Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:13 pm BST

PDB ID	:	5EPT
Title	:	Crystal Structure of S. cerevisiae TSA2 in the disulfide state
Authors	:	Nielsen, M.H.; Kidmose, R.T.; Jenner, L.B.
Deposited on	:	2015-11-12
Resolution	:	5.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

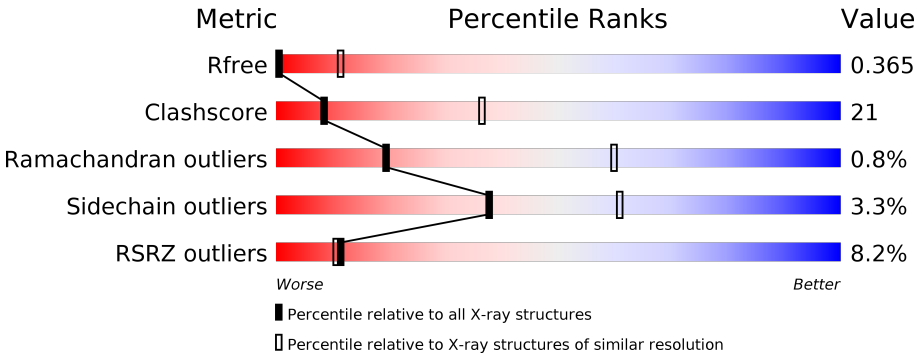
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 5.00 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	1140 (6.20-3.80)
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RSRZ outliers	127900	1010 (6.22-3.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	217	12% 46% 31% • • 19%
1	B	217	8% 52% 24% • 20%
1	C	217	7% 57% 21% 21%
1	D	217	9% 51% 25% • • 22%
1	E	217	7% 50% 30% • 18%
1	F	217	6% 46% 30% • • 22%

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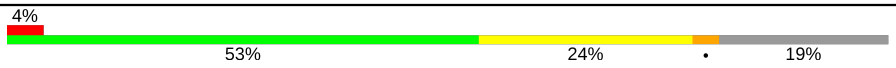
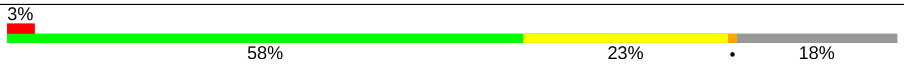
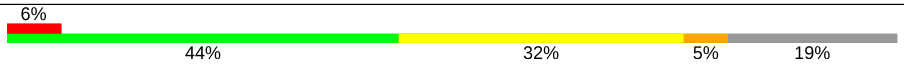
Mol	Chain	Length	Quality of chain
1	G	217	
1	H	217	
1	I	217	
1	J	217	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13616 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 Peroxiredoxin TSA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	178	Total	C	N	O	S	0	0	0
			1394	906	230	255	3			
1	B	173	Total	C	N	O	S	0	0	0
			1342	869	223	247	3			
1	C	172	Total	C	N	O	S	0	0	0
			1344	873	222	247	2			
1	A	175	Total	C	N	O	S	0	0	0
			1365	887	225	250	3			
1	G	175	Total	C	N	O	S	0	0	0
			1365	887	225	250	3			
1	I	177	Total	C	N	O	S	0	0	0
			1387	902	229	253	3			
1	D	170	Total	C	N	O	S	0	0	0
			1330	864	220	244	2			
1	E	178	Total	C	N	O	S	0	0	0
			1394	906	230	255	3			
1	J	175	Total	C	N	O	S	0	0	0
			1365	887	225	250	3			
1	F	170	Total	C	N	O	S	0	0	0
			1330	864	220	244	2			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-20	MET	-	initiating methionine	UNP Q04120
H	-19	ALA	-	expression tag	UNP Q04120
H	-18	HIS	-	expression tag	UNP Q04120
H	-17	HIS	-	expression tag	UNP Q04120
H	-16	HIS	-	expression tag	UNP Q04120
H	-15	HIS	-	expression tag	UNP Q04120
H	-14	HIS	-	expression tag	UNP Q04120
H	-13	HIS	-	expression tag	UNP Q04120
H	-12	VAL	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	ASP	-	expression tag	UNP Q04120
H	-10	ASP	-	expression tag	UNP Q04120
H	-9	ASP	-	expression tag	UNP Q04120
H	-8	ASP	-	expression tag	UNP Q04120
H	-7	LYS	-	expression tag	UNP Q04120
H	-6	GLU	-	expression tag	UNP Q04120
H	-5	ASN	-	expression tag	UNP Q04120
H	-4	LEU	-	expression tag	UNP Q04120
H	-3	TYR	-	expression tag	UNP Q04120
H	-2	PHE	-	expression tag	UNP Q04120
H	-1	GLN	-	expression tag	UNP Q04120
H	0	GLY	-	expression tag	UNP Q04120
B	-20	MET	-	initiating methionine	UNP Q04120
B	-19	ALA	-	expression tag	UNP Q04120
B	-18	HIS	-	expression tag	UNP Q04120
B	-17	HIS	-	expression tag	UNP Q04120
B	-16	HIS	-	expression tag	UNP Q04120
B	-15	HIS	-	expression tag	UNP Q04120
B	-14	HIS	-	expression tag	UNP Q04120
B	-13	HIS	-	expression tag	UNP Q04120
B	-12	VAL	-	expression tag	UNP Q04120
B	-11	ASP	-	expression tag	UNP Q04120
B	-10	ASP	-	expression tag	UNP Q04120
B	-9	ASP	-	expression tag	UNP Q04120
B	-8	ASP	-	expression tag	UNP Q04120
B	-7	LYS	-	expression tag	UNP Q04120
B	-6	GLU	-	expression tag	UNP Q04120
B	-5	ASN	-	expression tag	UNP Q04120
B	-4	LEU	-	expression tag	UNP Q04120
B	-3	TYR	-	expression tag	UNP Q04120
B	-2	PHE	-	expression tag	UNP Q04120
B	-1	GLN	-	expression tag	UNP Q04120
B	0	GLY	-	expression tag	UNP Q04120
C	-20	MET	-	initiating methionine	UNP Q04120
C	-19	ALA	-	expression tag	UNP Q04120
C	-18	HIS	-	expression tag	UNP Q04120
C	-17	HIS	-	expression tag	UNP Q04120
C	-16	HIS	-	expression tag	UNP Q04120
C	-15	HIS	-	expression tag	UNP Q04120
C	-14	HIS	-	expression tag	UNP Q04120
C	-13	HIS	-	expression tag	UNP Q04120
C	-12	VAL	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	ASP	-	expression tag	UNP Q04120
C	-10	ASP	-	expression tag	UNP Q04120
C	-9	ASP	-	expression tag	UNP Q04120
C	-8	ASP	-	expression tag	UNP Q04120
C	-7	LYS	-	expression tag	UNP Q04120
C	-6	GLU	-	expression tag	UNP Q04120
C	-5	ASN	-	expression tag	UNP Q04120
C	-4	LEU	-	expression tag	UNP Q04120
C	-3	TYR	-	expression tag	UNP Q04120
C	-2	PHE	-	expression tag	UNP Q04120
C	-1	GLN	-	expression tag	UNP Q04120
C	0	GLY	-	expression tag	UNP Q04120
A	-20	MET	-	initiating methionine	UNP Q04120
A	-19	ALA	-	expression tag	UNP Q04120
A	-18	HIS	-	expression tag	UNP Q04120
A	-17	HIS	-	expression tag	UNP Q04120
A	-16	HIS	-	expression tag	UNP Q04120
A	-15	HIS	-	expression tag	UNP Q04120
A	-14	HIS	-	expression tag	UNP Q04120
A	-13	HIS	-	expression tag	UNP Q04120
A	-12	VAL	-	expression tag	UNP Q04120
A	-11	ASP	-	expression tag	UNP Q04120
A	-10	ASP	-	expression tag	UNP Q04120
A	-9	ASP	-	expression tag	UNP Q04120
A	-8	ASP	-	expression tag	UNP Q04120
A	-7	LYS	-	expression tag	UNP Q04120
A	-6	GLU	-	expression tag	UNP Q04120
A	-5	ASN	-	expression tag	UNP Q04120
A	-4	LEU	-	expression tag	UNP Q04120
A	-3	TYR	-	expression tag	UNP Q04120
A	-2	PHE	-	expression tag	UNP Q04120
A	-1	GLN	-	expression tag	UNP Q04120
A	0	GLY	-	expression tag	UNP Q04120
G	-20	MET	-	initiating methionine	UNP Q04120
G	-19	ALA	-	expression tag	UNP Q04120
G	-18	HIS	-	expression tag	UNP Q04120
G	-17	HIS	-	expression tag	UNP Q04120
G	-16	HIS	-	expression tag	UNP Q04120
G	-15	HIS	-	expression tag	UNP Q04120
G	-14	HIS	-	expression tag	UNP Q04120
G	-13	HIS	-	expression tag	UNP Q04120
G	-12	VAL	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-11	ASP	-	expression tag	UNP Q04120
G	-10	ASP	-	expression tag	UNP Q04120
G	-9	ASP	-	expression tag	UNP Q04120
G	-8	ASP	-	expression tag	UNP Q04120
G	-7	LYS	-	expression tag	UNP Q04120
G	-6	GLU	-	expression tag	UNP Q04120
G	-5	ASN	-	expression tag	UNP Q04120
G	-4	LEU	-	expression tag	UNP Q04120
G	-3	TYR	-	expression tag	UNP Q04120
G	-2	PHE	-	expression tag	UNP Q04120
G	-1	GLN	-	expression tag	UNP Q04120
G	0	GLY	-	expression tag	UNP Q04120
I	-20	MET	-	initiating methionine	UNP Q04120
I	-19	ALA	-	expression tag	UNP Q04120
I	-18	HIS	-	expression tag	UNP Q04120
I	-17	HIS	-	expression tag	UNP Q04120
I	-16	HIS	-	expression tag	UNP Q04120
I	-15	HIS	-	expression tag	UNP Q04120
I	-14	HIS	-	expression tag	UNP Q04120
I	-13	HIS	-	expression tag	UNP Q04120
I	-12	VAL	-	expression tag	UNP Q04120
I	-11	ASP	-	expression tag	UNP Q04120
I	-10	ASP	-	expression tag	UNP Q04120
I	-9	ASP	-	expression tag	UNP Q04120
I	-8	ASP	-	expression tag	UNP Q04120
I	-7	LYS	-	expression tag	UNP Q04120
I	-6	GLU	-	expression tag	UNP Q04120
I	-5	ASN	-	expression tag	UNP Q04120
I	-4	LEU	-	expression tag	UNP Q04120
I	-3	TYR	-	expression tag	UNP Q04120
I	-2	PHE	-	expression tag	UNP Q04120
I	-1	GLN	-	expression tag	UNP Q04120
I	0	GLY	-	expression tag	UNP Q04120
D	-20	MET	-	initiating methionine	UNP Q04120
D	-19	ALA	-	expression tag	UNP Q04120
D	-18	HIS	-	expression tag	UNP Q04120
D	-17	HIS	-	expression tag	UNP Q04120
D	-16	HIS	-	expression tag	UNP Q04120
D	-15	HIS	-	expression tag	UNP Q04120
D	-14	HIS	-	expression tag	UNP Q04120
D	-13	HIS	-	expression tag	UNP Q04120
D	-12	VAL	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	ASP	-	expression tag	UNP Q04120
D	-10	ASP	-	expression tag	UNP Q04120
D	-9	ASP	-	expression tag	UNP Q04120
D	-8	ASP	-	expression tag	UNP Q04120
D	-7	LYS	-	expression tag	UNP Q04120
D	-6	GLU	-	expression tag	UNP Q04120
D	-5	ASN	-	expression tag	UNP Q04120
D	-4	LEU	-	expression tag	UNP Q04120
D	-3	TYR	-	expression tag	UNP Q04120
D	-2	PHE	-	expression tag	UNP Q04120
D	-1	GLN	-	expression tag	UNP Q04120
D	0	GLY	-	expression tag	UNP Q04120
E	-20	MET	-	initiating methionine	UNP Q04120
E	-19	ALA	-	expression tag	UNP Q04120
E	-18	HIS	-	expression tag	UNP Q04120
E	-17	HIS	-	expression tag	UNP Q04120
E	-16	HIS	-	expression tag	UNP Q04120
E	-15	HIS	-	expression tag	UNP Q04120
E	-14	HIS	-	expression tag	UNP Q04120
E	-13	HIS	-	expression tag	UNP Q04120
E	-12	VAL	-	expression tag	UNP Q04120
E	-11	ASP	-	expression tag	UNP Q04120
E	-10	ASP	-	expression tag	UNP Q04120
E	-9	ASP	-	expression tag	UNP Q04120
E	-8	ASP	-	expression tag	UNP Q04120
E	-7	LYS	-	expression tag	UNP Q04120
E	-6	GLU	-	expression tag	UNP Q04120
E	-5	ASN	-	expression tag	UNP Q04120
E	-4	LEU	-	expression tag	UNP Q04120
E	-3	TYR	-	expression tag	UNP Q04120
E	-2	PHE	-	expression tag	UNP Q04120
E	-1	GLN	-	expression tag	UNP Q04120
E	0	GLY	-	expression tag	UNP Q04120
J	-20	MET	-	initiating methionine	UNP Q04120
J	-19	ALA	-	expression tag	UNP Q04120
J	-18	HIS	-	expression tag	UNP Q04120
J	-17	HIS	-	expression tag	UNP Q04120
J	-16	HIS	-	expression tag	UNP Q04120
J	-15	HIS	-	expression tag	UNP Q04120
J	-14	HIS	-	expression tag	UNP Q04120
J	-13	HIS	-	expression tag	UNP Q04120
J	-12	VAL	-	expression tag	UNP Q04120

