



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:06 PM UTC

PDB ID : 5EPT / pdb_00005ept
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

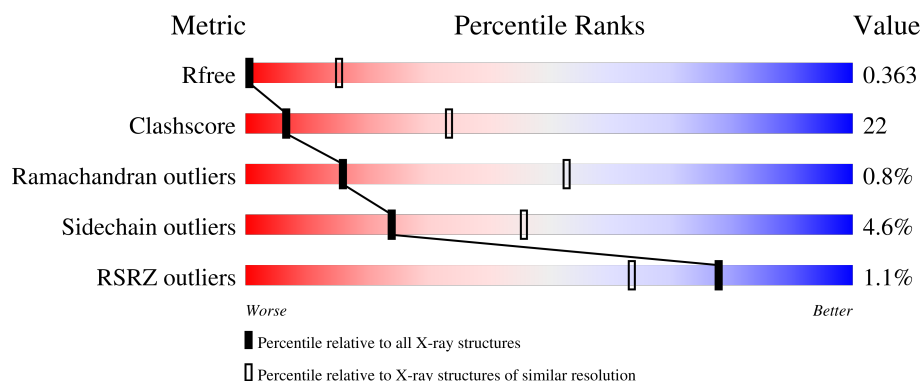
1 Overall quality at a glance

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.



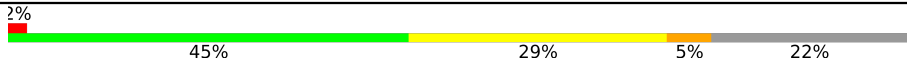
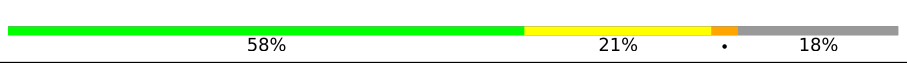
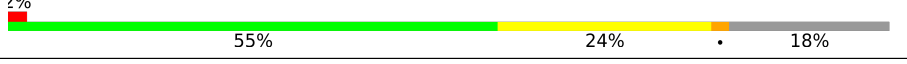
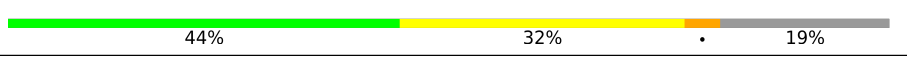
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

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

Mol	Chain	Length	Quality of chain
1	A	217	0% 45% 31% • 19%
1	B	217	2% 52% 24% • 20%
1	C	217	56% 22% • 21%
1	D	217	50% 26% • 22%
1	E	217	50% 30% • 18%

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Mol	Chain	Length	Quality of chain
1	F	217	
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
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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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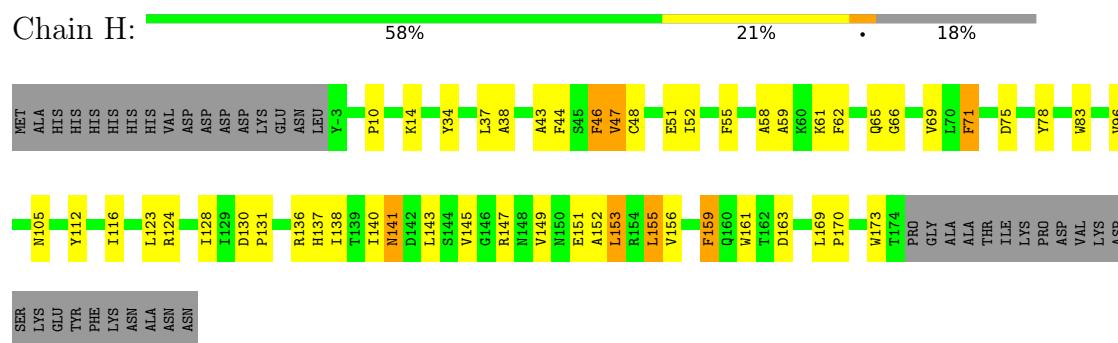
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Chain	Residue	Modelled	Actual	Comment	Reference
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J	-10	ASP	-	expression tag	UNP Q04120
J	-9	ASP	-	expression tag	UNP Q04120
J	-8	ASP	-	expression tag	UNP Q04120
J	-7	LYS	-	expression tag	UNP Q04120
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

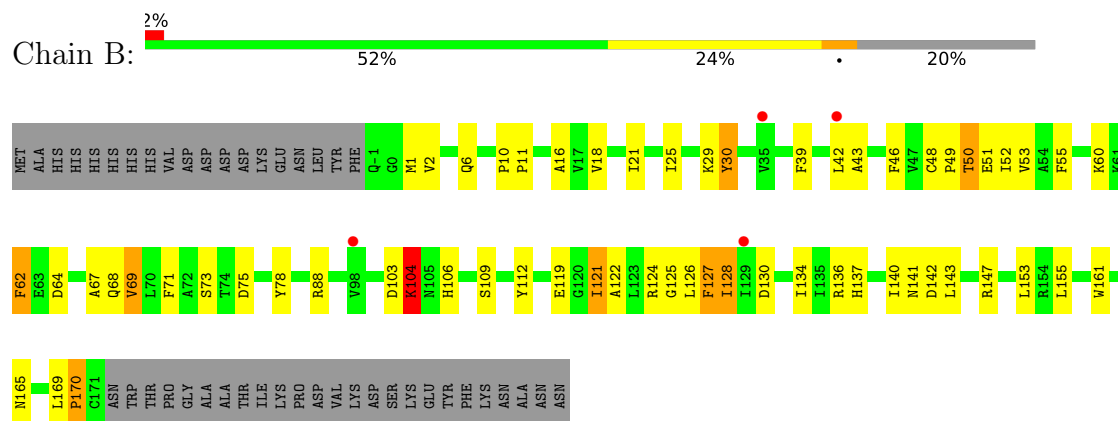
3 Residue-property plots

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.

