



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2020 – 04:09 PM JST

PDB ID : 7CTO  
Title : Staphylococcus aureus MsrB  
Authors : Kim, H.J.  
Deposited on : 2020-08-19  
Resolution : 3.47 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

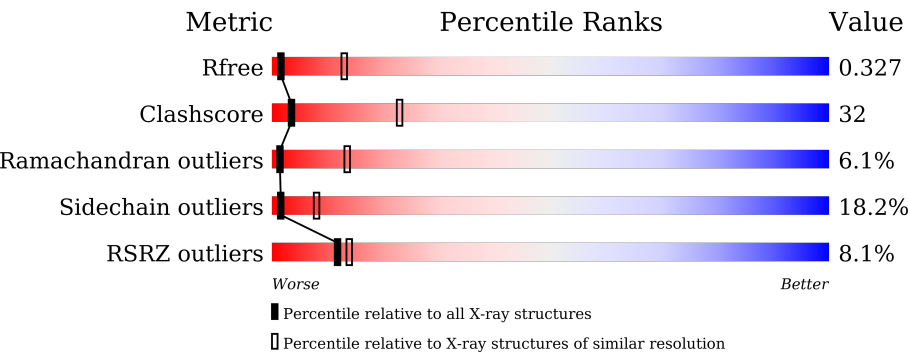
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	159	<div><div>9%</div><div>40%37%6%16%</div></div>
1	B	159	<div><div>3%</div><div>37%38%11%13%</div></div>
1	C	159	<div><div>7%</div><div>37%38%10%14%</div></div>
1	D	159	<div><div>6%</div><div>45%30%11%14%</div></div>
1	E	159	<div><div>8%</div><div>32%44%9%14%</div></div>
1	F	159	<div><div>9%</div><div>40%34%10%15%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6564 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 Peptide methionine sulfoxide reductase MsrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1076	684	172	216	4			
1	B	139	Total	C	N	O	S	0	0	0
			1121	713	179	225	4			
1	C	136	Total	C	N	O	S	0	0	0
			1093	694	175	220	4			
1	D	136	Total	C	N	O	S	0	0	0
			1095	695	174	222	4			
1	E	136	Total	C	N	O	S	0	0	0
			1095	697	174	220	4			
1	F	135	Total	C	N	O	S	0	0	0
			1084	688	173	219	4			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP W8TTH3
A	-15	HIS	-	expression tag	UNP W8TTH3
A	-14	HIS	-	expression tag	UNP W8TTH3
A	-13	HIS	-	expression tag	UNP W8TTH3
A	-12	HIS	-	expression tag	UNP W8TTH3
A	-11	HIS	-	expression tag	UNP W8TTH3
A	-10	HIS	-	expression tag	UNP W8TTH3
A	-9	GLU	-	expression tag	UNP W8TTH3
A	-8	ASN	-	expression tag	UNP W8TTH3
A	-7	LEU	-	expression tag	UNP W8TTH3
A	-6	TYR	-	expression tag	UNP W8TTH3
A	-5	PHE	-	expression tag	UNP W8TTH3
A	-4	GLN	-	expression tag	UNP W8TTH3
A	-3	GLY	-	expression tag	UNP W8TTH3
A	-2	ALA	-	expression tag	UNP W8TTH3
A	-1	ALA	-	expression tag	UNP W8TTH3
A	0	SER	-	expression tag	UNP W8TTH3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP W8TTH3
B	-15	HIS	-	expression tag	UNP W8TTH3
B	-14	HIS	-	expression tag	UNP W8TTH3
B	-13	HIS	-	expression tag	UNP W8TTH3
B	-12	HIS	-	expression tag	UNP W8TTH3
B	-11	HIS	-	expression tag	UNP W8TTH3
B	-10	HIS	-	expression tag	UNP W8TTH3
B	-9	GLU	-	expression tag	UNP W8TTH3
B	-8	ASN	-	expression tag	UNP W8TTH3
B	-7	LEU	-	expression tag	UNP W8TTH3
B	-6	TYR	-	expression tag	UNP W8TTH3
B	-5	PHE	-	expression tag	UNP W8TTH3
B	-4	GLN	-	expression tag	UNP W8TTH3
B	-3	GLY	-	expression tag	UNP W8TTH3
B	-2	ALA	-	expression tag	UNP W8TTH3
B	-1	ALA	-	expression tag	UNP W8TTH3
B	0	SER	-	expression tag	UNP W8TTH3
C	-16	MET	-	initiating methionine	UNP W8TTH3
C	-15	HIS	-	expression tag	UNP W8TTH3
C	-14	HIS	-	expression tag	UNP W8TTH3
C	-13	HIS	-	expression tag	UNP W8TTH3
C	-12	HIS	-	expression tag	UNP W8TTH3
C	-11	HIS	-	expression tag	UNP W8TTH3
C	-10	HIS	-	expression tag	UNP W8TTH3
C	-9	GLU	-	expression tag	UNP W8TTH3
C	-8	ASN	-	expression tag	UNP W8TTH3
C	-7	LEU	-	expression tag	UNP W8TTH3
C	-6	TYR	-	expression tag	UNP W8TTH3
C	-5	PHE	-	expression tag	UNP W8TTH3
C	-4	GLN	-	expression tag	UNP W8TTH3
C	-3	GLY	-	expression tag	UNP W8TTH3
C	-2	ALA	-	expression tag	UNP W8TTH3
C	-1	ALA	-	expression tag	UNP W8TTH3
C	0	SER	-	expression tag	UNP W8TTH3
D	-16	MET	-	initiating methionine	UNP W8TTH3
D	-15	HIS	-	expression tag	UNP W8TTH3
D	-14	HIS	-	expression tag	UNP W8TTH3
D	-13	HIS	-	expression tag	UNP W8TTH3
D	-12	HIS	-	expression tag	UNP W8TTH3
D	-11	HIS	-	expression tag	UNP W8TTH3
D	-10	HIS	-	expression tag	UNP W8TTH3
D	-9	GLU	-	expression tag	UNP W8TTH3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	ASN	-	expression tag	UNP W8TTH3
D	-7	LEU	-	expression tag	UNP W8TTH3
D	-6	TYR	-	expression tag	UNP W8TTH3
D	-5	PHE	-	expression tag	UNP W8TTH3
D	-4	GLN	-	expression tag	UNP W8TTH3
D	-3	GLY	-	expression tag	UNP W8TTH3
D	-2	ALA	-	expression tag	UNP W8TTH3
D	-1	ALA	-	expression tag	UNP W8TTH3
D	0	SER	-	expression tag	UNP W8TTH3
E	-16	MET	-	initiating methionine	UNP W8TTH3
E	-15	HIS	-	expression tag	UNP W8TTH3
E	-14	HIS	-	expression tag	UNP W8TTH3
E	-13	HIS	-	expression tag	UNP W8TTH3
E	-12	HIS	-	expression tag	UNP W8TTH3
E	-11	HIS	-	expression tag	UNP W8TTH3
E	-10	HIS	-	expression tag	UNP W8TTH3
E	-9	GLU	-	expression tag	UNP W8TTH3
E	-8	ASN	-	expression tag	UNP W8TTH3
E	-7	LEU	-	expression tag	UNP W8TTH3
E	-6	TYR	-	expression tag	UNP W8TTH3
E	-5	PHE	-	expression tag	UNP W8TTH3
E	-4	GLN	-	expression tag	UNP W8TTH3
E	-3	GLY	-	expression tag	UNP W8TTH3
E	-2	ALA	-	expression tag	UNP W8TTH3
E	-1	ALA	-	expression tag	UNP W8TTH3
E	0	SER	-	expression tag	UNP W8TTH3
F	-16	MET	-	initiating methionine	UNP W8TTH3
F	-15	HIS	-	expression tag	UNP W8TTH3
F	-14	HIS	-	expression tag	UNP W8TTH3
F	-13	HIS	-	expression tag	UNP W8TTH3
F	-12	HIS	-	expression tag	UNP W8TTH3
F	-11	HIS	-	expression tag	UNP W8TTH3
F	-10	HIS	-	expression tag	UNP W8TTH3
F	-9	GLU	-	expression tag	UNP W8TTH3
F	-8	ASN	-	expression tag	UNP W8TTH3
F	-7	LEU	-	expression tag	UNP W8TTH3
F	-6	TYR	-	expression tag	UNP W8TTH3
F	-5	PHE	-	expression tag	UNP W8TTH3
F	-4	GLN	-	expression tag	UNP W8TTH3
F	-3	GLY	-	expression tag	UNP W8TTH3
F	-2	ALA	-	expression tag	UNP W8TTH3
F	-1	ALA	-	expression tag	UNP W8TTH3