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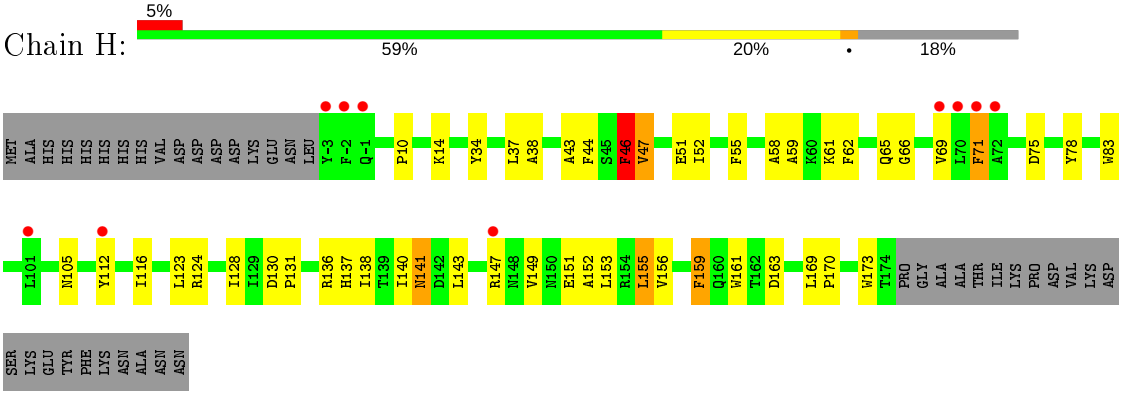
Chain	Residue	Modelled	Actual	Comment	Reference
J	-11	ASP	-	expression tag	UNP Q04120
J	-10	ASP	-	expression tag	UNP Q04120
J	-9	ASP	-	expression tag	UNP Q04120
J	-8	ASP	-	expression tag	UNP Q04120
J	-7	LYS	-	expression tag	UNP Q04120
J	-6	GLU	-	expression tag	UNP Q04120
J	-5	ASN	-	expression tag	UNP Q04120
J	-4	LEU	-	expression tag	UNP Q04120
J	-3	TYR	-	expression tag	UNP Q04120
J	-2	PHE	-	expression tag	UNP Q04120
J	-1	GLN	-	expression tag	UNP Q04120
J	0	GLY	-	expression tag	UNP Q04120
F	-20	MET	-	initiating methionine	UNP Q04120
F	-19	ALA	-	expression tag	UNP Q04120
F	-18	HIS	-	expression tag	UNP Q04120
F	-17	HIS	-	expression tag	UNP Q04120
F	-16	HIS	-	expression tag	UNP Q04120
F	-15	HIS	-	expression tag	UNP Q04120
F	-14	HIS	-	expression tag	UNP Q04120
F	-13	HIS	-	expression tag	UNP Q04120
F	-12	VAL	-	expression tag	UNP Q04120
F	-11	ASP	-	expression tag	UNP Q04120
F	-10	ASP	-	expression tag	UNP Q04120
F	-9	ASP	-	expression tag	UNP Q04120
F	-8	ASP	-	expression tag	UNP Q04120
F	-7	LYS	-	expression tag	UNP Q04120
F	-6	GLU	-	expression tag	UNP Q04120
F	-5	ASN	-	expression tag	UNP Q04120
F	-4	LEU	-	expression tag	UNP Q04120
F	-3	TYR	-	expression tag	UNP Q04120
F	-2	PHE	-	expression tag	UNP Q04120
F	-1	GLN	-	expression tag	UNP Q04120
F	0	GLY	-	expression tag	UNP Q04120

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

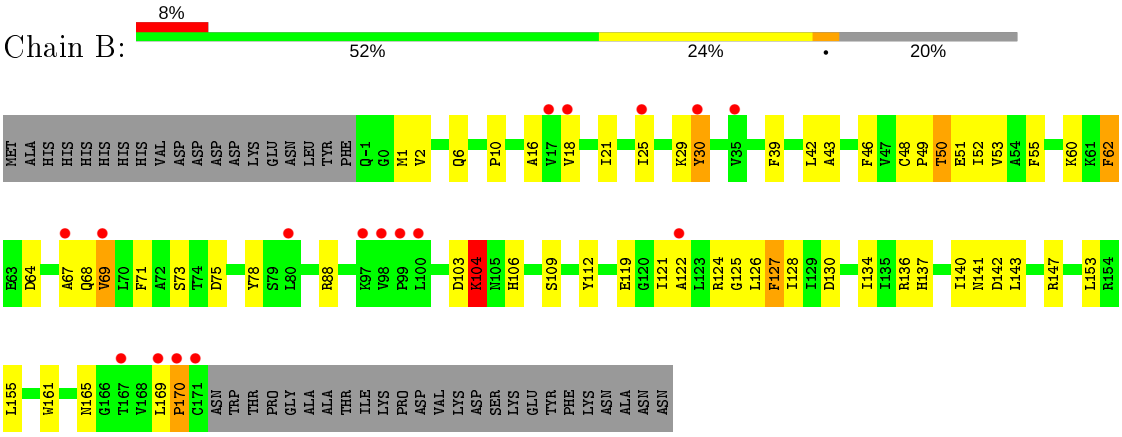
- Molecule 1: Peroxiredoxin TSA2

Chain H:



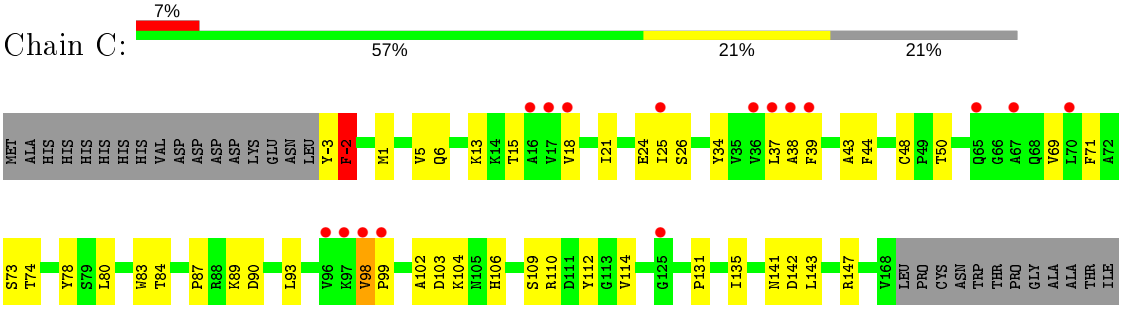
- Molecule 1: Peroxiredoxin TSA2

Chain B:

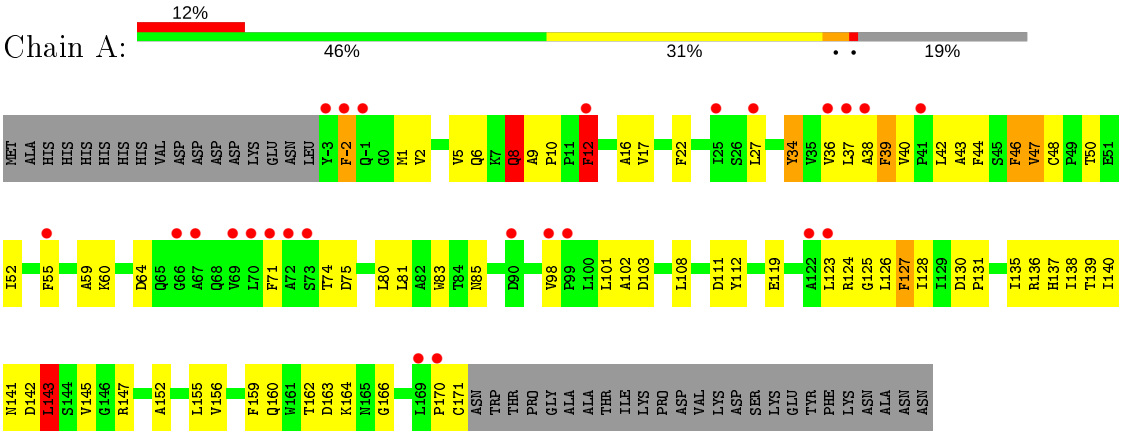


- Molecule 1: Peroxiredoxin TSA2

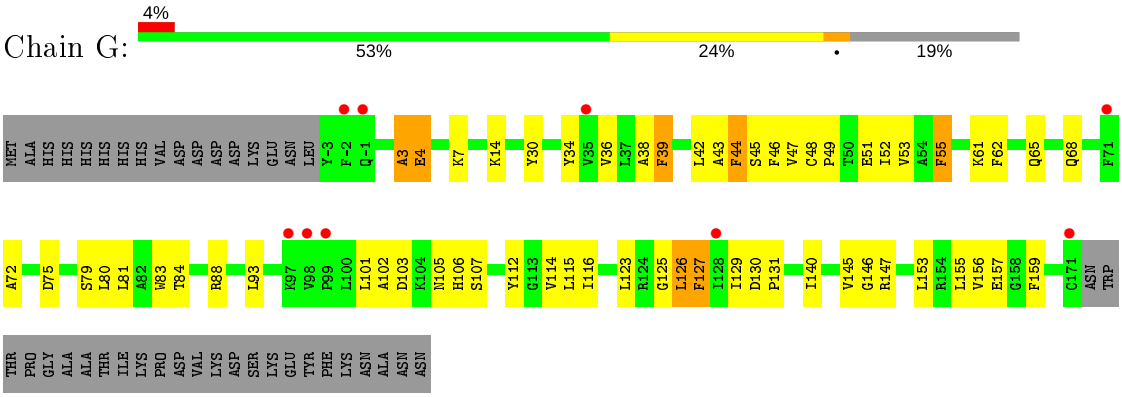
Chain C:



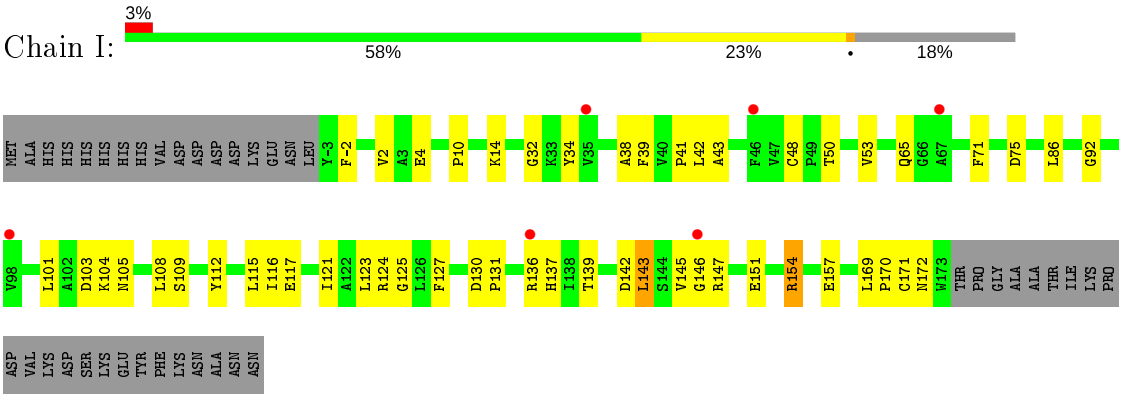
• Molecule 1: Peroxiredoxin TSA2



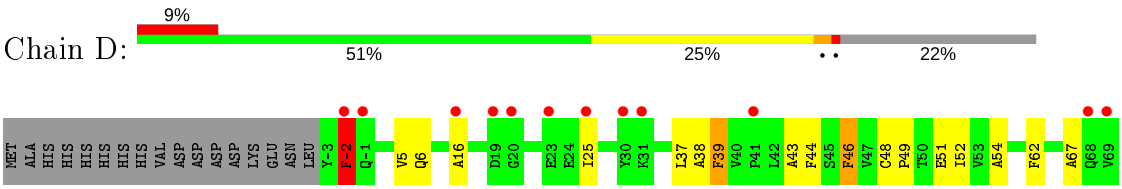
• Molecule 1: Peroxiredoxin TSA2

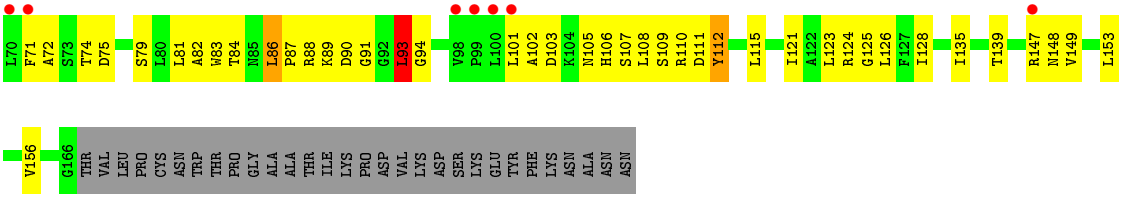


• Molecule 1: Peroxiredoxin TSA2



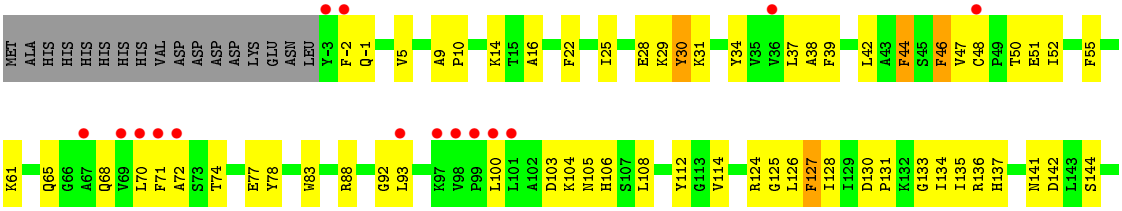
• Molecule 1: Peroxiredoxin TSA2

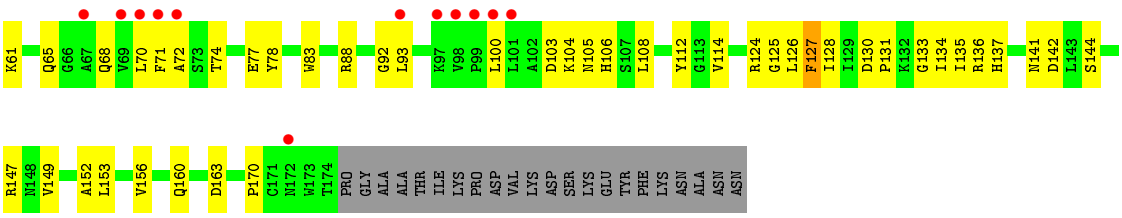




• Molecule 1: Peroxiredoxin TSA2

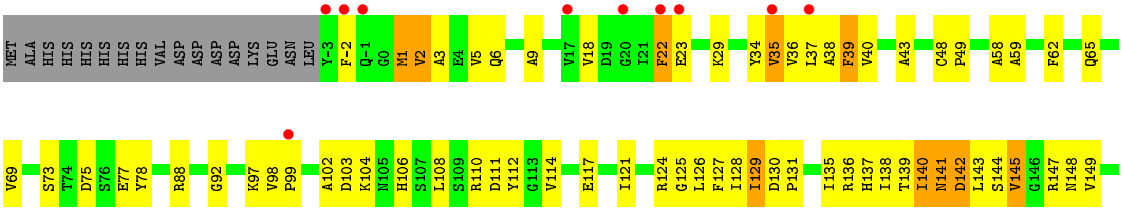
Chain E:

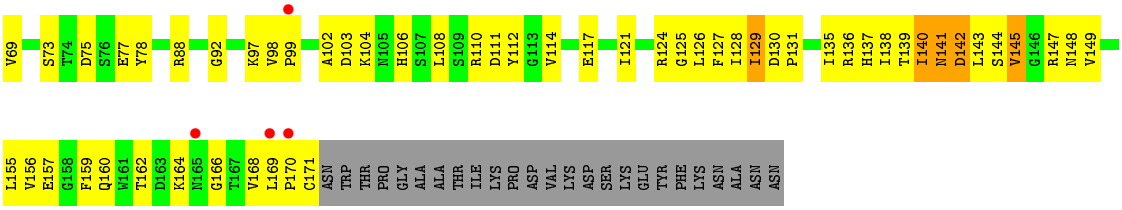




• Molecule 1: Peroxiredoxin TSA2

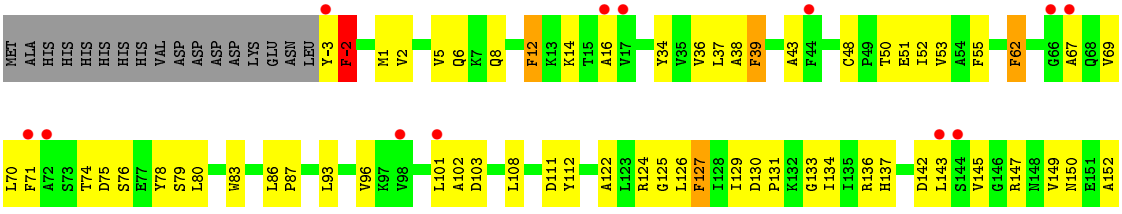
Chain J:

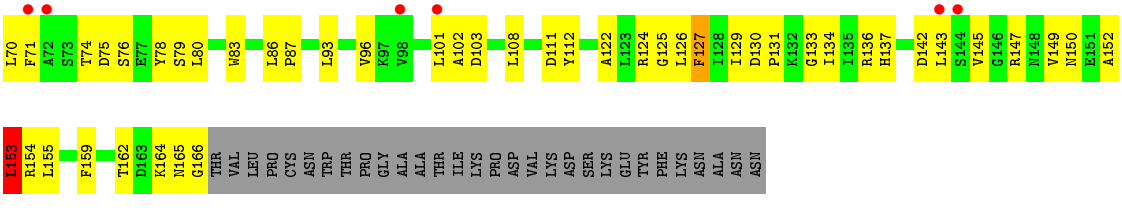




• Molecule 1: Peroxiredoxin TSA2

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.46Å 167.21Å 221.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.35 – 5.00 46.35 – 4.02	Depositor EDS
% Data completeness (in resolution range)	83.2 (46.35-5.00) 47.4 (46.35-4.02)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.64 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.274 , 0.375 0.276 , 0.365	Depositor DCC
R_{free} test set	1348 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	132.4	Xtriage
Anisotropy	1.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 317.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13616	wwPDB-VP
Average B, all atoms (Å^2)	350.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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	0.36	1/1395 (0.1%)	0.74	3/1890 (0.2%)
1	B	0.34	0/1370	0.61	0/1856
1	C	0.31	0/1373	0.64	1/1859 (0.1%)
1	D	0.33	0/1359	0.69	4/1839 (0.2%)
1	E	0.34	0/1426	0.75	2/1934 (0.1%)
1	F	0.30	0/1359	0.69	3/1839 (0.2%)
1	G	0.34	0/1395	0.61	0/1890
1	H	0.31	0/1426	0.66	2/1934 (0.1%)
1	I	0.32	0/1419	0.62	0/1924
1	J	0.31	0/1395	0.68	1/1890 (0.1%)
All	All	0.33	1/13917 (0.0%)	0.67	16/18855 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	I	0	1
1	J	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	GLN	CD-OE1	5.29	1.35	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	46	PHE	CB-CG-CD2	-8.20	115.06	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	46	PHE	CB-CG-CD2	-7.72	115.39	120.80
1	H	46	PHE	CB-CG-CD1	7.69	126.18	120.80
1	D	93	LEU	CB-CG-CD1	-6.61	99.77	111.00
1	F	-2	PHE	CB-CG-CD1	6.56	125.39	120.80
1	D	86	LEU	CA-CB-CG	6.55	130.36	115.30
1	E	46	PHE	CB-CG-CD1	6.48	125.33	120.80
1	D	-2	PHE	CB-CG-CD2	-6.45	116.29	120.80
1	D	-2	PHE	CB-CG-CD1	6.43	125.30	120.80
1	A	12	PHE	CB-CG-CD1	6.03	125.02	120.80
1	A	12	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	F	-2	PHE	CB-CG-CD2	-5.80	116.74	120.80
1	F	153	LEU	CA-CB-CG	5.51	127.97	115.30
1	C	-2	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	A	143	LEU	CA-CB-CG	5.17	127.19	115.30
1	J	1	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	GLN	Sidechain
1	B	50	THR	Peptide
1	I	-2	PHE	Peptide
1	J	140	ILE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1365	0	1388	77	0
1	B	1342	0	1370	61	0
1	C	1344	0	1367	35	0
1	D	1330	0	1351	65	0
1	E	1394	0	1412	67	0
1	F	1330	0	1350	72	0
1	G	1365	0	1388	70	0
1	H	1394	0	1411	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1387	0	1404	52	0
1	J	1365	0	1388	77	0
All	All	13616	0	13829	571	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 21.

