0.43	0/12950	0.68	4/17420 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	124	SER	C-N-CD	6.28	141.59	128.40
1	B	43	TYR	N-CA-C	-5.53	96.07	111.00
1	H	43	TYR	N-CA-C	-5.14	97.12	111.00
1	D	124	SER	C-N-CD	5.07	139.05	128.40

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	78	0
1	B	1265	0	1204	84	0
1	C	1265	0	1204	94	0
1	D	1265	0	1204	80	0
1	E	1265	0	1204	88	0
1	F	1265	0	1204	90	0
1	G	1265	0	1204	92	0
1	H	1265	0	1204	95	0
1	I	1265	0	1204	88	0
1	J	1265	0	1204	75	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	811	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 33.

All (811) 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:A:13:LEU:HD23	1:A:23:ARG:HB2	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:100:LEU:C	1:B:100:LEU:HD23	2.08	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:H:119:VAL:HG12	1:H:120:GLY:N	2.03	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: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: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:C:124:SER:O	1:C:125:PRO:C	2.32	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:8:ILE:HG13	1:H:9:LYS:N	2.11	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:B:122:MSE:HE3	1:C:122:MSE:SE	2.48	0.63
1:H:33:ASP:C	1:H:35:SER:H	2.02	0.63
1:C:122:MSE:HE2	1:C:123:VAL:C	2.19	0.63
1:J:33:ASP:C	1:J:35:SER:H	2.01	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
1:I:91:LEU:HA	1:I:96:ARG:NH2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:56:ARG:NH2	1:G:106:ILE:HD11	2.11	0.61
1:B:100:LEU:C	1:B:100:LEU:CD2	2.70	0.60
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:152:GLN:C	1:A:153:LYS:HD2	2.24	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: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: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: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:F:77:SER:C	1:F:79:GLU:H	2.10	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:33:ASP:C	1:H:35:SER:N	2.61	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:PHE:CD2	1:I:118:LEU:HD22	2.44	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:A:124:SER:HG	1:H:39:TRP:HD1	1.56	0.52
1:B:33:ASP:C	1:B:35:SER:H	2.13	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:D:82:LEU:HD13	1:D:150:VAL:HG11	1.91	0.52
1:E:125:PRO:O	1:E:126:GLY:C	2.47	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:B:119:VAL:HG12	1:B:120:GLY:N	2.25	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:E:100:LEU:C	1:E:100:LEU:HD23	2.30	0.51
1:J:143:MSE:HG3	1:J:144:TYR:CD2	2.45	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:E:70:SER:C	1:E:71:LEU:HD12	2.30	0.51
1:A:122:MSE:HE2	1:A:123:VAL:C	2.31	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
1:H:124:SER:O	1:H:126:GLY:N	2.44	0.51
1:A:101:VAL:HG21	1:A:107:PHE:CD2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:137:GLN:HG3	1:G:155:SER:C	2.31	0.50
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:H:149:ALA:HB1	1:J:146:GLN:CD	2.32	0.50
1:A:151:VAL:O	1:A:155:SER:HB3	2.11	0.50
1:G:53:HIS:CD2	1:G:155:SER:HA	2.46	0.50
1:H:45:LEU:HD23	1:H:45:LEU:C	2.31	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: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:E:100:LEU:C	1:E:100:LEU:CD2	2.80	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:I:33:ASP:C	1:I:35:SER:H	2.14	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
1:G:146:GLN:HG2	1:G:147:HIS:N	2.26	0.50
1:C:147:HIS:O	1:C:151:VAL:HG23	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MSE:HE3	1:F:2:GLN:HB3	1.93	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: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: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
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:J:100:LEU:C	1:J:100:LEU:HD23	2.34	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:E:119:VAL:CG1	1:E:120:GLY:N	2.76	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:F:101:VAL:O	1:F:101:VAL:HG23	2.13	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:B:124:SER:O	1:B:125:PRO:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:17:VAL:C	1:E:19:GLY:H	2.17	0.48
1:E:56:ARG:C	1:E:57:LEU:HD12	2.33	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
1:F:72:THR:OG1	1:F:112:ASN:ND2	2.46	0.47
1:H:36:ARG:NE	1:H:131:ASP:OD2	2.47	0.47
1:H:59:ALA:C	1:H:103:LYS:HB3	2.35	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:A:125:PRO:O	1:A:126:GLY:C	2.53	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:E:28:SER:C	1:E:30:THR:H	2.18	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:H:77:SER:C	1:H:79:GLU:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:H:122:MSE:SE	1:H:122:MSE:C	3.03	0.47
1:I:73:ILE:HG22	1:I:75:MSE:HG3	1.95	0.47
1:A:100:LEU:C	1:A:100:LEU:HD13	2.35	0.46