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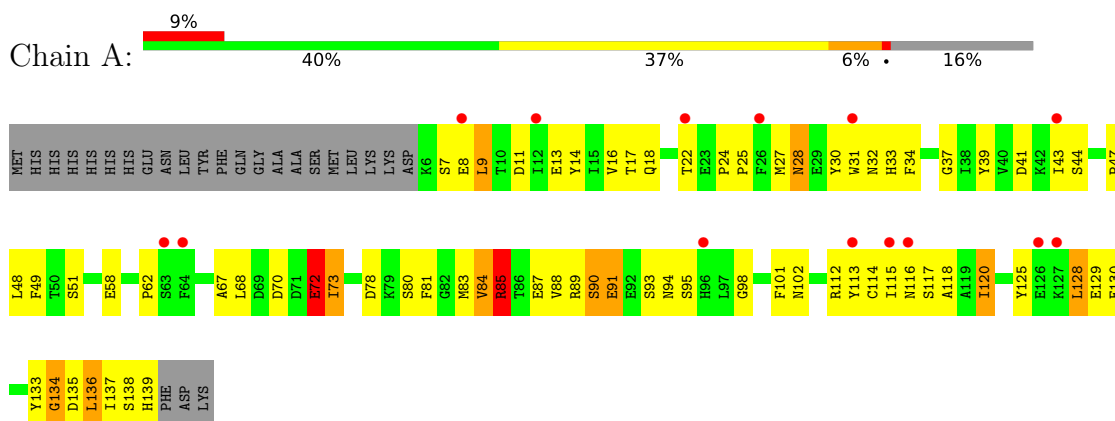
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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP W8TTH3

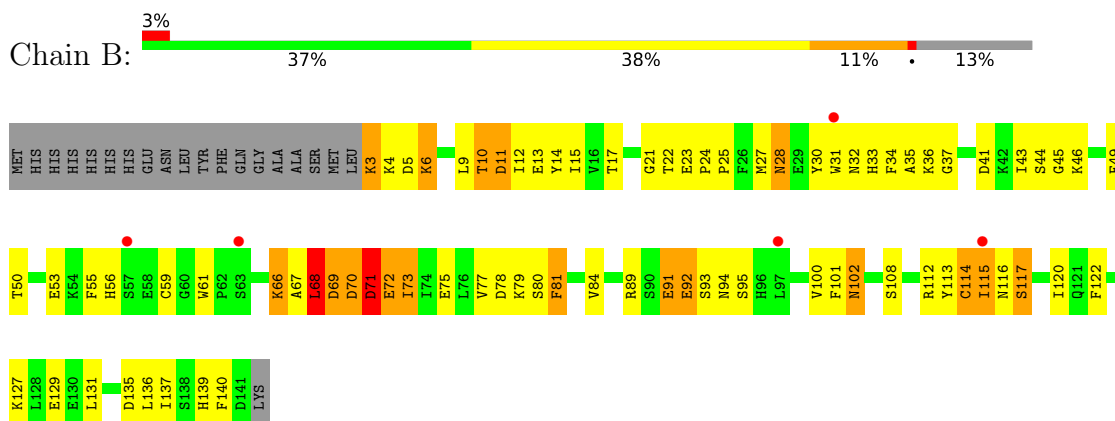
### 3 Residue-property plots

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.

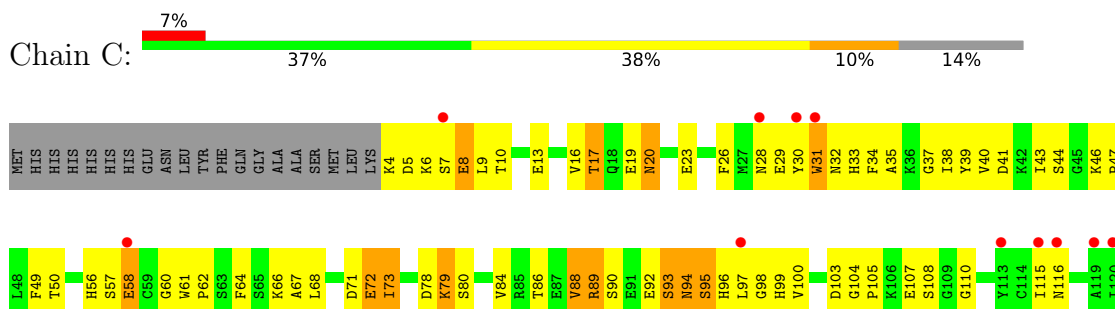
#### • Molecule 1: Peptide methionine sulfoxide reductase MsrB