All (571) 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:B:125:GLY:O	1:B:147:ARG:NH1	1.94	1.01
1:B:169:LEU:O	1:B:170:PRO:O	1.76	1.01
1:G:46:PHE:HE2	1:F:78:TYR:CE1	1.78	1.01
1:H:170:PRO:C	1:G:48:CYS:SG	2.41	1.00
1:D:86:LEU:HG	1:D:91:GLY:HA2	1.41	0.99
1:B:50:THR:N	1:A:171:CYS:SG	2.36	0.98
1:I:151:GLU:OE1	1:I:154:ARG:NH2	1.97	0.97
1:H:170:PRO:O	1:G:48:CYS:SG	2.23	0.95
1:G:53:VAL:HG21	1:G:88:ARG:CZ	2.00	0.91
1:I:125:GLY:O	1:I:147:ARG:NH1	2.04	0.91
1:G:46:PHE:HE2	1:F:78:TYR:HE1	1.12	0.90
1:G:51:GLU:OE2	1:G:146:GLY:HA3	1.71	0.90
1:D:43:ALA:N	1:D:75:ASP:OD2	2.07	0.88
1:I:39:PHE:O	1:I:147:ARG:NH2	2.06	0.87
1:J:125:GLY:O	1:J:147:ARG:NH1	2.07	0.87
1:G:46:PHE:CE2	1:F:78:TYR:CE1	2.65	0.85
1:E:14:LYS:NZ	1:E:105:ASN:OD1	2.11	0.83
1:G:46:PHE:CE2	1:F:78:TYR:HE1	1.97	0.82
1:B:51:GLU:HG2	1:A:171:CYS:HA	1.64	0.78
1:D:51:GLU:OE1	1:D:124:ARG:NH1	2.16	0.78
1:D:87:PRO:O	1:D:91:GLY:N	2.17	0.78
1:B:39:PHE:O	1:B:147:ARG:NH2	2.19	0.76
1:H:46:PHE:HD1	1:H:46:PHE:H	1.34	0.75
1:G:103:ASP:OD2	1:G:107:SER:N	2.21	0.74
1:H:14:LYS:NZ	1:H:105:ASN:OD1	2.20	0.73
1:H:51:GLU:OE2	1:H:124:ARG:NH1	2.21	0.73
1:B:1:MET:SD	1:B:10:PRO:HB3	2.29	0.73
1:J:65:GLN:NE2	1:J:157:GLU:OE2	2.22	0.73
1:G:61:LYS:O	1:G:65:GLN:NE2	2.23	0.72
1:D:16:ALA:HB3	1:D:25:ILE:HD13	1.70	0.72
1:E:130:ASP:OD1	1:E:134:ILE:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ASP:OD2	1:D:108:LEU:N	2.23	0.71
1:G:44:PHE:CD2	1:F:79:SER:HA	2.26	0.69
1:D:106:HIS:NE2	1:E:104:LYS:O	2.26	0.69
1:A:34:TYR:CE1	1:A:131:PRO:HD3	2.28	0.68
1:H:170:PRO:HB2	1:G:48:CYS:SG	2.33	0.68
1:B:50:THR:OG1	1:A:171:CYS:SG	2.52	0.68
1:H:43:ALA:N	1:H:75:ASP:OD2	2.26	0.67
1:D:81:LEU:O	1:D:84:THR:OG1	2.10	0.65
1:E:125:GLY:O	1:E:147:ARG:NH1	2.28	0.65
1:G:47:VAL:HG21	1:G:52:ILE:HG21	1.78	0.65
1:J:103:ASP:OD2	1:J:108:LEU:N	2.30	0.65
1:F:-2:PHE:CD1	1:F:1:MET:HB3	2.32	0.64
1:F:150:ASN:O	1:F:154:ARG:HB2	1.98	0.64
1:E:141:ASN:OD1	1:F:137:HIS:ND1	2.31	0.64
1:A:125:GLY:O	1:A:147:ARG:NH2	2.31	0.64
1:B:51:GLU:N	1:A:171:CYS:SG	2.71	0.64
1:D:83:TRP:O	1:D:93:LEU:HD11	1.98	0.64
1:D:93:LEU:HD12	1:D:94:GLY:N	2.12	0.64
1:E:34:TYR:CE1	1:E:131:PRO:HD3	2.32	0.63
1:E:88:ARG:HA	1:E:92:GLY:O	1.99	0.63
1:G:55:PHE:CE1	1:G:147:ARG:HB2	2.33	0.63
1:B:141:ASN:OD1	1:A:137:HIS:ND1	2.31	0.62
1:I:48:CYS:HB3	1:J:171:CYS:H	1.64	0.62
1:B:43:ALA:N	1:B:75:ASP:OD2	2.32	0.62
1:G:42:LEU:HB2	1:G:45:SER:HB3	1.80	0.62
1:I:142:ASP:OD1	1:J:6:GLN:NE2	2.32	0.62
1:H:62:PHE:O	1:H:66:GLY:N	2.33	0.61
1:J:6:GLN:N	1:J:135:ILE:O	2.33	0.61
1:A:142:ASP:OD1	1:A:143:LEU:HD23	2.01	0.61
1:B:103:ASP:OD2	1:B:109:SER:N	2.26	0.61
1:E:46:PHE:O	1:E:46:PHE:CD1	2.53	0.60
1:I:123:LEU:HD22	1:I:143:LEU:HD21	1.83	0.60
1:A:160:GLN:O	1:A:164:LYS:NZ	2.35	0.60
1:F:164:LYS:O	1:F:166:GLY:N	2.34	0.60
1:A:103:ASP:OD2	1:A:108:LEU:N	2.35	0.59
1:I:123:LEU:HD11	1:J:5:VAL:HG11	1.84	0.59
1:B:50:THR:OG1	1:A:171:CYS:CB	2.50	0.59
1:D:93:LEU:HD12	1:D:94:GLY:H	1.67	0.59
1:A:48:CYS:O	1:A:50:THR:N	2.35	0.59
1:G:53:VAL:HG21	1:G:88:ARG:NH1	2.18	0.59
1:D:46:PHE:N	1:D:46:PHE:CD1	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:-2:PHE:H	1:F:-2:PHE:HD1	1.51	0.58
1:D:84:THR:HA	1:D:93:LEU:HD11	1.86	0.58
1:F:34:TYR:CD1	1:F:131:PRO:HD3	2.38	0.58
1:J:130:ASP:HB3	1:J:136:ARG:NH2	2.18	0.58
1:D:83:TRP:C	1:D:93:LEU:HD11	2.24	0.58
1:A:162:THR:O	1:A:166:GLY:N	2.35	0.57
1:G:49:PRO:HB2	1:G:88:ARG:HH21	1.69	0.57
1:E:29:LYS:HD2	1:E:30:TYR:CE1	2.39	0.57
1:J:110:ARG:NH2	1:J:117:GLU:OE2	2.37	0.57
1:I:171:CYS:N	1:J:48:CYS:SG	2.78	0.57
1:J:48:CYS:HB3	1:J:49:PRO:HD2	1.85	0.57
1:I:116:ILE:HG12	1:I:123:LEU:HD21	1.87	0.57
1:H:141:ASN:N	1:H:141:ASN:OD1	2.37	0.57
1:E:126:LEU:C	1:E:127:PHE:HD1	2.09	0.57
1:F:43:ALA:N	1:F:75:ASP:OD2	2.38	0.56
1:F:14:LYS:HE3	1:F:103:ASP:HA	1.85	0.56
1:F:-2:PHE:N	1:F:-2:PHE:CD1	2.74	0.56
1:J:35:VAL:HG23	1:J:129:ILE:HB	1.87	0.56
1:B:50:THR:CA	1:A:171:CYS:SG	2.93	0.56
1:J:43:ALA:HB2	1:J:75:ASP:OD2	2.06	0.56
1:C:84:THR:HA	1:C:93:LEU:O	2.06	0.56
1:E:103:ASP:OD2	1:E:108:LEU:N	2.39	0.56
1:D:74:THR:HA	1:D:103:ASP:O	2.06	0.55
1:E:30:TYR:CE2	1:E:68:GLN:HG2	2.42	0.55
1:G:53:VAL:HG21	1:G:88:ARG:NE	2.19	0.55
1:A:119:GLU:O	1:J:104:LYS:NZ	2.38	0.55
1:B:29:LYS:HB2	1:B:30:TYR:CD1	2.40	0.55
1:D:46:PHE:O	1:D:49:PRO:HD2	2.07	0.55
1:J:144:SER:O	1:J:145:VAL:HG23	2.06	0.55
1:B:130:ASP:OD1	1:B:134:ILE:N	2.40	0.55
1:B:62:PHE:CD2	1:B:69:VAL:HG13	2.42	0.55
1:C:37:LEU:CD2	1:C:112:TYR:CE2	2.90	0.55
1:E:30:TYR:N	1:E:30:TYR:CD1	2.75	0.55
1:E:30:TYR:N	1:E:30:TYR:HD1	2.05	0.55
1:G:44:PHE:HD2	1:F:79:SER:HA	1.69	0.55
1:E:74:THR:HA	1:E:103:ASP:O	2.08	0.54
1:B:18:VAL:O	1:B:21:ILE:HG12	2.08	0.54
1:I:137:HIS:NE2	1:I:139:THR:OG1	2.40	0.54
1:D:62:PHE:O	1:D:67:ALA:N	2.36	0.54
1:J:1:MET:HG2	1:J:2:VAL:N	2.22	0.54
1:B:30:TYR:N	1:B:30:TYR:CD1	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:CYS:SG	1:A:170:PRO:HB2	2.48	0.54
1:F:76:SER:O	1:F:80:LEU:N	2.35	0.54
1:F:38:ALA:HA	1:F:125:GLY:O	2.08	0.53
1:J:103:ASP:OD1	1:J:106:HIS:N	2.41	0.53
1:J:59:ALA:HB1	1:J:98:VAL:HG13	1.90	0.53
1:F:-2:PHE:N	1:F:-2:PHE:HD1	2.07	0.53
1:G:44:PHE:CE1	1:G:83:TRP:HB2	2.43	0.53
1:B:136:ARG:NH2	1:A:142:ASP:OD2	2.36	0.53
1:E:170:PRO:HB2	1:F:48:CYS:HB2	1.89	0.53
1:F:34:TYR:CE1	1:F:131:PRO:HD3	2.44	0.53
1:J:160:GLN:O	1:J:164:LYS:HB2	2.09	0.53
1:D:82:ALA:HB1	1:E:44:PHE:CE2	2.44	0.53
1:D:87:PRO:C	1:D:91:GLY:HA3	2.29	0.53
1:F:83:TRP:CD2	1:F:93:LEU:HD23	2.43	0.53
1:H:155:LEU:O	1:H:159:PHE:CD1	2.62	0.53
1:J:156:VAL:O	1:J:160:GLN:HB2	2.09	0.53
1:F:74:THR:HA	1:F:103:ASP:O	2.09	0.53
1:H:151:GLU:O	1:H:155:LEU:HG	2.09	0.53
1:H:55:PHE:HB2	1:H:71:PHE:HZ	1.74	0.53
1:I:154:ARG:NH2	1:J:148:ASN:HD22	2.07	0.53
1:E:38:ALA:HA	1:E:125:GLY:O	2.09	0.52
1:H:78:TYR:CE2	1:I:42:LEU:HD13	2.43	0.52
1:B:30:TYR:CE2	1:B:68:GLN:HG2	2.45	0.52
1:G:55:PHE:CE1	1:G:147:ARG:CB	2.91	0.52
1:I:124:ARG:HA	1:I:147:ARG:HH21	1.75	0.52
1:D:37:LEU:HD23	1:D:112:TYR:CE2	2.44	0.52
1:E:34:TYR:CE2	1:E:160:GLN:HG3	2.45	0.52
1:G:49:PRO:O	1:G:53:VAL:HG23	2.09	0.52
1:J:34:TYR:CD1	1:J:131:PRO:HD3	2.44	0.52
1:D:82:ALA:CB	1:E:44:PHE:CE2	2.93	0.52
1:E:51:GLU:OE1	1:E:147:ARG:O	2.27	0.52
1:J:141:ASN:O	1:J:142:ASP:HB2	2.10	0.52
1:J:9:ALA:HA	1:J:135:ILE:HD11	1.91	0.52