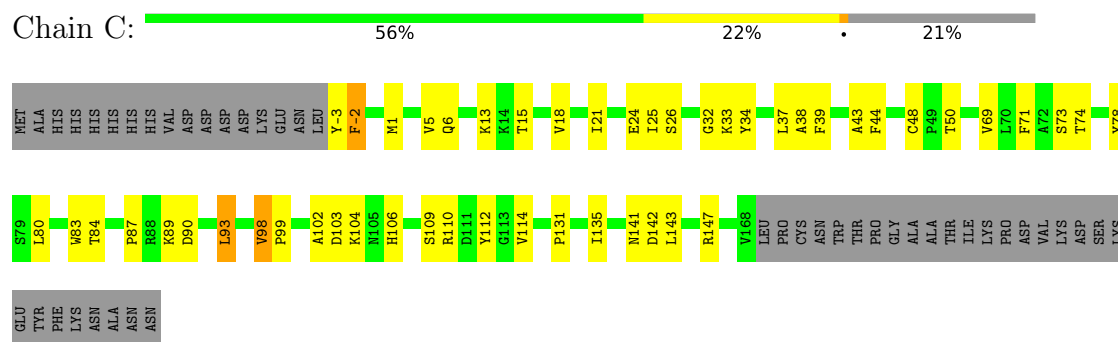
• Molecule 1: Peroxiredoxin TSA2



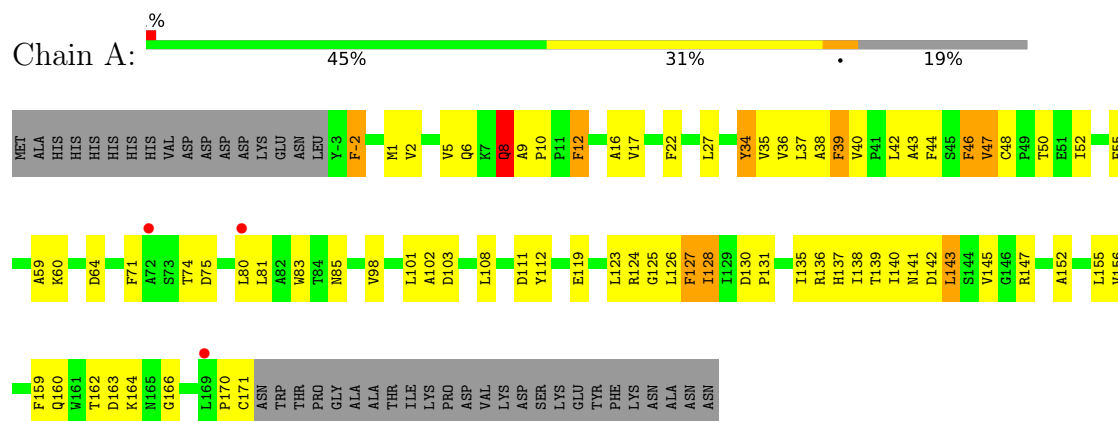
• Molecule 1: Peroxiredoxin TSA2



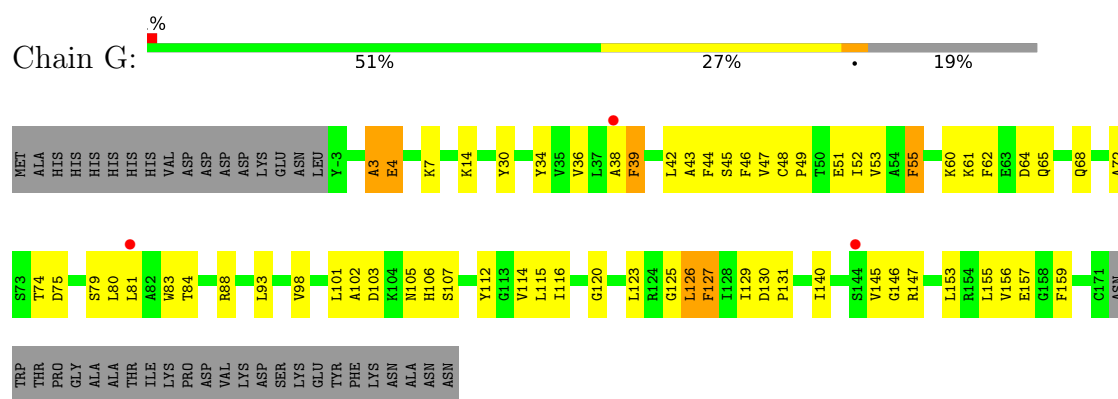
• Molecule 1: Peroxiredoxin TSA2



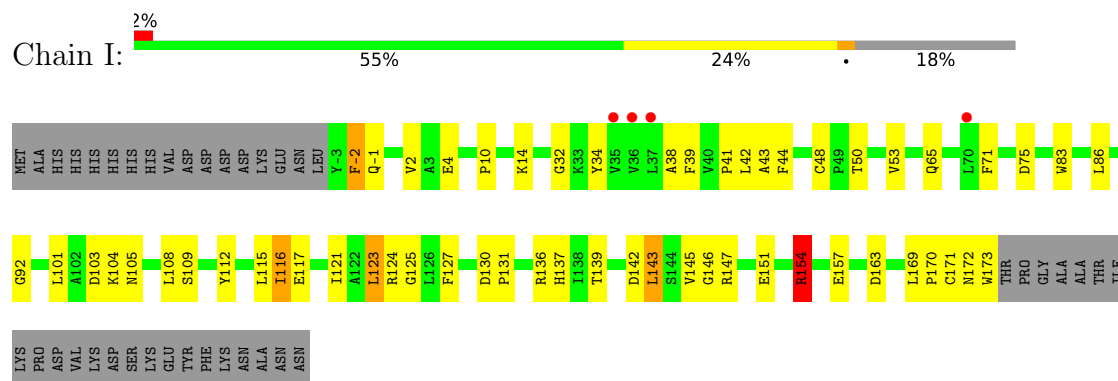
- Molecule 1: Peroxiredoxin TSA2



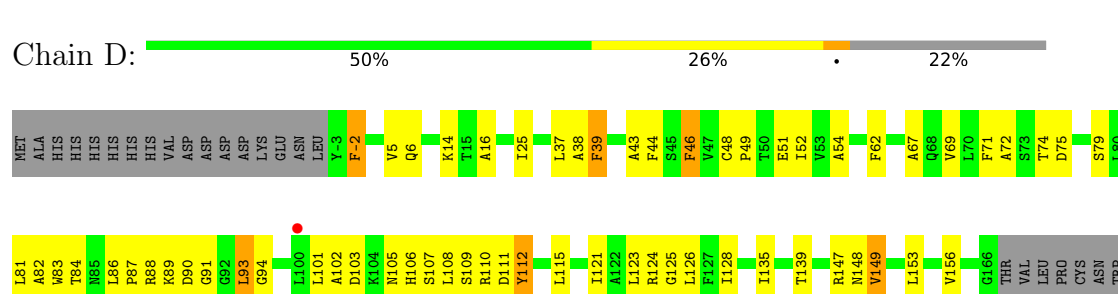
- Molecule 1: Peroxiredoxin TSA2



- Molecule 1: Peroxiredoxin TSA2



- Molecule 1: Peroxiredoxin TSA2



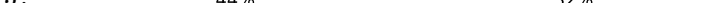
THR	PRO	GLY	ALA	ALA	THR	ILE	LYS	PRO	ASP	VAL	LYS	ASP	SER	LYS	GLU	TYR	PHE	LYS	ASN	ALA	ASN	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Peroxiredoxin TSA2

Chain E:  50% 30% 2% 18%

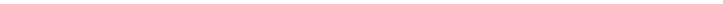