#### • Molecule 1: Peptide methionine sulfoxide reductase MsrB

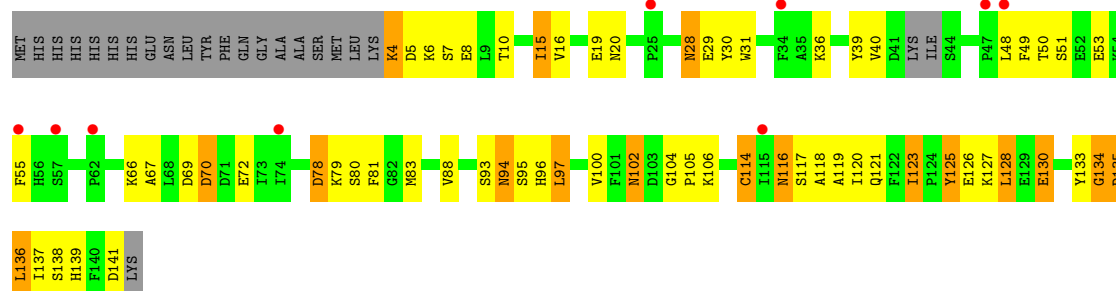


#### • Molecule 1: Peptide methionine sulfoxide reductase MsrB

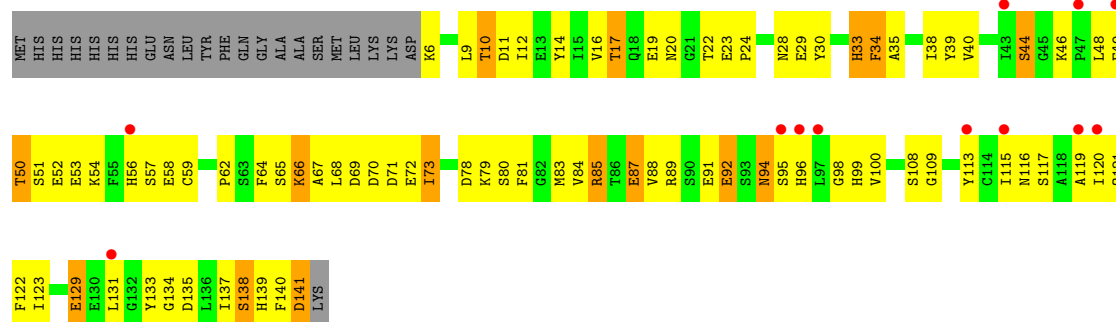




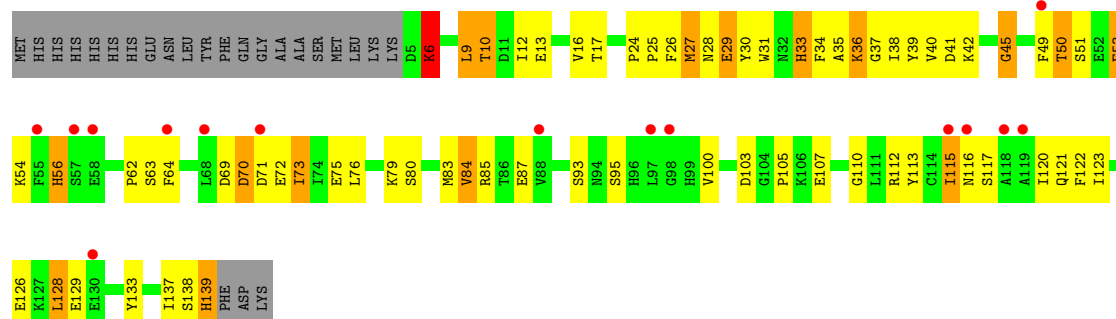
• Molecule 1: Peptide methionine sulfoxide reductase MsrB



• Molecule 1: Peptide methionine sulfoxide reductase MsrB



• Molecule 1: Peptide methionine sulfoxide reductase MsrB





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.83Å 122.19Å 73.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.68 – 3.47 83.68 – 3.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (83.68-3.47) 99.8 (83.68-3.47)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.216 , 0.323 0.230 , 0.327	Depositor DCC
$R_{free}$ test set	686 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	111.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 107.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.76	0/1104	0.91	0/1491
1	B	0.69	0/1150	0.97	0/1551
1	C	0.73	0/1121	0.90	0/1513
1	D	0.72	0/1123	0.92	0/1515
1	E	0.71	0/1124	0.90	0/1518
1	F	0.71	0/1112	0.88	0/1502
All	All	0.72	0/6734	0.92	0/9090

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1076	0	1008	64	0
1	B	1121	0	1051	92	0
1	C	1093	0	1025	71	0
1	D	1095	0	1013	66	0
1	E	1095	0	1021	68	0
1	F	1084	0	1012	58	0
All	All	6564	0	6130	408	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 32.