1:E:29:LYS:HB3	1:E:30:TYR:CD1	2.44	0.52
1:E:44:PHE:HD1	1:E:44:PHE:N	2.08	0.52
1:F:62:PHE:CD1	1:F:153:LEU:HD23	2.45	0.52
1:F:75:ASP:O	1:F:102:ALA:HB1	2.10	0.52
1:B:10:PRO:HB2	1:B:112:TYR:HE1	1.74	0.52
1:E:128:ILE:HB	1:E:137:HIS:HB3	1.92	0.52
1:H:155:LEU:HB2	1:H:159:PHE:CE1	2.45	0.52
1:D:72:ALA:HA	1:D:101:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:PHE:CG	1:J:69:VAL:HG23	2.45	0.52
1:D:86:LEU:CG	1:D:91:GLY:HA2	2.29	0.51
1:F:6:GLN:HA	1:F:134:ILE:HG23	1.93	0.51
1:A:74:THR:HA	1:A:103:ASP:O	2.10	0.51
1:C:142:ASP:OD1	1:C:143:LEU:N	2.38	0.51
1:A:125:GLY:N	1:A:147:ARG:HH22	2.07	0.51
1:E:-2:PHE:O	1:E:-1:GLN:HB3	2.10	0.51
1:D:86:LEU:C	1:D:91:GLY:HA3	2.31	0.51
1:G:34:TYR:CE1	1:G:131:PRO:HD3	2.45	0.51
1:B:112:TYR:HB3	1:B:127:PHE:CE2	2.46	0.51
1:D:-2:PHE:HD1	1:D:-2:PHE:H	1.58	0.51
1:G:38:ALA:HA	1:G:125:GLY:O	2.10	0.51
1:A:124:ARG:NH2	1:A:143:LEU:O	2.44	0.51
1:G:72:ALA:HA	1:G:101:LEU:O	2.11	0.51
1:D:84:THR:HA	1:D:93:LEU:CD1	2.40	0.51
1:G:44:PHE:CE2	1:F:79:SER:HA	2.45	0.51
1:I:123:LEU:CD1	1:J:5:VAL:HG11	2.40	0.51
1:I:34:TYR:CE1	1:I:131:PRO:HD3	2.46	0.51
1:J:39:PHE:O	1:J:147:ARG:NH2	2.43	0.51
1:F:62:PHE:O	1:F:67:ALA:N	2.41	0.51
1:J:34:TYR:CE1	1:J:131:PRO:HD3	2.46	0.51
1:B:127:PHE:N	1:B:127:PHE:CD1	2.78	0.51
1:G:65:GLN:NE2	1:G:157:GLU:OE2	2.44	0.50
1:I:130:ASP:OD2	1:I:136:ARG:HD3	2.11	0.50
1:J:140:ILE:HG12	1:J:140:ILE:O	2.11	0.50
1:E:44:PHE:N	1:E:44:PHE:CD1	2.80	0.50
1:C:34:TYR:CE1	1:C:131:PRO:HD3	2.46	0.50
1:D:46:PHE:N	1:D:46:PHE:HD1	2.07	0.50
1:J:77:GLU:HB3	1:J:102:ALA:CB	2.42	0.50
1:B:121:ILE:HD12	1:B:122:ALA:O	2.11	0.50
1:G:43:ALA:HB2	1:G:80:LEU:HD23	1.92	0.50
1:B:60:LYS:HE2	1:B:64:ASP:OD1	2.12	0.50
1:B:50:THR:HA	1:B:53:VAL:HG22	1.94	0.50
1:E:141:ASN:OD1	1:F:137:HIS:CE1	2.65	0.50
1:G:126:LEU:C	1:G:127:PHE:HD1	2.15	0.50
1:J:88:ARG:HA	1:J:92:GLY:O	2.10	0.50
1:H:46:PHE:CD1	1:H:46:PHE:N	2.78	0.50
1:J:1:MET:CG	1:J:2:VAL:N	2.75	0.50
1:G:81:LEU:O	1:G:84:THR:HG22	2.12	0.49
1:J:162:THR:O	1:J:166:GLY:HA2	2.11	0.49
1:F:51:GLU:O	1:F:55:PHE:CD2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:N	1:A:127:PHE:HD1	2.10	0.49
1:H:37:LEU:HD23	1:H:112:TYR:HE2	1.78	0.49
1:I:117:GLU:OE1	1:I:117:GLU:N	2.43	0.49
1:B:62:PHE:CE1	1:B:153:LEU:HD21	2.47	0.49
1:C:80:LEU:HD12	1:C:102:ALA:HB2	1.94	0.49
1:E:30:TYR:CD2	1:E:68:GLN:HG2	2.47	0.49
1:H:10:PRO:HB2	1:H:112:TYR:HE1	1.77	0.49
1:A:-2:PHE:CE1	1:A:1:MET:HG2	2.48	0.49
1:C:-2:PHE:CE1	1:C:1:MET:CG	2.95	0.49
1:D:38:ALA:HA	1:D:125:GLY:O	2.11	0.49
1:E:9:ALA:N	1:E:133:GLY:O	2.31	0.49
1:J:124:ARG:HG3	1:J:142:ASP:O	2.12	0.49
1:C:48:CYS:HB2	1:C:50:THR:HG23	1.95	0.49
1:A:112:TYR:HB3	1:A:127:PHE:CE2	2.48	0.49
1:H:124:ARG:O	1:H:140:ILE:HA	2.12	0.49
1:B:6:GLN:OE1	1:A:123:LEU:HD21	2.13	0.48
1:D:89:LYS:CG	1:D:90:ASP:H	2.25	0.48
1:E:103:ASP:OD1	1:E:106:HIS:N	2.45	0.48
1:G:55:PHE:CZ	1:G:147:ARG:CB	2.95	0.48
1:H:37:LEU:HD23	1:H:112:TYR:CE2	2.48	0.48
1:J:126:LEU:HG	1:J:147:ARG:HD2	1.93	0.48
1:G:55:PHE:CZ	1:G:147:ARG:HB3	2.49	0.48
1:A:8:GLN:HG3	1:A:9:ALA:N	2.28	0.48
1:E:77:GLU:OE1	1:E:104:LYS:NZ	2.39	0.48
1:F:150:ASN:O	1:F:154:ARG:CB	2.60	0.48
1:G:39:PHE:CE2	1:G:114:VAL:HG21	2.48	0.48
1:G:44:PHE:CZ	1:G:79:SER:O	2.66	0.48
1:A:12:PHE:CD2	1:A:108:LEU:HD21	2.48	0.48
1:C:141:ASN:OD1	1:C:147:ARG:HG2	2.14	0.48
1:E:28:GLU:OE1	1:E:31:LYS:NZ	2.40	0.48
1:J:58:ALA:CB	1:J:149:VAL:HG21	2.42	0.48
1:A:34:TYR:OH	1:A:163:ASP:OD2	2.27	0.48
1:C:-2:PHE:CD1	1:C:1:MET:HG2	2.48	0.48
1:E:127:PHE:HD1	1:E:127:PHE:N	2.11	0.48
1:F:108:LEU:HD11	1:F:112:TYR:CE2	2.48	0.48
1:J:39:PHE:CE2	1:J:114:VAL:HG21	2.49	0.48
1:B:73:SER:O	1:B:103:ASP:N	2.31	0.48
1:C:25:ILE:CD1	1:C:99:PRO:HB3	2.44	0.48
1:E:30:TYR:CE2	1:E:70:LEU:HD21	2.49	0.48
1:J:125:GLY:HA2	1:J:139:THR:O	2.13	0.48
1:D:52:ILE:HG12	1:D:71:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:TYR:CD2	1:G:156:VAL:HG13	2.48	0.48
1:I:48:CYS:HB3	1:J:171:CYS:N	2.28	0.48
1:F:12:PHE:HE2	1:F:108:LEU:HD22	1.77	0.48
1:G:3:ALA:O	1:G:4:GLU:HB2	2.14	0.48
1:B:30:TYR:N	1:B:30:TYR:HD1	2.12	0.48
1:G:34:TYR:CD1	1:G:130:ASP:HA	2.48	0.48
1:E:34:TYR:OH	1:E:160:GLN:HA	2.14	0.48
1:I:103:ASP:O	1:I:105:ASN:N	2.47	0.48
1:B:141:ASN:OD1	1:A:137:HIS:CE1	2.68	0.47
1:A:44:PHE:CE2	1:A:83:TRP:HB2	2.49	0.47
1:H:58:ALA:O	1:H:62:PHE:CD2	2.67	0.47
1:A:126:LEU:C	1:A:127:PHE:HD1	2.16	0.47
1:A:43:ALA:HB2	1:A:75:ASP:OD2	2.14	0.47
1:E:39:PHE:CE2	1:E:114:VAL:HG21	2.49	0.47
1:I:123:LEU:HD22	1:I:143:LEU:CD2	2.43	0.47
1:C:87:PRO:O	1:C:90:ASP:OD1	2.33	0.47
1:D:84:THR:CA	1:D:93:LEU:HD11	2.44	0.47
1:B:62:PHE:O	1:B:67:ALA:N	2.33	0.47
1:D:93:LEU:CD1	1:D:94:GLY:N	2.76	0.47
1:E:127:PHE:CD1	1:E:127:PHE:N	2.82	0.47
1:F:12:PHE:CD2	1:F:108:LEU:HD13	2.49	0.47
1:F:127:PHE:N	1:F:127:PHE:HD1	2.13	0.47
1:E:153:LEU:O	1:E:156:VAL:N	2.46	0.47
1:F:38:ALA:O	1:F:71:PHE:HA	2.15	0.47
1:H:47:VAL:O	1:H:47:VAL:HG12	2.15	0.47
1:J:3:ALA:HB2	1:J:112:TYR:HA	1.96	0.47
1:B:137:HIS:ND1	1:A:141:ASN:OD1	2.37	0.47
1:B:29:LYS:HB2	1:B:30:TYR:CE1	2.49	0.47
1:C:-2:PHE:CE1	1:C:1:MET:HG2	2.50	0.47
1:F:62:PHE:HB3	1:F:67:ALA:HB3	1.96	0.47
1:A:127:PHE:N	1:A:127:PHE:CD1	2.81	0.47
1:A:12:PHE:CE1	1:A:27:LEU:HB2	2.50	0.47
1:D:54:ALA:HB1	1:D:149:VAL:CG2	2.44	0.47
1:F:127:PHE:N	1:F:127:PHE:CD1	2.81	0.47
1:F:124:ARG:HD2	1:F:145:VAL:O	2.14	0.47
1:H:44:PHE:CZ	1:H:83:TRP:HB2	2.50	0.47
1:J:112:TYR:CD1	1:J:127:PHE:CE2	3.03	0.47
1:D:54:ALA:HB1	1:D:149:VAL:HG22	1.96	0.47
1:F:34:TYR:HA	1:F:129:ILE:O	2.15	0.47
1:I:42:LEU:HD21	1:I:121:ILE:HG21	1.97	0.47
1:I:130:ASP:HB3	1:I:131:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:50:THR:O	1:I:53:VAL:HG22	2.15	0.47
1:A:12:PHE:N	1:A:12:PHE:CD1	2.82	0.47
1:E:16:ALA:CB	1:E:25:ILE:HD12	2.45	0.46
1:E:44:PHE:CE1	1:E:83:TRP:HA	2.50	0.46
1:G:49:PRO:HA	1:G:52:ILE:HD11	1.97	0.46
1:J:126:LEU:C	1:J:127:PHE:HD1	2.18	0.46
1:J:36:VAL:HG22	1:J:128:ILE:HD13	1.96	0.46
1:B:127:PHE:N	1:B:127:PHE:HD1	2.12	0.46
1:D:38:ALA:C	1:D:39:PHE:HD1	2.19	0.46
1:D:89:LYS:CG	1:D:90:ASP:N	2.79	0.46
1:C:114:VAL:O	1:C:114:VAL:HG23	2.15	0.46
1:E:39:PHE:CE1	1:E:72:ALA:HB3	2.50	0.46
1:D:82:ALA:HB2	1:E:44:PHE:CD2	2.49	0.46
1:F:62:PHE:N	1:F:62:PHE:CD1	2.83	0.46
1:J:2:VAL:O	1:J:111:ASP:O	2.34	0.46
1:B:161:TRP:CE3	1:B:165:ASN:OD1	2.69	0.46