V166		Q65	HIS	ALA	MET
Q160		Q68	HIS	HIS	
D163		V69	HIS	HIS	
P170		L70	HIS	HIS	
T174		A72	HIS	HIS	
PRO		S73	VAL	ASP	
GLY		T74	ASP	ASP	
ALA		Y78	ASP	ASP	
THR		W83	LYS	GLU	
ILE		R88	LYS	ASN	
PRO		G82	LYS	LEU	
ASP		L93	F-2	Y-3	
VAL		L100	F-1		
LYS		D103	V5		
ASP		K104	A9		
SER		N105	P10		
LYS		H106	K14		
GLU		S107	T15		
TYR		L108	A16		
PHE		Y112	F22		
LYS		G113	I25		
ASN		V114	E28		
ALA		R124	K29		
ASN		L126	Y30		
ASN		F127	K31		
ASN		I128	Y34		
ASN		I129	L37		
ASN		D130	A38		
ASN		P131	F39		
ASN		K132	L42		
ASN		G133	A43		
ASN		L134	F44		
ASN		I135	S45		
ASN		R136	F46		
ASN		H137	V47		
ASN		N141	C48		
ASN		D142	P49		
ASN		L143	T50		
ASN		S144	E51		
ASN		R147	I52		
ASN		F148	F55		
ASN		V149	Y61		
ASN		A152			
ASN		L153			