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
1:C:100:LEU:HD13	1:C:100:LEU:O	2.15	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:J:33:ASP:C	1:J:35:SER:N	2.69	0.46
1:B:45:LEU:HB2	1:B:118:LEU:HD12	1.98	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:C:100:LEU:HD13	1:C:100:LEU:C	2.37	0.46
1:D:124:SER:O	1:D:125:PRO:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:52:SER:HB3	1:I:109:SER:H	1.80	0.46
1:I:66:HIS:HD2	1:I:119:VAL:C	2.20	0.46
1:J:86:GLN:HE22	1:J:112:ASN:CG	2.18	0.45
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:22:TYR:CG	1:B:23:ARG:N	2.83	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: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:H:125:PRO:O	1:H:126:GLY:C	2.55	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:C:47:ARG:C	1:C:49:GLY:H	2.20	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:D:8:ILE:O	1:D:8:ILE:HD12	2.16	0.45
1:E:122:MSE:HE2	1:E:123:VAL:C	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:59:ALA:C	1:G:103:LYS:HB3	2.37	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:E:65:PHE:O	1:F:66:HIS:HA	2.17	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:I:59:ALA:HB1	1:I:125:PRO:HD2	1.99	0.44
1:J:122:MSE:SE	1:J:122:MSE:C	3.06	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:G:56:ARG:C	1:G:57:LEU:HD12	2.38	0.44
1:J:37:GLN:HA	1:J:37:GLN:NE2	2.31	0.44
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:C:147:HIS:O	1:C:148:LYS:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:146:GLN:H	1:C:146:GLN:HE21	1.64	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:33:ASP:C	1:G:35:SER:H	2.22	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: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: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:59:ALA:C	1:D:103:LYS:HB3	2.39	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:D:39:TRP:CD1	1:J:124:SER:HB2	2.53	0.43
1:J:125:PRO:O	1:J:126:GLY:C	2.57	0.43
1:A:149:ALA:O	1:A:153:LYS:HD3	2.19	0.43
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: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:E:47:ARG:HH21	1:E:47:ARG:HG2	1.84	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:D:141:LEU:HD12	1:D:141:LEU:HA	1.77	0.42
1:D:151:VAL:HG12	1:D:151:VAL:O	2.18	0.42
1:E:13:LEU:HD23	1:E:23:ARG:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:45:LEU:HD23	1:F:45:LEU:C	2.40	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: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:E:33:ASP:C	1:E:35:SER:N	2.72	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
1:D:33:ASP:HB3	1:D:34:PRO:CD	2.49	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:77:SER:HB2	1:H:78:PRO:HD2	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:123:VAL:O	1:G:124:SER:C	2.58	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: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: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
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:108:GLY:O	1:H:109:SER:HB2	2.20	0.41
1:H:147:HIS:HB3	1:H:150:VAL:HG12	2.02	0.41
1:I:82:LEU:HD12	1:I:83:THR:H	1.86	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: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:J:53:HIS:O	1:J:55:HIS:CD2	2.74	0.41
1:B:125:PRO:O	1:B:126:GLY:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:O	1:A:54:PHE:C	2.59	0.41
1:D:58:THR:O	1:D:58:THR:CG2	2.63	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: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: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: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: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: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:E:25:SER:C	1:E:26:TYR:CD1	2.94	0.40
1:G:56:ARG:HE	1:G:106:ILE:CG1	2.34	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:C:59:ALA:C	1:C:103:LYS:HB3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:E:23:ARG:HD3	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
1:F:77:SER:C	1:F:79:GLU:N	2.74	0.40
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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/170 (92%)	134 (86%)	17 (11%)	5 (3%)	4	9
1	B	156/170 (92%)	139 (89%)	11 (7%)	6 (4%)	3	7
1	C	156/170 (92%)	136 (87%)	14 (9%)	6 (4%)	3	7
1	D	156/170 (92%)	132 (85%)	18 (12%)	6 (4%)	3	7
1	E	156/170 (92%)	134 (86%)	15 (10%)	7 (4%)	2	5
1	F	156/170 (92%)	123 (79%)	24 (15%)	9 (6%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	156/170 (92%)	117 (75%)	30 (19%)	9 (6%)	1 2
1	H	156/170 (92%)	137 (88%)	18 (12%)	1 (1%)	25 50
1	I	156/170 (92%)	129 (83%)	22 (14%)	5 (3%)	4 9
1	J	156/170 (92%)	140 (90%)	12 (8%)	4 (3%)	5 13
All	All	1560/1700 (92%)	1321 (85%)	181 (12%)	58 (4%)	3 7