All (408) 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:C:49:PHE:CE1	1:C:67:ALA:HB2	1.89	1.06
1:E:88:VAL:HG12	1:E:98:GLY:C	1.80	1.02
1:E:88:VAL:HG12	1:E:98:GLY:O	1.68	0.92
1:C:89:ARG:NH1	1:C:94:ASN:HD21	1.68	0.91
1:E:23:GLU:HG2	1:E:116:ASN:OD1	1.69	0.91
1:B:46:LYS:NZ	1:B:72:GLU:HB3	1.88	0.89
1:F:36:LYS:H	1:F:36:LYS:HD2	1.39	0.87
1:B:30:TYR:HB2	1:B:117:SER:HB3	1.57	0.86
1:D:20:ASN:HA	1:D:96:HIS:CD2	2.13	0.84
1:F:39:TYR:HD2	1:F:120:ILE:HG21	1.42	0.82
1:B:46:LYS:HZ3	1:B:72:GLU:HB3	1.46	0.81
1:D:50:THR:HG23	1:D:53:GLU:HG2	1.61	0.80
1:E:54:LYS:HG3	1:E:64:PHE:CE2	2.17	0.79
1:C:32:ASN:O	1:C:34:PHE:CD1	2.35	0.79
1:F:36:LYS:N	1:F:36:LYS:HD2	1.97	0.79
1:B:69:ASP:N	1:B:69:ASP:OD1	2.15	0.77
1:D:102:ASN:H	1:D:102:ASN:HD22	1.29	0.77
1:C:32:ASN:O	1:C:34:PHE:HD1	1.66	0.76
1:E:78:ASP:HB2	1:E:87:GLU:HB3	1.67	0.76
1:B:28:ASN:HB3	1:B:117:SER:OG	1.86	0.76
1:F:41:ASP:OD2	1:F:93:SER:HB3	1.84	0.76
1:B:66:LYS:HA	1:B:113:TYR:CE1	2.22	0.75
1:D:127:LYS:HD3	1:D:130:GLU:OE1	1.88	0.74
1:A:72:GLU:O	1:A:91:GLU:CD	2.26	0.74
1:F:39:TYR:CD2	1:F:120:ILE:HG21	2.22	0.74
1:F:33:HIS:CE1	1:F:35:ALA:HB3	2.22	0.73
1:D:48:LEU:HD13	1:D:97:LEU:HD11	1.68	0.73
1:D:102:ASN:ND2	1:D:102:ASN:N	2.37	0.73
1:D:123:ILE:O	1:D:128:LEU:HD11	1.89	0.73
1:E:20:ASN:HA	1:E:96:HIS:CD2	2.24	0.73
1:E:46:LYS:HD2	1:E:92:GLU:HG2	1.70	0.72
1:D:127:LYS:O	1:D:130:GLU:HB2	1.89	0.72
1:D:102:ASN:HD22	1:D:102:ASN:N	1.88	0.71
1:D:94:ASN:O	1:D:94:ASN:CG	2.30	0.70
1:D:50:THR:CG2	1:D:53:GLU:HG2	2.22	0.70
1:D:39:TYR:HB3	1:D:120:ILE:HG23	1.73	0.70
1:D:30:TYR:HD2	1:D:117:SER:HB2	1.55	0.69
1:F:17:THR:HB	1:F:95:SER:HB2	1.73	0.69
1:A:90:SER:O	1:A:94:ASN:HA	1.92	0.68
1:D:30:TYR:CD2	1:D:117:SER:HB2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:LYS:HG3	1:E:67:ALA:O	1.93	0.68
1:C:79:LYS:HD3	1:C:84:VAL:HG22	1.76	0.68
1:B:28:ASN:ND2	1:B:28:ASN:H	1.91	0.68
1:D:28:ASN:O	1:D:30:TYR:N	2.25	0.67
1:E:49:PHE:CE1	1:E:67:ALA:HA	2.29	0.67
1:D:116:ASN:H	1:D:116:ASN:HD22	1.41	0.67
1:A:128:LEU:HD23	1:A:133:TYR:HB2	1.77	0.67
1:A:134:GLY:O	1:A:137:ILE:HG12	1.95	0.67
1:F:39:TYR:CE2	1:F:122:PHE:HB2	2.30	0.67
1:B:72:GLU:OE1	1:B:72:GLU:HA	1.94	0.67
1:D:28:ASN:HB3	1:D:117:SER:OG	1.95	0.66
1:D:88:VAL:O	1:D:97:LEU:HB2	1.95	0.66
1:B:68:LEU:HD12	1:B:68:LEU:C	2.16	0.66
1:A:22:THR:O	1:E:24:PRO:HB3	1.96	0.66
1:C:40:VAL:HG12	1:C:47:PRO:HA	1.77	0.66
1:D:48:LEU:CD1	1:D:97:LEU:HD11	2.27	0.66
1:A:113:TYR:O	1:A:115:ILE:HG12	1.97	0.65
1:B:72:GLU:O	1:B:91:GLU:HB3	1.97	0.65
1:F:64:PHE:O	1:F:113:TYR:HD1	1.79	0.64
1:A:91:GLU:CD	1:A:91:GLU:N	2.51	0.64
1:D:116:ASN:H	1:D:116:ASN:ND2	1.95	0.64
1:C:10:THR:OG1	1:C:13:GLU:HG3	1.97	0.64
1:F:17:THR:HB	1:F:95:SER:CB	2.28	0.64
1:E:54:LYS:CG	1:E:64:PHE:CE2	2.81	0.63
1:D:118:ALA:C	1:D:120:ILE:H	2.01	0.63
1:D:40:VAL:HG22	1:D:121:GLN:O	1.98	0.63
1:D:55:PHE:CZ	1:D:105:PRO:CD	2.81	0.63
1:C:89:ARG:NH1	1:C:94:ASN:ND2	2.44	0.63
1:E:23:GLU:CG	1:E:116:ASN:OD1	2.46	0.63
1:C:9:LEU:HD11	1:C:43:ILE:HD11	1.81	0.63
1:D:16:VAL:O	1:D:96:HIS:HB3	1.99	0.63
1:B:17:THR:HB	1:B:95:SER:HB2	1.80	0.63
1:C:17:THR:HG22	1:C:95:SER:HB3	1.80	0.63
1:C:34:PHE:CE1	1:C:56:HIS:CE1	2.87	0.62
1:D:48:LEU:HD13	1:D:97:LEU:CD1	2.29	0.62
1:B:33:HIS:NE2	1:B:122:PHE:CD1	2.66	0.62
1:E:28:ASN:HD21	1:E:62:PRO:HD3	1.65	0.62
1:F:79:LYS:HA	1:F:83:MET:O	1.99	0.62
1:B:28:ASN:CB	1:B:117:SER:OG	2.47	0.62
1:B:37:GLY:O	1:B:140:PHE:HZ	1.83	0.62
1:A:28:ASN:HD21	1:A:62:PRO:HD3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ASP:C	1:D:78:ASP:OD1	2.38	0.61
1:B:49:PHE:CE1	1:B:67:ALA:HA	2.35	0.61
1:B:46:LYS:HZ1	1:B:72:GLU:HB3	1.64	0.61
1:E:28:ASN:ND2	1:E:62:PRO:HD3	2.16	0.61
1:C:30:TYR:HA	1:C:33:HIS:HB3	1.81	0.61
1:C:94:ASN:ND2	1:C:94:ASN:O	2.32	0.60
1:D:128:LEU:H	1:D:128:LEU:HD13	1.66	0.60
1:A:102:ASN:HD21	1:C:84:VAL:H	1.50	0.60
1:D:127:LYS:CD	1:D:130:GLU:OE1	2.49	0.60
1:E:85:ARG:HH12	1:E:99:HIS:CE1	2.20	0.60
1:D:134:GLY:O	1:D:136:LEU:N	2.35	0.60
1:B:49:PHE:HE2	1:B:115:ILE:HD13	1.65	0.60
1:E:20:ASN:HA	1:E:96:HIS:CG	2.37	0.59
1:C:73:ILE:HD11	1:C:97:LEU:HD12	1.83	0.59
1:B:112:ARG:NH1	1:B:114:CYS:SG	2.76	0.59
1:B:35:ALA:HB3	1:B:122:PHE:CZ	2.37	0.59
1:A:133:TYR:O	1:A:135:ASP:N	2.35	0.59
1:B:84:VAL:HG11	1:E:100:VAL:HG13	1.84	0.59
1:F:30:TYR:CD2	1:F:117:SER:HB2	2.37	0.59
1:F:16:VAL:HG13	1:F:116:ASN:HD22	1.68	0.59
1:C:33:HIS:HD2	1:C:39:TYR:OH	1.86	0.58
1:F:6:LYS:O	1:F:6:LYS:HG2	2.02	0.58
1:C:28:ASN:HD21	1:C:62:PRO:HD3	1.69	0.58
1:B:28:ASN:HB3	1:B:117:SER:HG	1.67	0.58
1:B:17:THR:CB	1:B:95:SER:HB2	2.34	0.58
1:C:46:LYS:NZ	1:C:72:GLU:OE2	2.27	0.58
1:B:66:LYS:HA	1:B:113:TYR:HE1	1.68	0.58
1:D:20:ASN:HA	1:D:96:HIS:CG	2.39	0.58
1:A:90:SER:HA	1:A:91:GLU:OE2	2.04	0.58
1:D:100:VAL:HG13	1:F:84:VAL:HG11	1.85	0.58
1:E:54:LYS:HG3	1:E:64:PHE:CD2	2.38	0.58
1:A:9:LEU:HD21	1:A:43:ILE:CD1	2.34	0.58
1:E:39:TYR:HA	1:E:121:GLN:O	2.03	0.58
1:A:72:GLU:O	1:A:91:GLU:OE2	2.22	0.57
1:F:39:TYR:HD2	1:F:120:ILE:CG2	2.17	0.57
1:B:89:ARG:NH2	1:B:94:ASN:HD21	2.02	0.57
1:F:56:HIS:N	1:F:56:HIS:ND1	2.53	0.57
1:A:78:ASP:OD1	1:A:80:SER:HB2	2.04	0.57
1:A:84:VAL:O	1:A:85:ARG:HB2	2.04	0.57
1:F:37:GLY:HA3	1:F:122:PHE:HE1	1.70	0.57
1:C:49:PHE:HB3	1:C:64:PHE:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:N	1:C:98:GLY:O	2.38	0.56
1:E:34:PHE:HD1	1:E:34:PHE:N	2.04	0.56
1:B:25:PRO:HG3	1:B:61:TRP:CZ2	2.40	0.56
1:E:48:LEU:C	1:E:49:PHE:CD2	2.78	0.56
1:D:118:ALA:O	1:D:120:ILE:N	2.38	0.56
1:D:127:LYS:O	1:D:130:GLU:N	2.39	0.56
1:A:41:ASP:OD2	1:A:93:SER:HB3	2.06	0.56
1:B:73:ILE:HD13	1:B:73:ILE:O	2.06	0.56
1:E:50:THR:OG1	1:E:51:SER:N	2.38	0.56
1:E:71:ASP:O	1:E:91:GLU:OE1	2.24	0.56
1:B:67:ALA:O	1:B:69:ASP:N	2.39	0.55
1:C:44:SER:HB3	1:C:93:SER:HB2	1.87	0.55
1:D:4:LYS:N	1:D:7:SER:OG	2.39	0.55
1:F:84:VAL:HG12	1:F:84:VAL:O	2.06	0.55
1:B:41:ASP:OD2	1:B:93:SER:HB3	2.07	0.55