- Molecule 1: Peroxiredoxin TSA2

Chain J:  44% 32% . 19%

F159	D75	MET
Q160	S76	ALA
W161	E77	HIS
T162	Y78	HIS
D163		HIS
K164	R88	HIS
M165		HIS
G166	G92	VAL
T167		ASP
V168	K97	ASP
L169	V98	ASP
P170	P99	ASP
C171		ASP
ASN	A102	LYS
TRP	D103	GLU
THR	K104	ASN
PRO	N105	LEU
GLY	H106	Y-3
ALA	S107	F-2
ALA	L108	
THR	S109	M1
ILE	R110	V2
LYS	D111	A3
PRO	Y112	E4
ASP	G113	V5
VAL	V114	Q6
LYS		
ASP	E117	A9
SER		
LYS	I121	V18
GLU		
TYR	R124	F22
PHE	G125	E23
LYS	L126	
ASN	F127	K29
ALA	I128	
ASN	I129	Y34
ASN	D130	V35
ASN	P131	V36
		L37
		A38
	I135	F39
	R136	V40
	H137	
	L138	A43
	T139	
	I140	C48
	N141	P49
	D142	
	L143	A58
	S144	A59
	V145	
	G146	F62
	R147	
	N148	Q65
	V149	
		V69
	L155	S73
	V156	W74
	E157	
	G158	

- Molecule 1: Peroxiredoxin TSA2

Chain F: 

R154	V69	HET
L155	F71	ALA
F159		HIS
		HIS
T162	T74	HIS
D163	D75	HIS
K164	S76	HIS
L165	E77	HIS
M165	S78	VAL
G166	S79	ASP
	L80	ASP
THR		ASP
VAL		ASP
LEU	W83	ASP
PRO		LYS
CYS	L86	GLU
ASN	P87	ASN
TRP		LEU
THR	L93	Y-3
PRO		F-2
GLY	V96	
ALA		M1
ALA	L100	V2
THR	L101	
ILE	A102	V5
LYS	D103	Q6
PRO		K7
ASP	L108	Q8
VAL		
LYS	D111	F12
ASP	Y112	K13
SER		K14
LYS	A122	T15
GLU	L123	A16
TYR	R124	
PHE	G125	
LYS	L126	G20
ASN	F127	
LYS		S26
ASN	I128	
ASN	I129	Y34
ASN	D130	V35
	P131	V36
		L37
	G133	A38
	I134	F39
	I135	
	R136	A43
	H137	
	D142	C48
	L143	P49
		T50
	S144	E51
	V145	I52
	G146	V53
	R147	A54
	F148	F55
	V149	
	N150	F62
	E151	
	A152	A67
	I153	A69

4 Data and refinement statistics

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 – 5.00	Depositor EDS
% Data completeness (in resolution range)	83.2 (46.35-5.00) 78.0 (46.35-5.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.64 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.274 , 0.375 0.282 , 0.363	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 , 394.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	1/1395 (0.1%)	0.67	0/1890
1	B	0.26	0/1370	0.56	0/1856
1	C	0.25	0/1373	0.59	0/1859
1	D	0.31	0/1359	0.60	0/1839
1	E	0.27	0/1426	0.67	0/1934
1	F	0.22	0/1359	0.63	0/1839
1	G	0.29	0/1395	0.62	0/1890
1	H	0.24	0/1426	0.58	0/1934
1	I	0.25	0/1419	0.56	1/1924 (0.1%)
1	J	0.23	0/1395	0.65	0/1890
All	All	0.27	1/13917 (0.0%)	0.62	1/18855 (0.0%)

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	6.33	1.35	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	154	ARG	CB-CG-CD	5.04	122.88	111.30

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

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	78	0
1	B	1342	0	1370	64	0
1	C	1344	0	1367	36	0
1	D	1330	0	1351	66	0
1	E	1394	0	1412	67	0
1	F	1330	0	1350	78	0
1	G	1365	0	1388	72	0
1	H	1394	0	1411	52	0
1	I	1387	0	1404	55	0
1	J	1365	0	1388	79	0
All	All	13616	0	13829	591	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 22.