1:E:39:PHE:CE2	1:E:114:VAL:CG2	2.97	0.46
1:J:22:PHE:HD1	1:J:22:PHE:N	2.14	0.46
1:A:59:ALA:HB2	1:A:98:VAL:HG13	1.97	0.46
1:B:78:TYR:HB3	1:C:44:PHE:CG	2.51	0.46
1:H:65:GLN:O	1:H:65:GLN:OE1	2.33	0.46
1:A:81:LEU:HG	1:A:85:ASN:OD1	2.16	0.46
1:F:62:PHE:N	1:F:62:PHE:HD1	2.14	0.46
1:G:30:TYR:CE1	1:G:68:GLN:HG2	2.51	0.46
1:A:130:ASP:HB2	1:A:131:PRO:CD	2.45	0.46
1:B:126:LEU:C	1:B:127:PHE:CD1	2.89	0.46
1:J:22:PHE:N	1:J:22:PHE:CD1	2.84	0.46
1:A:152:ALA:O	1:A:156:VAL:HG23	2.15	0.46
1:A:-2:PHE:CE1	1:A:1:MET:CG	2.99	0.46
1:D:115:LEU:HD12	1:D:121:ILE:O	2.15	0.46
1:G:83:TRP:O	1:G:93:LEU:HB3	2.16	0.45
1:C:39:PHE:HE2	1:C:109:SER:HA	1.80	0.45
1:E:55:PHE:CE1	1:E:149:VAL:HG23	2.51	0.45
1:E:5:VAL:HA	1:E:135:ILE:O	2.17	0.45
1:H:169:LEU:HD11	1:H:173:TRP:CZ3	2.51	0.45
1:I:2:VAL:O	1:I:4:GLU:HG3	2.17	0.45
1:A:60:LYS:NZ	1:A:64:ASP:OD2	2.36	0.45
1:E:130:ASP:HB2	1:E:131:PRO:CD	2.47	0.45
1:F:48:CYS:SG	1:F:51:GLU:HG2	2.57	0.45
1:H:62:PHE:CZ	1:H:153:LEU:HD22	2.52	0.45
1:E:136:ARG:NH2	1:E:163:ASP:OD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:PRO:C	1:G:88:ARG:HH21	2.19	0.45
1:H:61:LYS:HE3	1:H:153:LEU:HD11	1.99	0.45
1:H:55:PHE:HB2	1:H:71:PHE:CZ	2.50	0.45
1:J:110:ARG:HA	1:J:110:ARG:NE	2.31	0.45
1:J:160:GLN:O	1:J:164:LYS:CB	2.64	0.45
1:A:40:VAL:HG11	1:A:52:ILE:HG13	1.98	0.45
1:B:124:ARG:O	1:B:140:ILE:HA	2.16	0.45
1:G:36:VAL:HA	1:G:127:PHE:O	2.16	0.45
1:B:42:LEU:HD13	1:C:78:TYR:CD2	2.51	0.45
1:H:55:PHE:O	1:H:59:ALA:HB2	2.17	0.45
1:I:41:PRO:HG3	1:I:124:ARG:NH2	2.32	0.45
1:C:13:LYS:HA	1:C:26:SER:HA	1.99	0.45
1:E:55:PHE:HB2	1:E:71:PHE:HZ	1.81	0.45
1:F:36:VAL:HA	1:F:127:PHE:O	2.16	0.45
1:F:149:VAL:O	1:F:152:ALA:HB3	2.16	0.45
1:I:32:GLY:HA2	1:I:131:PRO:HA	1.98	0.45
1:C:69:VAL:HG12	1:C:98:VAL:HG21	1.99	0.45
1:G:106:HIS:HB3	1:G:115:LEU:CD1	2.47	0.45
1:A:124:ARG:O	1:A:140:ILE:HA	2.17	0.45
1:C:74:THR:HA	1:C:103:ASP:O	2.17	0.45
1:D:112:TYR:N	1:D:112:TYR:CD1	2.85	0.45
1:F:39:PHE:CD1	1:F:39:PHE:N	2.84	0.45
1:F:50:THR:O	1:F:53:VAL:HG22	2.17	0.45
1:H:34:TYR:CD1	1:H:130:ASP:HA	2.52	0.45
1:I:32:GLY:HA2	1:I:131:PRO:CA	2.47	0.45
1:A:10:PRO:HD2	1:A:112:TYR:CE1	2.51	0.44
1:A:136:ARG:HH22	1:A:163:ASP:CG	2.19	0.44
1:E:152:ALA:O	1:E:156:VAL:HG23	2.17	0.44
1:H:51:GLU:OE2	1:H:124:ARG:CZ	2.64	0.44
1:A:34:TYR:OH	1:A:160:GLN:HA	2.17	0.44
1:J:117:GLU:N	1:J:117:GLU:OE1	2.47	0.44
1:B:62:PHE:HB3	1:B:67:ALA:HB3	1.99	0.44
1:C:-3:TYR:CZ	1:C:1:MET:HB2	2.52	0.44
1:D:147:ARG:O	1:D:148:ASN:HB2	2.17	0.44
1:D:25:ILE:N	1:D:25:ILE:HD12	2.32	0.44
1:D:87:PRO:O	1:D:89:LYS:N	2.51	0.44
1:F:5:VAL:O	1:F:6:GLN:HB2	2.16	0.44
1:G:55:PHE:CZ	1:G:147:ARG:HB2	2.52	0.44
1:I:143:LEU:HD23	1:I:143:LEU:N	2.31	0.44
1:A:126:LEU:O	1:A:138:ILE:HA	2.18	0.44
1:C:18:VAL:O	1:C:21:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:ILE:HD11	1:G:123:LEU:HD12	1.98	0.44
1:H:153:LEU:N	1:H:153:LEU:HD23	2.32	0.44
1:A:155:LEU:O	1:A:159:PHE:HD2	2.00	0.44
1:F:37:LEU:O	1:F:126:LEU:HA	2.18	0.44
1:F:8:GLN:HG3	1:F:133:GLY:O	2.17	0.44
1:G:49:PRO:HB2	1:G:88:ARG:HE	1.82	0.44
1:I:38:ALA:HB1	1:I:147:ARG:NH1	2.32	0.44
1:J:137:HIS:NE2	1:J:139:THR:OG1	2.50	0.44
1:A:43:ALA:CB	1:A:75:ASP:OD2	2.65	0.44
1:D:93:LEU:H	1:D:93:LEU:HD12	1.81	0.44
1:G:46:PHE:O	1:G:47:VAL:CG1	2.66	0.44
1:A:12:PHE:H	1:A:12:PHE:HD1	1.64	0.44
1:B:49:PRO:O	1:B:52:ILE:HB	2.18	0.44
1:F:43:ALA:CB	1:F:75:ASP:OD2	2.66	0.44
1:J:5:VAL:O	1:J:6:GLN:HB2	2.17	0.44
1:A:46:PHE:HB2	1:A:47:VAL:H	1.62	0.44
1:A:22:PHE:CE1	1:A:81:LEU:HD13	2.53	0.44
1:I:124:ARG:HA	1:I:147:ARG:NH2	2.32	0.44
1:J:5:VAL:HB	1:J:138:ILE:HD12	1.99	0.44
1:J:40:VAL:HG22	1:J:73:SER:HB3	2.00	0.44
1:C:34:TYR:CD1	1:C:131:PRO:HD3	2.53	0.43
1:C:73:SER:OG	1:C:80:LEU:HD21	2.18	0.43
1:E:47:VAL:HG21	1:E:124:ARG:NH2	2.32	0.43
1:E:44:PHE:HE1	1:E:83:TRP:HB2	1.82	0.43
1:F:39:PHE:HD1	1:F:39:PHE:N	2.15	0.43
1:G:14:LYS:HD2	1:G:103:ASP:OD1	2.18	0.43
1:G:46:PHE:C	1:G:47:VAL:HG13	2.38	0.43
1:I:169:LEU:HB3	1:I:172:ASN:HB2	1.99	0.43
1:F:126:LEU:C	1:F:127:PHE:HD1	2.22	0.43
1:I:145:VAL:HG12	1:I:146:GLY:O	2.18	0.43
1:J:1:MET:CG	1:J:2:VAL:H	2.31	0.43
1:A:123:LEU:HD23	1:A:143:LEU:CD2	2.48	0.43
1:B:104:LYS:O	1:B:106:HIS:ND1	2.48	0.43
1:D:39:PHE:HE2	1:D:109:SER:HA	1.83	0.43
1:I:116:ILE:HG12	1:I:123:LEU:CD2	2.48	0.43
1:J:159:PHE:O	1:J:162:THR:HG22	2.18	0.43
1:B:137:HIS:CE1	1:A:139:THR:HG23	2.53	0.43
1:C:38:ALA:O	1:C:71:PHE:HA	2.18	0.43
1:C:90:ASP:OD1	1:C:90:ASP:N	2.49	0.43
1:E:37:LEU:CD2	1:E:112:TYR:HE2	2.31	0.43
1:F:52:ILE:HA	1:F:55:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:LEU:O	1:G:159:PHE:CD2	2.71	0.43
1:H:62:PHE:CZ	1:H:153:LEU:CD2	3.01	0.43
1:I:115:LEU:HD12	1:I:121:ILE:O	2.19	0.43
1:B:62:PHE:CD1	1:B:153:LEU:HD21	2.53	0.43
1:F:2:VAL:O	1:F:111:ASP:O	2.37	0.43
1:H:123:LEU:HA	1:H:143:LEU:HD21	2.00	0.43
1:H:34:TYR:CD1	1:H:131:PRO:HD3	2.53	0.43
1:J:34:TYR:OH	1:J:160:GLN:HA	2.18	0.43
1:D:128:ILE:O	1:D:135:ILE:HA	2.18	0.43
1:H:58:ALA:HB2	1:H:149:VAL:HG21	2.00	0.43
1:B:128:ILE:HB	1:B:137:HIS:HB3	2.00	0.43
1:H:130:ASP:HB2	1:H:131:PRO:CD	2.49	0.43
1:H:138:ILE:HG22	1:H:140:ILE:HD12	1.99	0.43
1:I:112:TYR:HB3	1:I:127:PHE:CE2	2.54	0.43
1:I:43:ALA:N	1:I:75:ASP:OD2	2.47	0.43
1:A:5:VAL:HG12	1:A:6:GLN:HG3	2.00	0.43
1:B:51:GLU:HB3	1:B:55:PHE:CE2	2.54	0.43
1:D:37:LEU:CD2	1:D:112:TYR:CE2	3.02	0.43
1:D:93:LEU:HD12	1:D:93:LEU:N	2.33	0.43
1:J:18:VAL:HG22	1:J:99:PRO:HB3	2.00	0.43
1:A:47:VAL:O	1:A:47:VAL:HG12	2.19	0.43
1:B:62:PHE:N	1:B:62:PHE:CD1	2.86	0.43
1:C:43:ALA:HB1	1:C:83:TRP:CE2	2.53	0.43
1:C:5:VAL:HG11	1:D:123:LEU:CD1	2.48	0.43
1:G:34:TYR:HA	1:G:129:ILE:O	2.19	0.43
1:E:142:ASP:OD2	1:F:136:ARG:HA	2.19	0.43
1:G:112:TYR:HD1	1:G:127:PHE:CE2	2.37	0.43
1:J:39:PHE:N	1:J:39:PHE:CD1	2.87	0.43
1:A:12:PHE:CE2	1:A:108:LEU:HD21	2.54	0.42
1:E:142:ASP:OD2	1:F:136:ARG:HD2	2.18	0.42
1:F:126:LEU:C	1:F:127:PHE:CD1	2.92	0.42
1:F:16:ALA:HB2	1:F:101:LEU:HG	2.01	0.42
1:H:71:PHE:CD1	1:H:71:PHE:N	2.87	0.42
1:J:39:PHE:N	1:J:39:PHE:HD1	2.17	0.42
1:A:16:ALA:HB2	1:A:101:LEU:HD22	2.00	0.42
1:D:107:SER:O	1:D:110:ARG:HB3	2.18	0.42
1:H:136:ARG:NH1	1:H:163:ASP:OD2	2.52	0.42
1:I:48:CYS:HB2	1:J:170:PRO:HB3	2.01	0.42
1:J:137:HIS:CD2	1:J:155:LEU:HD13	2.54	0.42
1:D:103:ASP:OD1	1:D:105:ASN:OD1	2.37	0.42