1:D:128:LEU:H	1:D:128:LEU:CD1	2.19	0.55
1:E:88:VAL:CG1	1:E:98:GLY:C	2.67	0.55
1:C:46:LYS:HD3	1:C:92:GLU:HB3	1.89	0.55
1:B:9:LEU:O	1:B:11:ASP:N	2.40	0.55
1:E:34:PHE:N	1:E:34:PHE:CD1	2.74	0.55
1:E:88:VAL:O	1:E:88:VAL:HG13	2.06	0.55
1:C:49:PHE:CD1	1:C:67:ALA:HB2	2.39	0.55
1:D:55:PHE:CZ	1:D:105:PRO:HD3	2.40	0.55
1:F:54:LYS:HB2	1:F:64:PHE:CE2	2.42	0.55
1:E:50:THR:CG2	1:E:68:LEU:HD13	2.38	0.54
1:E:17:THR:HG22	1:E:95:SER:HB2	1.88	0.54
1:A:128:LEU:C	1:A:130:GLU:H	2.11	0.54
1:A:94:ASN:ND2	1:A:94:ASN:O	2.40	0.54
1:A:81:PHE:O	1:A:83:MET:HG3	2.08	0.54
1:B:3:LYS:O	1:B:6:LYS:N	2.40	0.54
1:B:25:PRO:C	1:B:27:MET:H	2.10	0.54
1:B:81:PHE:CD1	1:B:81:PHE:N	2.75	0.54
1:A:88:VAL:N	1:A:98:GLY:O	2.41	0.53
1:B:66:LYS:C	1:B:68:LEU:H	2.12	0.53
1:D:15:ILE:O	1:D:19:GLU:N	2.39	0.53
1:E:88:VAL:HG13	1:E:98:GLY:H	1.73	0.53
1:C:49:PHE:HB3	1:C:64:PHE:CE2	2.43	0.53
1:E:66:LYS:HA	1:E:113:TYR:CE1	2.42	0.53
1:F:62:PRO:HD2	1:F:115:ILE:O	2.08	0.53
1:D:117:SER:O	1:D:120:ILE:HB	2.08	0.53
1:A:28:ASN:HD22	1:A:117:SER:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ILE:O	1:E:122:PHE:HA	2.08	0.53
1:C:9:LEU:HD21	1:C:43:ILE:CD1	2.39	0.52
1:F:80:SER:HB2	1:F:85:ARG:HH21	1.72	0.52
1:B:9:LEU:O	1:B:10:THR:C	2.47	0.52
1:C:93:SER:OG	1:C:95:SER:OG	2.27	0.52
1:A:13:GLU:HA	1:A:118:ALA:HB1	1.92	0.52
1:B:139:HIS:H	1:B:139:HIS:CD2	2.27	0.52
1:B:35:ALA:CB	1:B:122:PHE:CZ	2.92	0.52
1:A:84:VAL:HG22	1:C:86:THR:HG21	1.90	0.52
1:A:80:SER:HB3	1:A:81:PHE:CD2	2.45	0.52
1:B:102:ASN:N	1:B:102:ASN:ND2	2.57	0.52
1:C:90:SER:O	1:C:94:ASN:HA	2.10	0.52
1:F:37:GLY:HA3	1:F:122:PHE:CE1	2.45	0.52
1:D:128:LEU:N	1:D:128:LEU:CD1	2.73	0.51
1:E:85:ARG:NH1	1:E:99:HIS:CE1	2.78	0.51
1:A:90:SER:O	1:A:94:ASN:CA	2.58	0.51
1:D:104:GLY:O	1:D:105:PRO:C	2.47	0.51
1:A:84:VAL:HG13	1:A:85:ARG:N	2.26	0.51
1:A:90:SER:O	1:A:94:ASN:N	2.43	0.51
1:F:28:ASN:HB2	1:F:117:SER:OG	2.10	0.51
1:B:10:THR:OG1	1:B:13:GLU:HB2	2.11	0.51
1:F:24:PRO:HB2	1:F:27:MET:HG3	1.92	0.51
1:D:93:SER:O	1:D:93:SER:OG	2.19	0.51
1:D:36:LYS:HA	1:D:51:SER:CB	2.41	0.50
1:D:30:TYR:HB2	1:D:117:SER:CB	2.41	0.50
1:E:29:GLU:HG2	1:E:30:TYR:N	2.26	0.50
1:E:80:SER:HB3	1:E:81:PHE:CD2	2.47	0.50
1:E:30:TYR:OH	1:E:121:GLN:NE2	2.44	0.50
1:B:15:ILE:HG22	1:B:21:GLY:HA3	1.94	0.50
1:C:105:PRO:HD2	1:C:108:SER:OG	2.11	0.50
1:D:114:CYS:O	1:D:114:CYS:SG	2.70	0.50
1:D:39:TYR:HB3	1:D:120:ILE:CG2	2.42	0.50
1:E:141:ASP:OD2	1:E:141:ASP:N	2.44	0.50
1:F:70:ASP:HA	1:F:73:ILE:HD13	1.93	0.50
1:C:49:PHE:CZ	1:C:67:ALA:HB2	2.44	0.50
1:A:125:TYR:HA	1:A:128:LEU:HD12	1.94	0.49
1:D:20:ASN:OD1	1:D:96:HIS:HB2	2.12	0.49
1:E:123:ILE:HD13	1:E:133:TYR:CE1	2.47	0.49
1:F:69:ASP:HB3	1:F:72:GLU:HG2	1.95	0.49
1:D:128:LEU:O	1:D:133:TYR:HB2	2.12	0.49
1:F:9:LEU:HB2	1:F:13:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:TYR:HA	1:F:33:HIS:HB3	1.95	0.49
1:A:44:SER:HB3	1:A:93:SER:HB3	1.94	0.49
1:C:20:ASN:HA	1:C:96:HIS:CD2	2.48	0.49
1:B:17:THR:HG22	1:B:95:SER:HB2	1.95	0.49
1:D:116:ASN:N	1:D:116:ASN:ND2	2.61	0.49
1:B:80:SER:HB3	1:B:81:PHE:CE1	2.48	0.49
1:F:137:ILE:O	1:F:139:HIS:N	2.46	0.49
1:C:93:SER:HG	1:C:95:SER:HG	1.57	0.48
1:D:20:ASN:CA	1:D:96:HIS:CD2	2.91	0.48
1:F:36:LYS:N	1:F:36:LYS:CD	2.73	0.48
1:F:45:GLY:O	1:F:133:TYR:OH	2.30	0.48
1:B:80:SER:HB3	1:B:81:PHE:CZ	2.48	0.48
1:C:4:LYS:HA	1:C:8:GLU:OE2	2.14	0.48
1:C:32:ASN:O	1:C:34:PHE:CE1	2.66	0.48
1:E:94:ASN:ND2	1:E:94:ASN:O	2.46	0.48
1:B:13:GLU:O	1:B:17:THR:OG1	2.28	0.48
1:B:3:LYS:HA	1:B:3:LYS:HE2	1.95	0.48
1:C:72:GLU:OE1	1:C:72:GLU:O	2.31	0.48
1:A:30:TYR:HA	1:A:33:HIS:HB3	1.96	0.48
1:D:118:ALA:C	1:D:120:ILE:N	2.67	0.47
1:B:46:LYS:NZ	1:B:72:GLU:CB	2.71	0.47
1:E:137:ILE:O	1:E:139:HIS:N	2.47	0.47
1:B:44:SER:HB3	1:B:93:SER:HB2	1.96	0.47
1:D:79:LYS:HA	1:D:83:MET:O	2.15	0.47
1:A:25:PRO:HD2	1:E:22:THR:HG21	1.96	0.47
1:B:3:LYS:O	1:B:5:ASP:N	2.48	0.47
1:C:33:HIS:NE2	1:C:35:ALA:HB3	2.30	0.47
1:E:67:ALA:CB	1:E:73:ILE:HD11	2.45	0.47
1:F:25:PRO:HB2	1:F:26:PHE:CD2	2.49	0.47
1:A:73:ILE:HA	1:A:91:GLU:OE2	2.14	0.47
1:B:37:GLY:C	1:B:140:PHE:HZ	2.18	0.47
1:B:23:GLU:OE1	1:B:117:SER:N	2.48	0.47
1:A:31:TRP:O	1:A:31:TRP:CE3	2.68	0.47
1:B:10:THR:O	1:B:11:ASP:HB2	2.14	0.47
1:B:11:ASP:O	1:B:14:TYR:N	2.47	0.47
1:C:89:ARG:HA	1:C:97:LEU:HG	1.97	0.47
1:B:28:ASN:OD1	1:B:61:TRP:HD1	1.98	0.47
1:E:30:TYR:HB2	1:E:117:SER:HB2	1.96	0.47
1:A:84:VAL:HG21	1:C:100:VAL:HG13	1.96	0.47
1:A:125:TYR:HA	1:A:128:LEU:CD1	2.46	0.46
1:A:78:ASP:OD1	1:A:80:SER:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:VAL:HG13	1:E:84:VAL:HG21	1.97	0.46
1:C:73:ILE:HA	1:C:73:ILE:HD13	1.62	0.46
1:F:33:HIS:CD2	1:F:39:TYR:HH	2.32	0.46
1:B:23:GLU:HG2	1:B:116:ASN:OD1	2.14	0.46
1:F:33:HIS:CD2	1:F:39:TYR:OH	2.68	0.46
1:E:78:ASP:OD1	1:E:80:SER:CB	2.64	0.46
1:F:13:GLU:CD	1:F:42:LYS:HE2	2.35	0.46
1:E:20:ASN:OD1	1:E:89:ARG:NH1	2.48	0.46
1:F:105:PRO:C	1:F:107:GLU:H	2.18	0.46
1:B:102:ASN:N	1:B:102:ASN:HD22	2.14	0.46
1:B:139:HIS:N	1:B:139:HIS:CD2	2.83	0.46
1:C:41:ASP:HB3	1:C:44:SER:OG	2.16	0.46
1:A:8:GLU:HG3	1:A:8:GLU:O	2.16	0.46
1:B:115:ILE:HD11	1:B:120:ILE:HG23	1.97	0.46
1:B:46:LYS:HZ1	1:B:72:GLU:CB	2.28	0.46
1:B:17:THR:CG2	1:B:95:SER:HB2	2.46	0.46
1:F:69:ASP:HB3	1:F:72:GLU:CG	2.46	0.46
1:B:5:ASP:CG	1:B:6:LYS:N	2.69	0.46
1:A:37:GLY:O	1:A:51:SER:HB3	2.15	0.46
1:B:37:GLY:O	1:B:140:PHE:CZ	2.68	0.45
1:C:89:ARG:HH11	1:C:94:ASN:HD21	1.54	0.45
1:A:41:ASP:HB2	1:A:48:LEU:HD11	1.97	0.45
1:B:66:LYS:HA	1:B:113:TYR:CD1	2.50	0.45
1:C:29:GLU:HG2	1:C:30:TYR:H	1.82	0.45
1:C:17:THR:CG2	1:C:95:SER:HB3	2.46	0.45
1:A:49:PHE:CD1	1:A:67:ALA:HA	2.51	0.45
1:B:35:ALA:HB3	1:B:122:PHE:CE1	2.50	0.45
1:C:38:ILE:HG12	1:C:123:ILE:HB	1.99	0.45
1:D:70:ASP:OD1	1:D:70:ASP:N	2.49	0.45
1:F:10:THR:CG2	1:F:12:ILE:HG22	2.46	0.45
1:A:135:ASP:O	1:A:137:ILE:N	2.49	0.45
1:B:31:TRP:CE3	1:B:31:TRP:O	2.69	0.45
1:E:49:PHE:HA	1:E:68:LEU:HB2	1.99	0.45