All (591) 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:H:170:PRO:C	1:G:48:CYS:SG	2.41	1.04
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:H:46:PHE:HD1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:55:PHE:CE1	1:G:147:ARG:HB2	2.33	0.63
1:E:88:ARG:HA	1:E:92:GLY:O	1.99	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:D:83:TRP:C	1:D:93:LEU:HD11	2.24	0.62
1:I:142:ASP:OD1	1:J:6:GLN:NE2	2.32	0.62
1:E:126:LEU:C	1:E:127:PHE:HD1	2.09	0.61
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:B:103:ASP:OD2	1:B:109:SER:N	2.26	0.61
1:A:142:ASP:OD1	1:A:143:LEU:HD23	2.01	0.61
1:E:46:PHE:CD1	1:E:46:PHE:O	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:CD1	1:D:46:PHE:N	2.71	0.58
1:F:-2:PHE:HD1	1:F:-2:PHE:H	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: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:D:87:PRO:C	1:D:91:GLY:HA3	2.29	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:OD1	1:H:141:ASN:N	2.37	0.57
1:F:14:LYS:HE3	1:F:103:ASP:HA	1.85	0.56
1:F:43:ALA:N	1:F:75:ASP:OD2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:-2:PHE:CD1	1:F:-2:PHE:N	2.74	0.56
1:D:86:LEU:C	1:D:91:GLY:HA3	2.31	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:G:53:VAL:HG21	1:G:88:ARG:NE	2.19	0.55
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: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:CD1	1:E:30:TYR:N	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:G:126:LEU:C	1:G:127:PHE:HD1	2.15	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:CD1	1:B:30:TYR:N	2.76	0.54
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:59:ALA:HB1	1:J:98:VAL:HG13	1.90	0.53
1:J:103:ASP:OD1	1:J:106:HIS:N	2.41	0.53
1:G:44:PHE:CE1	1:G:83:TRP:HB2	2.43	0.53
1:F:-2:PHE:HD1	1:F:-2:PHE:N	2.07	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:J:160:GLN:O	1:J:164:LYS:HB2	2.09	0.53
1:F:34:TYR:CE1	1:F:131:PRO:HD3	2.44	0.53
1:H:155:LEU:O	1:H:159:PHE:CD1	2.62	0.53
1:D:82:ALA:HB1	1:E:44:PHE:CE2	2.44	0.53
1:F:83:TRP:CD2	1:F:93:LEU:HD23	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:156:VAL:O	1:J:160:GLN:HB2	2.09	0.53
1:H:151:GLU:O	1:H:155:LEU:HG	2.09	0.53
1:F:74:THR:HA	1:F:103:ASP:O	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:H:78:TYR:CE2	1:I:42:LEU:HD13	2.43	0.52
1:E:38:ALA:HA	1:E:125:GLY:O	2.09	0.52
1:B:30:TYR:CE2	1:B:68:GLN:HG2	2.45	0.52
1:A:126:LEU:C	1:A:127:PHE:HD1	2.16	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:G:49:PRO:O	1:G:53:VAL:HG23	2.09	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: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:9:ALA:HA	1:J:135:ILE:HD11	1.91	0.52
1:J:141:ASN:O	1:J:142:ASP:HB2	2.10	0.52
1:E:29:LYS:HB3	1:E:30:TYR:CD1	2.44	0.52
1:E:44:PHE:N	1:E:44:PHE:HD1	2.08	0.52
1:J:126:LEU:C	1:J:127:PHE:HD1	2.18	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:H:155:LEU:HB2	1:H:159:PHE:CE1	2.45	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:D:72:ALA:HA	1:D:101:LEU:O	2.10	0.52
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:C:142:ASP:OD1	1:C:143:LEU:N	2.38	0.51
1:A:74:THR:HA	1:A:103:ASP:O	2.10	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:G:34:TYR:CE1	1:G:131:PRO:HD3	2.45	0.51
1:D:38:ALA:C	1:D:39:PHE:HD1	2.19	0.51
1:B:112:TYR:HB3	1:B:127:PHE:CE2	2.46	0.51
1:G:38:ALA:HA	1:G:125:GLY:O	2.10	0.51
1:D:-2:PHE:HD1	1:D:-2:PHE:H	1.58	0.51
1:A:124:ARG:NH2	1:A:143:LEU:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ALA:HA	1:G:101:LEU:O	2.11	0.51
1:A:136:ARG:HH22	1:A:163:ASP:CG	2.19	0.51
1:G:44:PHE:CE2	1:F:79:SER:HA	2.45	0.51
1:I:34:TYR:CE1	1:I:131:PRO:HD3	2.46	0.51
1:I:123:LEU:CD1	1:J:5:VAL:HG11	2.40	0.51
1:D:84:THR:HA	1:D:93:LEU:CD1	2.40	0.51