1:D:44:PHE:CD1	1:D:86:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:-3:TYR:CD1	1:F:1:MET:SD	3.13	0.42
1:J:39:PHE:CD2	1:J:114:VAL:HG21	2.54	0.42
1:J:136:ARG:NH1	1:J:159:PHE:HD1	2.17	0.42
1:A:143:LEU:CD2	1:A:143:LEU:N	2.82	0.42
1:A:46:PHE:N	1:A:46:PHE:CD1	2.88	0.42
1:A:55:PHE:O	1:A:59:ALA:N	2.53	0.42
1:G:145:VAL:O	1:G:145:VAL:HG13	2.19	0.42
1:I:71:PHE:O	1:I:101:LEU:N	2.52	0.42
1:I:170:PRO:CB	1:J:48:CYS:H	2.33	0.42
1:A:34:TYR:CE2	1:A:160:GLN:HG2	2.55	0.42
1:A:42:LEU:HD13	1:J:78:TYR:CE2	2.54	0.42
1:D:79:SER:O	1:D:83:TRP:HB2	2.20	0.42
1:E:52:ILE:CG2	1:E:93:LEU:HD21	2.50	0.42
1:F:86:LEU:HD12	1:F:87:PRO:HD2	2.01	0.42
1:G:127:PHE:N	1:G:127:PHE:CD1	2.87	0.42
1:I:169:LEU:CB	1:I:172:ASN:HB2	2.50	0.42
1:C:6:GLN:N	1:C:135:ILE:O	2.50	0.42
1:F:62:PHE:CD2	1:F:69:VAL:HG22	2.55	0.42
1:G:127:PHE:HD1	1:G:127:PHE:N	2.17	0.42
1:H:71:PHE:HD1	1:H:71:PHE:N	2.18	0.42
1:I:14:LYS:HE3	1:I:108:LEU:CD1	2.50	0.42
1:D:112:TYR:N	1:D:112:TYR:HD1	2.18	0.42
1:E:61:LYS:O	1:E:65:GLN:OE1	2.38	0.42
1:G:75:ASP:O	1:G:102:ALA:HB1	2.20	0.42
1:I:154:ARG:O	1:I:154:ARG:HG3	2.18	0.42
1:A:128:ILE:HG12	1:A:156:VAL:HG22	2.01	0.42
1:A:55:PHE:HB2	1:A:71:PHE:HZ	1.85	0.42
1:A:80:LEU:HD12	1:A:102:ALA:HB2	2.02	0.42
1:C:106:HIS:O	1:C:110:ARG:HB3	2.20	0.42
1:B:78:TYR:HB3	1:C:44:PHE:HB2	2.02	0.42
1:D:44:PHE:CE1	1:D:86:LEU:HD23	2.55	0.42
1:I:32:GLY:O	1:I:131:PRO:HA	2.20	0.42
1:I:65:GLN:HG3	1:I:157:GLU:HG2	2.02	0.42
1:J:-2:PHE:N	1:J:-2:PHE:CD1	2.87	0.42
1:A:124:ARG:NH1	1:A:145:VAL:O	2.52	0.42
1:D:75:ASP:O	1:D:102:ALA:HB1	2.20	0.42
1:E:22:PHE:HZ	1:E:78:TYR:CD1	2.37	0.42
1:G:43:ALA:C	1:G:44:PHE:CG	2.91	0.42
1:H:52:ILE:HG23	1:H:71:PHE:CE2	2.55	0.42
1:A:39:PHE:N	1:A:39:PHE:HD1	2.17	0.42
1:G:34:TYR:CD1	1:G:131:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:112:TYR:HB3	1:I:127:PHE:CZ	2.55	0.42
1:J:121:ILE:HD13	1:J:143:LEU:HD21	2.02	0.42
1:A:17:VAL:HG11	1:A:81:LEU:HB2	2.02	0.41
1:E:16:ALA:HB1	1:E:100:LEU:O	2.20	0.41
1:E:71:PHE:HB2	1:E:100:LEU:HD23	2.02	0.41
1:G:83:TRP:CE2	1:G:93:LEU:HB2	2.55	0.41
1:H:152:ALA:O	1:H:156:VAL:HG23	2.20	0.41
1:A:39:PHE:CD1	1:A:39:PHE:N	2.87	0.41
1:B:53:VAL:CG1	1:B:88:ARG:HD3	2.51	0.41
1:G:39:PHE:N	1:G:39:PHE:CD1	2.88	0.41
1:G:43:ALA:O	1:G:44:PHE:CD2	2.73	0.41
1:B:46:PHE:CD2	1:C:78:TYR:CE1	3.08	0.41
1:F:124:ARG:O	1:F:147:ARG:NH1	2.54	0.41
1:I:38:ALA:HA	1:I:147:ARG:HH12	1.85	0.41
1:B:137:HIS:CE1	1:B:155:LEU:HD13	2.56	0.41
1:D:48:CYS:HB2	1:D:49:PRO:HD3	2.02	0.41
1:E:39:PHE:HZ	1:E:108:LEU:HG	1.84	0.41
1:F:142:ASP:OD1	1:F:143:LEU:N	2.45	0.41
1:H:116:ILE:HD11	1:H:123:LEU:CD2	2.50	0.41
1:H:161:TRP:CZ3	1:H:169:LEU:HB2	2.55	0.41
1:H:62:PHE:CD2	1:H:69:VAL:CG2	3.03	0.41
1:A:12:PHE:HE1	1:A:27:LEU:HB2	1.86	0.41
1:B:126:LEU:C	1:B:127:PHE:HD1	2.24	0.41
1:G:39:PHE:N	1:G:39:PHE:HD1	2.19	0.41
1:G:53:VAL:CG2	1:G:88:ARG:CZ	2.86	0.41
1:D:5:VAL:O	1:D:6:GLN:HB2	2.20	0.41
1:E:144:SER:HB2	1:F:162:THR:HG21	2.02	0.41
1:G:114:VAL:HG12	1:G:140:ILE:HD12	2.03	0.41
1:G:47:VAL:CG2	1:G:52:ILE:HG21	2.47	0.41
1:G:62:PHE:CD2	1:G:153:LEU:HD21	2.55	0.41
1:I:170:PRO:HB2	1:J:48:CYS:SG	2.60	0.41
1:D:88:ARG:CG	1:D:93:LEU:O	2.69	0.41
1:J:110:ARG:HE	1:J:110:ARG:HA	1.85	0.41
1:J:37:LEU:HG	1:J:39:PHE:HE1	1.86	0.41
1:B:119:GLU:O	1:C:104:LYS:HE2	2.20	0.41
1:B:142:ASP:OD1	1:B:143:LEU:N	2.48	0.41
1:F:93:LEU:CD1	1:F:96:VAL:HG13	2.51	0.41
1:I:109:SER:OG	1:I:115:LEU:HB2	2.20	0.41
1:D:126:LEU:HB3	1:D:139:THR:HB	2.03	0.41
1:G:4:GLU:HB3	1:G:7:LYS:CG	2.51	0.41
1:A:38:ALA:C	1:A:39:PHE:HD1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:TYR:HB3	1:C:44:PHE:CB	2.51	0.41
1:D:153:LEU:O	1:D:156:VAL:HG22	2.21	0.41
1:D:44:PHE:CE1	1:D:86:LEU:CD2	3.04	0.41
1:F:155:LEU:O	1:F:159:PHE:CD2	2.73	0.41
1:H:128:ILE:HG12	1:H:156:VAL:HG22	2.02	0.41
1:H:38:ALA:HB1	1:H:147:ARG:NH2	2.35	0.41
1:I:10:PRO:O	1:I:112:TYR:OH	2.25	0.41
1:J:59:ALA:CB	1:J:97:LYS:HB2	2.51	0.41
1:J:59:ALA:CB	1:J:98:VAL:HG13	2.49	0.41
1:B:50:THR:HG1	1:A:171:CYS:CB	2.31	0.41
1:D:89:LYS:HG3	1:D:90:ASP:N	2.36	0.41
1:E:37:LEU:HD23	1:E:112:TYR:HE2	1.86	0.41
1:E:29:LYS:HB3	1:E:30:TYR:CE1	2.56	0.41
1:F:130:ASP:OD1	1:F:134:ILE:N	2.50	0.41
1:G:49:PRO:HB2	1:G:88:ARG:NH2	2.36	0.41
1:I:86:LEU:HD22	1:I:92:GLY:N	2.36	0.41
1:I:142:ASP:HB3	1:J:159:PHE:HZ	1.86	0.41
1:A:5:VAL:HG13	1:A:135:ILE:O	2.21	0.40
1:B:103:ASP:O	1:B:103:ASP:OD1	2.39	0.40
1:B:78:TYR:HB3	1:C:44:PHE:CD2	2.56	0.40
1:F:108:LEU:O	1:F:111:ASP:N	2.54	0.40
1:F:112:TYR:HB3	1:F:127:PHE:CZ	2.56	0.40
1:F:-2:PHE:CD1	1:F:1:MET:SD	3.14	0.40
1:G:80:LEU:HD12	1:G:102:ALA:HB2	2.04	0.40
1:A:81:LEU:O	1:A:85:ASN:OD1	2.39	0.40
1:D:108:LEU:O	1:D:111:ASP:N	2.54	0.40
1:D:39:PHE:N	1:D:39:PHE:HD1	2.19	0.40
1:E:10:PRO:HD2	1:E:112:TYR:CE1	2.56	0.40
1:E:112:TYR:HB3	1:E:127:PHE:HE2	1.86	0.40
1:G:103:ASP:OD1	1:G:105:ASN:OD1	2.38	0.40
1:H:124:ARG:HG3	1:H:143:LEU:HD23	2.03	0.40
1:A:2:VAL:HA	1:A:111:ASP:O	2.21	0.40
1:C:15:THR:HG22	1:C:24:GLU:OE2	2.20	0.40
1:E:48:CYS:HB3	1:E:50:THR:HG23	2.03	0.40
1:I:116:ILE:HD11	1:I:143:LEU:HD11	2.03	0.40
1:J:124:ARG:HD3	1:J:147:ARG:HH21	1.87	0.40
1:J:23:GLU:OE2	1:J:29:LYS:NZ	2.54	0.40
1:J:38:ALA:HA	1:J:147:ARG:HH12	1.87	0.40
1:A:36:VAL:HG22	1:A:128:ILE:CD1	2.51	0.40
1:D:-2:PHE:CD1	1:D:-2:PHE:N	2.90	0.40
1:H:58:ALA:HB1	1:H:153:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:168:VAL:HG22	1:J:169:LEU:H	1.86	0.40
1:B:16:ALA:HB3	1:B:25:ILE:CG1	2.51	0.40
1:E:55:PHE:HB2	1:E:71:PHE:CZ	2.57	0.40
1:F:39:PHE:HD2	1:F:122:ALA:CB	2.34	0.40
1:F:69:VAL:O	1:F:70:LEU:HD23	2.22	0.40
1:H:128:ILE:HD13	1:H:137:HIS:HB3	2.04	0.40
1:H:169:LEU:HD12	1:H:170:PRO:HD2	2.04	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	173/217 (80%)	161 (93%)	11 (6%)	1 (1%)	25 65
1	B	171/217 (79%)	161 (94%)	7 (4%)	3 (2%)	8 41
1	C	170/217 (78%)	160 (94%)	10 (6%)	0	100 100
1	D	168/217 (77%)	155 (92%)	13 (8%)	0	100 100
1	E	176/217 (81%)	167 (95%)	9 (5%)	0	100 100
1	F	168/217 (77%)	156 (93%)	11 (6%)	1 (1%)	25 65
1	G	173/217 (80%)	162 (94%)	9 (5%)	2 (1%)	13 50
1	H	176/217 (81%)	166 (94%)	9 (5%)	1 (1%)	25 65
1	I	175/217 (81%)	164 (94%)	10 (6%)	1 (1%)	25 65
1	J	173/217 (80%)	153 (88%)	16 (9%)	4 (2%)	6 36
All	All	1723/2170 (79%)	1605 (93%)	105 (6%)	13 (1%)	19 60