1:B:41:ASP:OD2	1:B:93:SER:CB	2.64	0.45
1:F:29:GLU:HG2	1:F:30:TYR:CE1	2.51	0.45
1:E:20:ASN:N	1:E:20:ASN:OD1	2.47	0.45
1:B:49:PHE:CE2	1:B:115:ILE:HD13	2.50	0.45
1:B:129:GLU:OE1	1:B:137:ILE:CD1	2.64	0.45
1:D:55:PHE:CZ	1:D:105:PRO:HD2	2.51	0.45
1:E:10:THR:OG1	1:E:12:ILE:HG22	2.15	0.45
1:D:31:TRP:CE3	1:D:31:TRP:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:LEU:HA	1:F:128:LEU:HD12	1.81	0.45
1:A:94:ASN:O	1:A:94:ASN:CG	2.55	0.44
1:C:9:LEU:HD21	1:C:43:ILE:HD11	1.99	0.44
1:E:57:SER:O	1:E:58:GLU:C	2.56	0.44
1:C:137:ILE:HG22	1:C:137:ILE:O	2.16	0.44
1:C:47:PRO:HG2	1:C:136:LEU:HD11	1.99	0.44
1:D:137:ILE:HD12	1:D:138:SER:N	2.33	0.44
1:E:88:VAL:CG1	1:E:98:GLY:H	2.30	0.44
1:A:84:VAL:O	1:A:85:ARG:CB	2.65	0.44
1:E:129:GLU:HG3	1:E:134:GLY:HA3	1.98	0.44
1:D:4:LYS:N	1:D:7:SER:HG	2.15	0.44
1:A:31:TRP:C	1:A:31:TRP:CD2	2.90	0.44
1:B:25:PRO:C	1:B:27:MET:N	2.71	0.44
1:C:61:TRP:O	1:C:62:PRO:C	2.56	0.44
1:E:50:THR:HG22	1:E:68:LEU:HD13	1.98	0.44
1:C:4:LYS:N	1:C:8:GLU:HB3	2.33	0.44
1:F:54:LYS:HA	1:F:63:SER:O	2.18	0.44
1:A:84:VAL:CG2	1:C:86:THR:HG21	2.47	0.44
1:D:49:PHE:CD1	1:D:67:ALA:HA	2.52	0.44
1:E:30:TYR:HD2	1:E:117:SER:HB2	1.82	0.44
1:E:46:LYS:HD2	1:E:92:GLU:CG	2.46	0.44
1:C:72:GLU:OE1	1:C:90:SER:HA	2.19	0.43
1:E:28:ASN:HB2	1:E:117:SER:OG	2.18	0.43
1:E:17:THR:HG23	1:E:119:ALA:HB2	2.00	0.43
1:F:100:VAL:HA	1:F:112:ARG:O	2.18	0.43
1:A:17:THR:HB	1:A:18:GLN:HE21	1.83	0.43
1:A:49:PHE:CE1	1:A:67:ALA:HA	2.53	0.43
1:B:139:HIS:H	1:B:139:HIS:HD2	1.66	0.43
1:E:78:ASP:HB2	1:E:87:GLU:CB	2.45	0.43
1:F:75:GLU:HA	1:F:87:GLU:O	2.19	0.43
1:B:43:ILE:HB	1:B:93:SER:OG	2.19	0.43
1:C:115:ILE:HG22	1:C:116:ASN:O	2.17	0.43
1:C:17:THR:HG22	1:C:95:SER:CB	2.46	0.43
1:B:33:HIS:CD2	1:B:122:PHE:CD1	3.07	0.43
1:B:66:LYS:O	1:B:68:LEU:N	2.51	0.43
1:E:54:LYS:HD2	1:E:64:PHE:CZ	2.53	0.43
1:E:78:ASP:OD1	1:E:80:SER:OG	2.35	0.43
1:F:54:LYS:HB2	1:F:64:PHE:CZ	2.54	0.43
1:B:33:HIS:CE1	1:B:35:ALA:CB	3.02	0.43
1:A:24:PRO:HB3	1:E:22:THR:O	2.19	0.43
1:C:23:GLU:OE1	1:C:116:ASN:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:SER:O	1:C:58:GLU:HB2	2.19	0.43
1:D:30:TYR:HB2	1:D:117:SER:HB3	2.01	0.43
1:C:26:PHE:HB3	1:D:81:PHE:CZ	2.54	0.43
1:E:62:PRO:HD2	1:E:115:ILE:O	2.19	0.42
1:F:17:THR:CB	1:F:95:SER:HB2	2.44	0.42
1:A:133:TYR:O	1:A:134:GLY:C	2.57	0.42
1:A:41:ASP:OD2	1:A:93:SER:CB	2.68	0.42
1:D:4:LYS:O	1:D:8:GLU:HB3	2.19	0.42
1:B:36:LYS:HD3	1:B:36:LYS:N	2.34	0.42
1:F:30:TYR:CD1	1:F:33:HIS:CD2	3.08	0.42
1:F:49:PHE:HB3	1:F:64:PHE:CD2	2.54	0.42
1:C:26:PHE:CE1	1:C:60:GLY:HA2	2.53	0.42
1:D:30:TYR:HB2	1:D:117:SER:HB2	1.99	0.42
1:D:69:ASP:HB3	1:D:72:GLU:CG	2.50	0.42
1:F:34:PHE:HA	1:F:54:LYS:HZ2	1.84	0.42
1:F:50:THR:HG23	1:F:53:GLU:CG	2.49	0.42
1:F:84:VAL:O	1:F:84:VAL:CG1	2.67	0.42
1:A:39:TYR:HB3	1:A:120:ILE:CG2	2.49	0.42
1:B:66:LYS:C	1:B:68:LEU:N	2.72	0.42
1:C:33:HIS:CD2	1:C:39:TYR:OH	2.69	0.42
1:A:39:TYR:HB3	1:A:120:ILE:HG21	2.01	0.42
1:A:47:PRO:HG2	1:A:136:LEU:HD11	2.02	0.42
1:B:23:GLU:HB2	1:B:24:PRO:HD2	2.02	0.42
1:B:28:ASN:N	1:B:28:ASN:ND2	2.63	0.42
1:C:104:GLY:H	1:C:110:GLY:C	2.23	0.42
1:C:33:HIS:CE1	1:C:35:ALA:HB3	2.54	0.42
1:E:40:VAL:HG13	1:E:123:ILE:HD12	2.02	0.42
1:A:49:PHE:HA	1:A:68:LEU:HB2	2.01	0.42
1:C:20:ASN:N	1:C:20:ASN:ND2	2.67	0.42
1:C:6:LYS:C	1:C:8:GLU:H	2.22	0.42
1:E:19:GLU:O	1:E:20:ASN:C	2.57	0.42
1:A:73:ILE:HD13	1:A:73:ILE:H	1.85	0.42
1:D:69:ASP:OD1	1:D:70:ASP:N	2.53	0.42
1:E:94:ASN:CG	1:E:94:ASN:O	2.57	0.42
1:C:5:ASP:O	1:C:9:LEU:N	2.44	0.42
1:C:89:ARG:CB	1:C:95:SER:O	2.68	0.42
1:B:68:LEU:C	1:B:68:LEU:CD1	2.85	0.42
1:C:19:GLU:C	1:C:20:ASN:HD22	2.23	0.42
1:E:79:LYS:CD	1:E:84:VAL:HG12	2.50	0.42
1:B:70:ASP:OD2	1:B:70:ASP:N	2.53	0.41
1:A:16:VAL:HG12	1:A:17:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLU:HA	1:B:53:GLU:OE2	2.19	0.41
1:C:44:SER:HB2	1:C:46:LYS:HB2	2.01	0.41
1:F:25:PRO:HB2	1:F:26:PHE:HD2	1.85	0.41
1:F:33:HIS:HE1	1:F:35:ALA:HB3	1.77	0.41
1:A:17:THR:HB	1:A:95:SER:HB2	2.03	0.41
1:B:33:HIS:NE2	1:B:35:ALA:HB3	2.35	0.41
1:E:33:HIS:NE2	1:E:35:ALA:HB3	2.35	0.41
1:F:39:TYR:CD2	1:F:122:PHE:HB2	2.56	0.41
1:A:87:GLU:OE2	1:A:89:ARG:NE	2.49	0.41
1:B:33:HIS:CE1	1:B:35:ALA:HB3	2.54	0.41
1:D:136:LEU:HA	1:D:136:LEU:HD12	1.96	0.41
1:B:101:PHE:CD2	1:B:112:ARG:NH2	2.88	0.41
1:F:16:VAL:HG13	1:F:116:ASN:ND2	2.36	0.41
1:A:28:ASN:ND2	1:A:117:SER:OG	2.44	0.41
1:B:77:VAL:HG12	1:B:78:ASP:N	2.35	0.41
1:C:139:HIS:CD2	1:C:139:HIS:N	2.86	0.41
1:F:37:GLY:HA3	1:F:123:ILE:O	2.20	0.41
1:B:70:ASP:HB2	1:B:71:ASP:H	1.45	0.41
1:E:48:LEU:O	1:E:49:PHE:CD2	2.73	0.41
1:F:9:LEU:HD13	1:F:9:LEU:N	2.36	0.41
1:A:32:ASN:O	1:A:34:PHE:HD1	2.04	0.41
1:B:32:ASN:HD21	1:B:56:HIS:CE1	2.39	0.41
1:B:68:LEU:HD12	1:B:68:LEU:O	2.21	0.41
1:C:37:GLY:HA3	1:C:123:ILE:O	2.21	0.41
1:C:66:LYS:O	1:C:66:LYS:HG3	2.20	0.41
1:D:36:LYS:HA	1:D:51:SER:OG	2.20	0.41
1:F:120:ILE:HG22	1:F:121:GLN:N	2.36	0.41
1:E:44:SER:OG	1:E:92:GLU:HG3	2.21	0.41
1:B:127:LYS:O	1:B:131:LEU:HD12	2.21	0.40
1:D:4:LYS:HG3	1:D:7:SER:OG	2.21	0.40
1:A:91:GLU:CD	1:A:91:GLU:H	2.22	0.40
1:B:34:PHE:HE2	1:B:55:PHE:HA	1.87	0.40
1:A:73:ILE:HD13	1:A:73:ILE:N	2.36	0.40
1:A:89:ARG:NH2	1:A:94:ASN:O	2.51	0.40
1:C:28:ASN:HD21	1:C:31:TRP:HB3	1.86	0.40
1:B:115:ILE:HD11	1:B:120:ILE:CG2	2.51	0.40
1:A:101:PHE:O	1:A:112:ARG:N	2.51	0.40
1:B:49:PHE:CD1	1:B:67:ALA:HA	2.56	0.40
1:B:44:SER:HB2	1:B:92:GLU:HG3	2.03	0.40
1:C:19:GLU:C	1:C:20:ASN:ND2	2.75	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	132/159 (83%)	101 (76%)	23 (17%)	8 (6%)	1	13
1	B	137/159 (86%)	103 (75%)	26 (19%)	8 (6%)	1	14
1	C	134/159 (84%)	92 (69%)	35 (26%)	7 (5%)	2	16
1	D	132/159 (83%)	99 (75%)	21 (16%)	12 (9%)	1	7
1	E	134/159 (84%)	99 (74%)	28 (21%)	7 (5%)	2	16
1	F	133/159 (84%)	107 (80%)	19 (14%)	7 (5%)	2	16
All	All	802/954 (84%)	601 (75%)	152 (19%)	49 (6%)	1	13