1:J:39:PHE:O	1:J:147:ARG:NH2	2.43	0.51
1:J:34:TYR:CE1	1:J:131:PRO:HD3	2.46	0.51
1:F:62:PHE:O	1:F:67:ALA:N	2.41	0.51
1:B:127:PHE:CD1	1:B:127:PHE:N	2.78	0.51
1:B:126:LEU:C	1:B:127:PHE:CD1	2.89	0.50
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:B:1:MET:HE1	1:B:11:PRO:HD2	1.93	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:49:PRO:C	1:G:88:ARG:HH21	2.19	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
1:H:37:LEU:HD23	1:H:112:TYR:HE2	1.78	0.49
1:A:127:PHE:HD1	1:A:127:PHE:N	2.10	0.49
1:I:117:GLU:N	1:I:117:GLU:OE1	2.43	0.49
1:H:10:PRO:HB2	1:H:112:TYR:HE1	1.77	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:C:-2:PHE:CE1	1:C:1:MET:CG	2.95	0.49
1:A:-2:PHE:CE1	1:A:1:MET:HG2	2.48	0.49
1:D:38:ALA:HA	1:D:125:GLY:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:44:PHE:H	1:E:83:TRP:CD1	2.31	0.49
1:H:124:ARG:O	1:H:140:ILE:HA	2.12	0.49
1:G:60:LYS:NZ	1:G:64:ASP:OD1	2.44	0.49
1:H:37:LEU:HD23	1:H:112:TYR:CE2	2.48	0.48
1:B:6:GLN:OE1	1:A:123:LEU:HD21	2.13	0.48
1:G:46:PHE:C	1:G:47:VAL:HG13	2.38	0.48
1:G:55:PHE:CZ	1:G:147:ARG:CB	2.95	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: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: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:F:150:ASN:O	1:F:154:ARG:CB	2.60	0.48
1:C:141:ASN:OD1	1:C:147:ARG:HG2	2.14	0.48
1:A:12:PHE:CD2	1:A:108:LEU:HD21	2.48	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:C:-2:PHE:CD1	1:C:1:MET:HG2	2.48	0.48
1:A:34:TYR:OH	1:A:163:ASP:OD2	2.27	0.48
1:E:127:PHE:HD1	1:E:127:PHE:N	2.11	0.48
1:J:39:PHE:CE2	1:J:114:VAL:HG21	2.49	0.48
1:F:108:LEU:HD11	1:F:112:TYR:CE2	2.48	0.48
1:F:126:LEU:C	1:F:127:PHE:HD1	2.22	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: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:D:52:ILE:HG12	1:D:71:PHE:CE2	2.48	0.48
1:G:3:ALA:O	1:G:4:GLU:HB2	2.14	0.48
1:F:12:PHE:HE2	1:F:108:LEU:HD22	1.77	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:I:103:ASP:O	1:I:105:ASN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:TYR:OH	1:E:160:GLN:HA	2.14	0.48
1:H:58:ALA:O	1:H:62:PHE:CD2	2.67	0.47
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:A:43:ALA:HB2	1:A:75:ASP:OD2	2.14	0.47
1:I:123:LEU:HD22	1:I:143:LEU:CD2	2.43	0.47
1:E:39:PHE:CE2	1:E:114:VAL:HG21	2.49	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:N	1:E:127:PHE:CD1	2.82	0.47
1:F:12:PHE:CD2	1:F:108:LEU:HD13	2.49	0.47
1:F:126:LEU:C	1:F:127:PHE:CD1	2.92	0.47
1:F:127:PHE:HD1	1:F:127:PHE:N	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:HG12	1:H:47:VAL:O	2.15	0.47
1:J:3:ALA:HB2	1:J:112:TYR:HA	1.96	0.47
1:H:44:PHE:CZ	1:H:83:TRP:HB2	2.50	0.47
1:B:29:LYS:HB2	1:B:30:TYR:CE1	2.49	0.47
1:B:137:HIS:ND1	1:A:141:ASN:OD1	2.37	0.47
1:C:-2:PHE:CE1	1:C:1:MET:HG2	2.50	0.47
1:A:12:PHE:CE1	1:A:27:LEU:HB2	2.50	0.47
1:A:127:PHE:N	1:A:127:PHE:CD1	2.81	0.47
1:D:54:ALA:HB1	1:D:149:VAL:CG2	2.44	0.47
1:F:62:PHE:HB3	1:F:67:ALA:HB3	1.96	0.47
1:F:124:ARG:HD2	1:F:145:VAL:O	2.14	0.47
1:F:127:PHE:CD1	1:F:127:PHE:N	2.81	0.47
1:J:112:TYR:CD1	1:J:127:PHE:CE2	3.03	0.47
1:I:42:LEU:HD21	1:I:121:ILE:HG21	1.97	0.47
1:I:50:THR:O	1:I:53:VAL:HG22	2.15	0.47
1:I:130:ASP:HB3	1:I:131:PRO:CD	2.44	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:A:12:PHE:N	1:A:12:PHE:CD1	2.82	0.47
1:G:49:PRO:HA	1:G:52:ILE:HD11	1.97	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:O	1:C:114:VAL:HG23	2.15	0.46
1:G:43:ALA:C	1:G:44:PHE:CG	2.91	0.46
1:D:82:ALA:HB2	1:E:44:PHE:CD2	2.49	0.46
1:E:39:PHE:CE1	1:E:72:ALA:HB3	2.50	0.46
1:J:2:VAL:O	1:J:111:ASP:O	2.34	0.46
1:F:62:PHE:CD1	1:F:62:PHE:N	2.83	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:H:65:GLN:OE1	1:H:65:GLN:O	2.33	0.46
1:B:78:TYR:HB3	1:C:44:PHE:CG	2.51	0.46