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

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Mol	Chain	Res	Type
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
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	135/139 (97%)	125 (93%)	10 (7%)	13 32
1	B	135/139 (97%)	121 (90%)	14 (10%)	7 16
1	C	135/139 (97%)	120 (89%)	15 (11%)	6 14
1	D	135/139 (97%)	119 (88%)	16 (12%)	5 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	135/139 (97%)	120 (89%)	15 (11%)	6 14
1	F	135/139 (97%)	123 (91%)	12 (9%)	9 22
1	G	135/139 (97%)	124 (92%)	11 (8%)	11 27
1	H	135/139 (97%)	123 (91%)	12 (9%)	9 22
1	I	135/139 (97%)	127 (94%)	8 (6%)	19 43
1	J	135/139 (97%)	122 (90%)	13 (10%)	8 19
All	All	1350/1390 (97%)	1224 (91%)	126 (9%)	9 21

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	23	ARG
1	A	25	SER
1	A	57	LEU
1	A	69	GLN
1	A	96	ARG
1	A	105	CYS
1	A	122	MSE
1	A	130	ASP
1	A	138	GLU
1	B	3	ASN
1	B	8	ILE
1	B	23	ARG
1	B	46	LEU
1	B	57	LEU
1	B	58	THR
1	B	69	GLN
1	B	75	MSE
1	B	96	ARG
1	B	101	VAL
1	B	123	VAL
1	B	141	LEU
1	B	146	GLN
1	B	152	GLN
1	C	8	ILE
1	C	23	ARG
1	C	46	LEU
1	C	48	THR
1	C	57	LEU

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Mol	Chain	Res	Type
1	C	69	GLN
1	C	96	ARG
1	C	119	VAL
1	C	122	MSE
1	C	124	SER
1	C	125	PRO
1	C	130	ASP
1	C	131	ASP
1	C	141	LEU
1	C	146	GLN
1	D	6	ASP
1	D	8	ILE
1	D	23	ARG
1	D	27	ARG
1	D	46	LEU
1	D	57	LEU
1	D	71	LEU
1	D	83	THR
1	D	96	ARG
1	D	101	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	18	GLU
1	E	22	TYR
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	122	MSE
1	E	123	VAL
1	E	131	ASP
1	E	141	LEU
1	E	146	GLN
1	F	5	ASP

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Mol	Chain	Res	Type
1	F	34	PRO
1	F	36	ARG
1	F	44	PHE
1	F	51	VAL
1	F	58	THR
1	F	69	GLN
1	F	96	ARG
1	F	105	CYS
1	F	113	GLN
1	F	122	MSE
1	F	146	GLN
1	G	26	TYR
1	G	27	ARG
1	G	32	PHE
1	G	69	GLN
1	G	84	THR
1	G	96	ARG
1	G	100	LEU
1	G	122	MSE
1	G	130	ASP
1	G	144	TYR
1	G	146	GLN
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	122	MSE
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	131	ASP
1	I	146	GLN

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Mol	Chain	Res	Type
1	J	16	HIS
1	J	18	GLU
1	J	22	TYR
1	J	37	GLN
1	J	58	THR
1	J	69	GLN
1	J	96	ARG
1	J	101	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 (79) 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	3	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	B	147	HIS
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	137	GLN
1	C	146	GLN
1	C	147	HIS
1	D	3	ASN