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	136	LEU
1	B	4	LYS
1	B	10	THR
1	B	11	ASP
1	B	68	LEU
1	B	71	ASP
1	D	28	ASN
1	D	29	GLU
1	D	125	TYR
1	D	134	GLY
1	D	135	ASP
1	E	135	ASP
1	E	138	SER
1	E	140	PHE
1	F	27	MET
1	F	138	SER
1	A	58	GLU
1	A	85	ARG
1	A	134	GLY

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Mol	Chain	Res	Type
1	B	12	ILE
1	B	92	GLU
1	C	72	GLU
1	C	93	SER
1	C	134	GLY
1	C	135	ASP
1	D	10	THR
1	D	94	ASN
1	D	119	ALA
1	D	139	HIS
1	E	33	HIS
1	F	45	GLY
1	F	110	GLY
1	A	129	GLU
1	C	58	GLU
1	F	6	LYS
1	F	33	HIS
1	C	103	ASP
1	D	15	ILE
1	D	80	SER
1	D	130	GLU
1	E	70	ASP
1	E	109	GLY
1	F	51	SER
1	A	114	CYS
1	A	72	GLU
1	C	16	VAL
1	E	16	VAL
1	B	45	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	119/141 (84%)	102 (86%)	17 (14%)	3	17
1	B	124/141 (88%)	100 (81%)	24 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	121/141 (86%)	100 (83%)	21 (17%)	2	10
1	D	121/141 (86%)	102 (84%)	19 (16%)	2	14
1	E	121/141 (86%)	92 (76%)	29 (24%)	0	3
1	F	120/141 (85%)	98 (82%)	22 (18%)	1	8
All	All	726/846 (86%)	594 (82%)	132 (18%)	1	8