1:A:59:ALA:HB2	1:A:98:VAL:HG13	1.97	0.46
1:B:126:LEU:C	1:B:127:PHE:HD1	2.24	0.46
1:A:81:LEU:HG	1:A:85:ASN:OD1	2.16	0.46
1:G:30:TYR:CE1	1:G:68:GLN:HG2	2.51	0.46
1:F:62:PHE:N	1:F:62:PHE:HD1	2.14	0.46
1:A:130:ASP:HB2	1:A:131:PRO:CD	2.45	0.46
1:D:89:LYS:CG	1:D:90:ASP:N	2.79	0.46
1:J:22:PHE:N	1:J:22:PHE:CD1	2.84	0.46
1:A:-2:PHE:CE1	1:A:1:MET:CG	2.99	0.46
1:A:152:ALA:O	1:A:156:VAL:HG23	2.15	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:A:38:ALA:C	1:A:39:PHE:HD1	2.24	0.45
1:E:5:VAL:HA	1:E:135:ILE:O	2.17	0.45
1:E:55:PHE:CE1	1:E:149:VAL:HG23	2.51	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:F:164:LYS:C	1:F:166:GLY:H	2.25	0.45
1:H:62:PHE:CZ	1:H:153:LEU:HD22	2.52	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:55:PHE:HB2	1:H:71:PHE:CZ	2.50	0.45
1:H:61:LYS:HE3	1:H:153:LEU:HD11	1.99	0.45
1:E:136:ARG:NH2	1:E:163:ASP:OD2	2.42	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:B:124:ARG:O	1:B:140:ILE:HA	2.16	0.45
1:A:40:VAL:HG11	1:A:52:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:VAL:HA	1:G:127:PHE:O	2.16	0.45
1:H:55:PHE:O	1:H:59:ALA:HB2	2.17	0.45
1:B:42:LEU:HD13	1:C:78:TYR:CD2	2.51	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:I:32:GLY:HA2	1:I:131:PRO:HA	1.98	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: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:H:34:TYR:CD1	1:H:130:ASP:HA	2.52	0.45
1:C:74:THR:HA	1:C:103:ASP:O	2.17	0.45
1:A:124:ARG:O	1:A:140:ILE:HA	2.17	0.45
1:I:32:GLY:HA2	1:I:131:PRO:CA	2.47	0.45
1:D:112:TYR:CD1	1:D:112:TYR:N	2.85	0.45
1:F:39:PHE:N	1:F:39:PHE:CD1	2.84	0.45
1:F:50:THR:O	1:F:53:VAL:HG22	2.17	0.45
1:H:51:GLU:OE2	1:H:124:ARG:CZ	2.64	0.44
1:A:10:PRO:HD2	1:A:112:TYR:CE1	2.51	0.44
1:E:152:ALA:O	1:E:156:VAL:HG23	2.17	0.44
1:A:34:TYR:OH	1:A:160:GLN:HA	2.17	0.44
1:J:117:GLU:OE1	1:J:117:GLU:N	2.47	0.44
1:F:12:PHE:CD1	1:F:12:PHE:C	2.95	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:G:55:PHE:CZ	1:G:147:ARG:HB2	2.52	0.44
1:I:143:LEU:N	1:I:143:LEU:HD23	2.31	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:D:147:ARG:O	1:D:148:ASN:HB2	2.17	0.44
1:F:5:VAL:O	1:F:6:GLN:HB2	2.16	0.44
1:H:153:LEU:HD23	1:H:153:LEU:N	2.32	0.44
1:C:18:VAL:O	1:C:21:ILE:HG12	2.17	0.44
1:A:126:LEU:O	1:A:138:ILE:HA	2.18	0.44
1:G:116:ILE:HD11	1:G:123:LEU:HD12	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:GLN:HG3	1:F:133:GLY:O	2.17	0.44
1:A:43:ALA:CB	1:A:75:ASP:OD2	2.65	0.44
1:A:126:LEU:C	1:A:127:PHE:CD1	2.96	0.44
1:G:46:PHE:O	1:G:47:VAL:CG1	2.66	0.44
1:I:136:ARG:HH22	1:I:163:ASP:CG	2.24	0.44
1:D:93:LEU:HD12	1:D:93:LEU:H	1.81	0.44
1:B:49:PRO:O	1:B:52:ILE:HB	2.18	0.44
1:A:12:PHE:H	1:A:12:PHE:HD1	1.64	0.44
1:J:5:VAL:O	1:J:6:GLN:HB2	2.17	0.44
1:F:43:ALA:CB	1:F:75:ASP:OD2	2.66	0.44
1:A:22:PHE:CE1	1:A:81:LEU:HD13	2.53	0.44
1:A:46:PHE:HB2	1:A:47:VAL:H	1.62	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:G:14:LYS:HD2	1:G:103:ASP:OD1	2.18	0.43
1:I:169:LEU:HB3	1:I:172:ASN:HB2	1.99	0.43
1:E:44:PHE:HE1	1:E:83:TRP:HB2	1.82	0.43
1:E:47:VAL:HG21	1:E:124:ARG:NH2	2.32	0.43
1:F:39:PHE:N	1:F:39:PHE:HD1	2.15	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:B:104:LYS:O	1:B:106:HIS:ND1	2.48	0.43
1:A:123:LEU:HD23	1:A:143:LEU:CD2	2.48	0.43
1:I:116:ILE:HG12	1:I:123:LEU:CD2	2.48	0.43
1:D:39:PHE:HE2	1:D:109:SER:HA	1.83	0.43
1:J:159:PHE:O	1:J:162:THR:HG22	2.18	0.43
1:H:62:PHE:CZ	1:H:153:LEU:CD2	3.01	0.43
1:B:103:ASP:O	1:B:104:LYS:C	2.61	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:G:155:LEU:O	1:G:159:PHE:CD2	2.71	0.43
1:I:115:LEU:HD12	1:I:121:ILE:O	2.19	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
1:H:34:TYR:CD1	1:H:131:PRO:HD3	2.53	0.43
1:H:123:LEU:HA	1:H:143:LEU:HD21	2.00	0.43