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Mol	Chain	Res	Type
1	D	15	GLN
1	D	55	HIS
1	D	69	GLN
1	D	86	GLN
1	D	112	ASN
1	D	113	GLN
1	D	137	GLN
1	D	146	GLN
1	D	152	GLN
1	E	2	GLN
1	E	15	GLN
1	E	37	GLN
1	E	55	HIS
1	E	69	GLN
1	E	112	ASN
1	E	137	GLN
1	E	146	GLN
1	E	147	HIS
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	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	I	53	HIS
1	I	69	GLN

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Mol	Chain	Res	Type
1	I	86	GLN
1	I	112	ASN
1	I	137	GLN
1	I	146	GLN
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
1	J	152	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 monosaccharides 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	152/170 (89%)	0.21	3 (1%) 65 67	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%)	-0.05	2 (1%) 77 78	27, 55, 86, 118	0
1	D	152/170 (89%)	0.26	7 (4%) 32 31	36, 60, 84, 115	0
1	E	152/170 (89%)	0.55	11 (7%) 15 13	39, 72, 98, 122	0
1	F	152/170 (89%)	0.56	11 (7%) 15 13	43, 77, 112, 132	0
1	G	152/170 (89%)	0.83	17 (11%) 5 4	65, 89, 115, 137	0
1	H	152/170 (89%)	-0.00	0 100 100	23, 47, 79, 115	0
1	I	152/170 (89%)	0.88	19 (12%) 3 3	53, 86, 116, 132	0
1	J	152/170 (89%)	0.30	5 (3%) 46 46	33, 59, 85, 127	0
All	All	1520/1700 (89%)	0.33	75 (4%) 29 28	16, 66, 106, 137	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	PRO	6.7
1	F	33	ASP	5.9
1	I	157	PRO	5.4
1	I	144	TYR	5.0
1	A	121	CYS	4.5
1	G	144	TYR	4.4
1	E	140	LEU	4.2
1	I	140	LEU	4.1
1	G	126	GLY	4.1
1	G	78	PRO	4.0
1	G	157	PRO	4.0
1	G	140	LEU	3.9
1	G	114	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	94	GLY	3.8
1	D	138	GLU	3.7
1	F	120	GLY	3.6
1	G	121	CYS	3.6
1	F	140	LEU	3.6
1	E	22	TYR	3.5
1	I	64	TYR	3.5
1	I	158	GLU	3.5
1	G	158	GLU	3.2
1	I	106	ILE	3.2
1	F	121	CYS	3.2
1	F	32	PHE	3.2
1	F	158	GLU	3.1
1	I	120	GLY	3.1
1	G	64	TYR	3.1
1	I	156	ARG	3.1
1	D	120	GLY	3.0
1	I	92	ALA	3.0
1	J	36	ARG	3.0
1	I	82	LEU	2.9
1	D	64	TYR	2.9
1	D	121	CYS	2.9
1	D	32	PHE	2.8
1	G	32	PHE	2.8
1	J	8	ILE	2.8
1	E	2	GLN	2.7
1	C	148	LYS	2.7
1	I	136	SER	2.7
1	G	38	LEU	2.7
1	I	141	LEU	2.7
1	G	119	VAL	2.7
1	E	29	GLU	2.7
1	J	121	CYS	2.7
1	C	140	LEU	2.6
1	I	99	PHE	2.6
1	E	114	ASP	2.6
1	I	155	SER	2.6
1	A	92	ALA	2.6
1	I	121	CYS	2.6
1	G	47	ARG	2.6
1	A	120	GLY	2.5
1	G	120	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	31	ALA	2.4
1	J	48	THR	2.4
1	E	34	PRO	2.3
1	I	45	LEU	2.3
1	F	63	TRP	2.2
1	D	91	LEU	2.2
1	I	142	ALA	2.2
1	E	120	GLY	2.2
1	I	66	HIS	2.1
1	G	133	GLU	2.1
1	E	97	PRO	2.1
1	D	47	ARG	2.1
1	J	114	ASP	2.1
1	E	38	LEU	2.1
1	F	89	LEU	2.0
1	G	11	LEU	2.0
1	F	157	PRO	2.0
1	E	23	ARG	2.0
1	E	141	LEU	2.0
1	I	65	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.