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	PRO
1	A	47	VAL
1	G	3	ALA
1	J	141	ASN
1	B	104	LYS
1	G	4	GLU
1	F	165	ASN
1	I	104	LYS
1	J	142	ASP
1	J	145	VAL
1	H	47	VAL
1	J	2	VAL
1	B	2	VAL

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	147/184 (80%)	138 (94%)	9 (6%)	18	46
1	B	145/184 (79%)	139 (96%)	6 (4%)	30	55
1	C	144/184 (78%)	141 (98%)	3 (2%)	53	72
1	D	142/184 (77%)	137 (96%)	5 (4%)	36	59
1	E	150/184 (82%)	146 (97%)	4 (3%)	44	65
1	F	142/184 (77%)	136 (96%)	6 (4%)	30	54
1	G	147/184 (80%)	142 (97%)	5 (3%)	37	60
1	H	150/184 (82%)	145 (97%)	5 (3%)	38	61
1	I	149/184 (81%)	147 (99%)	2 (1%)	69	82
1	J	147/184 (80%)	143 (97%)	4 (3%)	44	65
All	All	1463/1840 (80%)	1414 (97%)	49 (3%)	38	61

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	46	PHE

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Mol	Chain	Res	Type
1	H	71	PHE
1	H	141	ASN
1	H	155	LEU
1	H	159	PHE
1	B	30	TYR
1	B	62	PHE
1	B	69	VAL
1	B	71	PHE
1	B	104	LYS
1	B	127	PHE
1	C	-2	PHE
1	C	89	LYS
1	C	98	VAL
1	A	-2	PHE
1	A	8	GLN
1	A	12	PHE
1	A	34	TYR
1	A	37	LEU
1	A	39	PHE
1	A	46	PHE
1	A	127	PHE
1	A	143	LEU
1	G	39	PHE
1	G	44	PHE
1	G	55	PHE
1	G	126	LEU
1	G	127	PHE
1	I	143	LEU
1	I	154	ARG
1	D	-2	PHE
1	D	39	PHE
1	D	46	PHE
1	D	93	LEU
1	D	112	TYR
1	E	30	TYR
1	E	42	LEU
1	E	44	PHE
1	E	127	PHE
1	J	22	PHE
1	J	35	VAL
1	J	39	PHE
1	J	129	ILE

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Mol	Chain	Res	Type
1	F	-2	PHE
1	F	12	PHE
1	F	39	PHE
1	F	62	PHE
1	F	127	PHE
1	F	153	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	ASN
1	A	8	GLN
1	A	106	HIS
1	G	65	GLN
1	I	65	GLN
1	D	8	GLN
1	E	106	HIS
1	J	106	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	175/217 (80%)	0.46	25 (14%) 2 3	313, 374, 442, 476	0
1	B	173/217 (79%)	0.15	17 (9%) 7 8	311, 364, 413, 508	0
1	C	172/217 (79%)	0.27	16 (9%) 8 8	307, 370, 441, 493	0
1	D	170/217 (78%)	0.20	19 (11%) 5 6	314, 361, 444, 598	0
1	E	178/217 (82%)	0.24	16 (8%) 9 9	302, 350, 391, 445	0
1	F	170/217 (78%)	0.14	12 (7%) 16 13	266, 319, 375, 482	0
1	G	175/217 (80%)	-0.08	9 (5%) 28 24	239, 304, 378, 411	0
1	H	178/217 (82%)	0.05	10 (5%) 24 21	259, 302, 368, 462	0
1	I	177/217 (81%)	-0.03	6 (3%) 45 37	274, 332, 396, 413	0
1	J	175/217 (80%)	0.21	13 (7%) 14 12	306, 356, 422, 578	0
All	All	1743/2170 (80%)	0.16	143 (8%) 11 10	239, 348, 416, 598	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	-3	TYR	11.0
1	F	144	SER	9.4
1	D	69	VAL	7.6
1	A	122	ALA	7.4
1	A	98	VAL	6.3
1	B	98	VAL	5.7
1	J	170	PRO	5.5
1	E	101	LEU	5.3
1	A	99	PRO	5.2
1	C	98	VAL	5.2
1	I	146	GLY	5.1
1	A	169	LEU	4.8
1	D	99	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	99	PRO	4.7
1	E	98	VAL	4.7
1	E	71	PHE	4.5
1	C	67	ALA	4.3
1	D	70	LEU	4.2
1	E	100	LEU	4.2
1	B	122	ALA	4.0
1	C	18	VAL	3.9
1	E	-3	TYR	3.9
1	C	38	ALA	3.9
1	D	25	ILE	3.9
1	H	-3	TYR	3.8
1	G	-2	PHE	3.8
1	G	171	CYS	3.7
1	D	98	VAL	3.6
1	F	66	GLY	3.6
1	J	-1	GLN	3.5
1	C	25	ILE	3.5
1	I	46	PHE	3.5
1	F	98	VAL	3.5
1	C	17	VAL	3.5
1	E	97	LYS	3.5
1	D	41	PRO	3.4
1	A	67	ALA	3.4
1	A	25	ILE	3.3
1	B	67	ALA	3.2
1	B	170	PRO	3.2
1	H	71	PHE	3.2
1	H	72	ALA	3.2
1	A	38	ALA	3.2
1	A	71	PHE	3.2
1	C	37	LEU	3.1
1	B	99	PRO	3.1
1	A	70	LEU	3.1
1	B	169	LEU	3.1
1	J	-2	PHE	3.0
1	E	99	PRO	3.0
1	E	72	ALA	3.0
1	J	35	VAL	3.0
1	A	69	VAL	3.0
1	G	98	VAL	3.0
1	G	97	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	20	GLY	2.9
1	C	97	LYS	2.9
1	F	17	VAL	2.8
1	B	17	VAL	2.8
1	A	-2	PHE	2.8
1	E	69	VAL	2.8
1	D	-2	PHE	2.8
1	B	69	VAL	2.8
1	J	165	ASN	2.7
1	D	30	TYR	2.7
1	A	37	LEU	2.7
1	D	68	GLN	2.7
1	D	20	GLY	2.6
1	A	27	LEU	2.6
1	H	-2	PHE	2.6
1	A	41	PRO	2.6
1	B	171	CYS	2.6
1	B	97	LYS	2.6
1	A	123	LEU	2.6
1	H	-1	GLN	2.6
1	C	70	LEU	2.6
1	I	98	VAL	2.6
1	C	96	VAL	2.6
1	A	170	PRO	2.6
1	A	-1	GLN	2.5
1	H	70	LEU	2.5
1	D	-1	GLN	2.5
1	E	70	LEU	2.5
1	A	66	GLY	2.5
1	J	22	PHE	2.5
1	G	35	VAL	2.5
1	A	55	PHE	2.5
1	D	71	PHE	2.5
1	H	147	ARG	2.4
1	E	-2	PHE	2.4
1	I	67	ALA	2.4
1	D	100	LEU	2.4
1	B	18	VAL	2.4
1	D	147	ARG	2.4
1	J	17	VAL	2.4
1	C	39	PHE	2.3
1	F	16	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	35	VAL	2.3
1	C	16	ALA	2.3
1	B	30	TYR	2.3
1	B	167	THR	2.3
1	F	-3	TYR	2.3
1	J	169	LEU	2.3
1	F	44	PHE	2.3
1	C	125	GLY	2.3
1	E	93	LEU	2.2
1	A	73	SER	2.2
1	H	101	LEU	2.2
1	J	99	PRO	2.2
1	A	72	ALA	2.2
1	D	101	LEU	2.2
1	E	67	ALA	2.2
1	D	31	LYS	2.2
1	F	72	ALA	2.2
1	H	69	VAL	2.2
1	A	36	VAL	2.2
1	E	48	CYS	2.1
1	E	172	ASN	2.1
1	F	101	LEU	2.1
1	H	112	TYR	2.1
1	E	36	VAL	2.1
1	B	80	LEU	2.1
1	C	65	GLN	2.1
1	F	71	PHE	2.1
1	I	136	ARG	2.1
1	G	71	PHE	2.1
1	B	100	LEU	2.1
1	D	16	ALA	2.1
1	D	23	GLU	2.1
1	B	25	ILE	2.1
1	A	-3	TYR	2.1
1	J	23	GLU	2.1
1	C	36	VAL	2.1
1	J	37	LEU	2.1
1	A	90	ASP	2.0
1	G	-1	GLN	2.0
1	G	99	PRO	2.0
1	F	143	LEU	2.0
1	I	35	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	67	ALA	2.0
1	D	19	ASP	2.0
1	A	12	PHE	2.0
1	G	128	ILE	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 carbohydrates 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.