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	ASP
1	A	14	TYR
1	A	27	MET
1	A	28	ASN
1	A	70	ASP
1	A	72	GLU
1	A	73	ILE
1	A	84	VAL
1	A	85	ARG
1	A	90	SER
1	A	91	GLU
1	A	116	ASN
1	A	120	ILE
1	A	128	LEU
1	A	138	SER
1	A	139	HIS
1	B	3	LYS
1	B	6	LYS
1	B	22	THR
1	B	28	ASN
1	B	50	THR
1	B	59	CYS
1	B	66	LYS
1	B	68	LEU
1	B	69	ASP
1	B	70	ASP
1	B	71	ASP
1	B	72	GLU
1	B	73	ILE
1	B	75	GLU
1	B	79	LYS

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Mol	Chain	Res	Type
1	B	81	PHE
1	B	91	GLU
1	B	102	ASN
1	B	108	SER
1	B	114	CYS
1	B	115	ILE
1	B	117	SER
1	B	135	ASP
1	B	136	LEU
1	C	7	SER
1	C	8	GLU
1	C	17	THR
1	C	20	ASN
1	C	31	TRP
1	C	50	THR
1	C	68	LEU
1	C	71	ASP
1	C	73	ILE
1	C	78	ASP
1	C	79	LYS
1	C	80	SER
1	C	88	VAL
1	C	89	ARG
1	C	94	ASN
1	C	95	SER
1	C	99	HIS
1	C	107	GLU
1	C	136	LEU
1	C	137	ILE
1	C	139	HIS
1	D	4	LYS
1	D	5	ASP
1	D	6	LYS
1	D	66	LYS
1	D	70	ASP
1	D	78	ASP
1	D	95	SER
1	D	97	LEU
1	D	102	ASN
1	D	106	LYS
1	D	114	CYS
1	D	116	ASN

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Mol	Chain	Res	Type
1	D	123	ILE
1	D	125	TYR
1	D	126	GLU
1	D	128	LEU
1	D	135	ASP
1	D	136	LEU
1	D	141	ASP
1	E	6	LYS
1	E	9	LEU
1	E	10	THR
1	E	11	ASP
1	E	14	TYR
1	E	17	THR
1	E	34	PHE
1	E	44	SER
1	E	50	THR
1	E	52	GLU
1	E	53	GLU
1	E	56	HIS
1	E	59	CYS
1	E	65	SER
1	E	66	LYS
1	E	69	ASP
1	E	72	GLU
1	E	73	ILE
1	E	83	MET
1	E	85	ARG
1	E	87	GLU
1	E	92	GLU
1	E	94	ASN
1	E	108	SER
1	E	120	ILE
1	E	129	GLU
1	E	131	LEU
1	E	138	SER
1	E	141	ASP
1	F	6	LYS
1	F	9	LEU
1	F	10	THR
1	F	29	GLU
1	F	31	TRP
1	F	36	LYS

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Mol	Chain	Res	Type
1	F	38	ILE
1	F	40	VAL
1	F	50	THR
1	F	53	GLU
1	F	56	HIS
1	F	70	ASP
1	F	71	ASP
1	F	73	ILE
1	F	76	LEU
1	F	84	VAL
1	F	103	ASP
1	F	115	ILE
1	F	126	GLU
1	F	128	LEU
1	F	129	GLU
1	F	139	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	28	ASN
1	A	33	HIS
1	A	94	ASN
1	A	102	ASN
1	B	28	ASN
1	B	32	ASN
1	B	56	HIS
1	B	94	ASN
1	B	139	HIS
1	C	20	ASN
1	C	28	ASN
1	C	33	HIS
1	C	56	HIS
1	C	94	ASN
1	C	121	GLN
1	C	139	HIS
1	D	96	HIS
1	D	99	HIS
1	D	116	ASN
1	E	33	HIS
1	E	94	ASN

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Mol	Chain	Res	Type
1	E	121	GLN
1	F	33	HIS
1	F	94	ASN
1	F	116	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	134/159 (84%)	0.72	14 (10%) 6 8	71, 115, 152, 187	0
1	B	139/159 (87%)	0.33	5 (3%) 42 40	64, 97, 141, 178	0
1	C	136/159 (85%)	0.56	11 (8%) 12 14	71, 107, 145, 173	0
1	D	136/159 (85%)	0.47	9 (6%) 18 18	70, 129, 177, 236	0
1	E	136/159 (85%)	0.54	12 (8%) 10 12	80, 137, 173, 187	0
1	F	135/159 (84%)	0.62	15 (11%) 5 7	79, 126, 171, 205	0
All	All	816/954 (85%)	0.54	66 (8%) 12 14	64, 116, 169, 236	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	115	ILE	4.5
1	A	43	ILE	4.4
1	C	120	ILE	4.4
1	F	118	ALA	4.3
1	F	97	LEU	4.2
1	F	119	ALA	4.0
1	F	116	ASN	4.0
1	F	57	SER	3.7
1	E	131	LEU	3.6
1	A	63	SER	3.6
1	C	28	ASN	3.4
1	E	56	HIS	3.3
1	C	58	GLU	3.3
1	B	31	TRP	3.2
1	C	97	LEU	3.1
1	D	57	SER	3.0
1	E	43	ILE	2.9
1	A	8	GLU	2.9
1	E	115	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	127	LYS	2.8
1	F	58	GLU	2.8
1	F	68	LEU	2.8
1	F	55	PHE	2.8
1	C	116	ASN	2.7
1	E	47	PRO	2.7
1	E	95	SER	2.7
1	C	31	TRP	2.7
1	E	119	ALA	2.7
1	C	115	ILE	2.7
1	D	55	PHE	2.6
1	D	62	PRO	2.6
1	C	113	TYR	2.6
1	A	115	ILE	2.6
1	F	64	PHE	2.5
1	D	47	PRO	2.5
1	A	126	GLU	2.5
1	A	113	TYR	2.5
1	B	63	SER	2.5
1	A	12	ILE	2.5
1	E	96	HIS	2.4
1	B	97	LEU	2.4
1	C	30	TYR	2.4
1	A	64	PHE	2.4
1	E	120	ILE	2.4
1	F	49	PHE	2.3
1	E	97	LEU	2.3
1	F	130	GLU	2.3
1	B	115	ILE	2.3
1	B	57	SER	2.3
1	A	22	THR	2.2
1	E	49	PHE	2.2
1	A	116	ASN	2.2
1	A	31	TRP	2.2
1	D	74	ILE	2.2
1	A	96	HIS	2.2
1	F	71	ASP	2.1
1	C	119	ALA	2.1
1	D	25	PRO	2.1
1	D	115	ILE	2.1
1	D	34	PHE	2.1
1	D	48	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	26	PHE	2.1
1	F	98	GLY	2.0
1	F	88	VAL	2.0
1	C	7	SER	2.0
1	E	113	TYR	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.