1:B:62:PHE:CD1	1:B:153:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:34:TYR:OH	1:J:160:GLN:HA	2.18	0.43
1:F:2:VAL:O	1:F:111:ASP:O	2.37	0.43
1:H:58:ALA:HB2	1:H:149:VAL:HG21	2.00	0.43
1:D:128:ILE:O	1:D:135:ILE:HA	2.18	0.43
1:H:47:VAL:O	1:H:48:CYS:C	2.61	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:B:128:ILE:HB	1:B:137:HIS:HB3	2.00	0.43
1:I:43:ALA:N	1:I:75:ASP:OD2	2.47	0.43
1:I:112:TYR:HB3	1:I:127:PHE:CE2	2.54	0.43
1:B:51:GLU:HB3	1:B:55:PHE:CE2	2.54	0.43
1:A:5:VAL:HG12	1:A:6:GLN:HG3	2.00	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:B:62:PHE:CD1	1:B:62:PHE:N	2.86	0.43
1:C:5:VAL:HG11	1:D:123:LEU:CD1	2.48	0.43
1:C:43:ALA:HB1	1:C:83:TRP:CE2	2.53	0.43
1:G:34:TYR:HA	1:G:129:ILE:O	2.19	0.43
1:A:47:VAL:HG12	1:A:47:VAL:O	2.19	0.43
1:G:112:TYR:HD1	1:G:127:PHE:CE2	2.37	0.43
1:D:14:LYS:NZ	1:D:105:ASN:OD1	2.52	0.43
1:E:142:ASP:OD2	1:F:136:ARG:HA	2.19	0.43
1:J:39:PHE:N	1:J:39:PHE:CD1	2.87	0.43
1:J:140:ILE:O	1:J:141:ASN:C	2.62	0.43
1:F:12:PHE:O	1:F:26:SER:OG	2.19	0.43
1:H:71:PHE:CD1	1:H:71:PHE:N	2.87	0.42
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:J:39:PHE:N	1:J:39:PHE:HD1	2.17	0.42
1:F:16:ALA:HB2	1:F:101:LEU:HG	2.01	0.42
1:H:136:ARG:NH1	1:H:163:ASP:OD2	2.52	0.42
1:A:16:ALA:HB2	1:A:101:LEU:HD22	2.00	0.42
1:I:48:CYS:HB2	1:J:170:PRO:HB3	2.01	0.42
1:D:107:SER:O	1:D:110:ARG:HB3	2.18	0.42
1:J:137:HIS:CD2	1:J:155:LEU:HD13	2.54	0.42
1:D:44:PHE:CD1	1:D:86:LEU:HD23	2.54	0.42
1:D:103:ASP:OD1	1:D:105:ASN:OD1	2.37	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:F:-3:TYR:CD1	1:F:1:MET:SD	3.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:CD1	1:A:46:PHE:N	2.88	0.42
1:A:55:PHE:O	1:A:59:ALA:N	2.53	0.42
1:A:143:LEU:CD2	1:A:143:LEU:N	2.82	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: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: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:H:71:PHE:N	1:H:71:PHE:HD1	2.18	0.42
1:C:6:GLN:N	1:C:135:ILE:O	2.50	0.42
1:G:127:PHE:HD1	1:G:127:PHE:N	2.17	0.42
1:I:-2:PHE:O	1:I:-1:GLN:C	2.62	0.42
1:I:14:LYS:HE3	1:I:108:LEU:CD1	2.50	0.42
1:I:172:ASN:C	1:I:173:TRP:CE3	2.97	0.42
1:F:62:PHE:CD2	1:F:69:VAL:HG22	2.55	0.42
1:G:75:ASP:O	1:G:102:ALA:HB1	2.20	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:B:78:TYR:HB3	1:C:44:PHE:HB2	2.02	0.42
1:C:106:HIS:O	1:C:110:ARG:HB3	2.20	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:A:128:ILE:HG12	1:A:156:VAL:HG22	2.01	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:D:44:PHE:CE1	1:D:86:LEU:HD23	2.55	0.42
1:J:-2:PHE:CD1	1:J:-2:PHE:N	2.87	0.42
1:F:2:VAL:C	1:F:111:ASP:O	2.62	0.42
1:H:52:ILE:HG23	1:H:71:PHE:CE2	2.55	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:C:32:GLY:C	1:C:33:LYS:HG3	2.45	0.42
1:A:39:PHE:HD1	1:A:39:PHE:N	2.17	0.42
1:G:34:TYR:CD1	1:G:131:PRO:HD3	2.55	0.42
1:G:74:THR:OG1	1:G:120:GLY:O	2.28	0.42
1:G:145:VAL:O	1:G:145:VAL:HG13	2.19	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:H:152:ALA:O	1:H:156:VAL:HG23	2.20	0.41
1:A:17:VAL:HG11	1:A:81:LEU:HB2	2.02	0.41
1:G:83:TRP:CE2	1:G:93:LEU:HB2	2.55	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:F:12:PHE:C	1:F:12:PHE:HD1	2.28	0.41
1:B:53:VAL:CG1	1:B:88:ARG:HD3	2.51	0.41
1:A:39:PHE:N	1:A:39:PHE:CD1	2.87	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:I:38:ALA:HA	1:I:147:ARG:HH12	1.85	0.41
1:F:124:ARG:O	1:F:147:ARG:NH1	2.54	0.41
1:H:62:PHE:CD2	1:H:69:VAL:CG2	3.03	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: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:A:12:PHE:HE1	1:A:27:LEU:HB2	1.86	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: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:G:114:VAL:HG12	1:G:140:ILE:HD12	2.03	0.41
1:I:170:PRO:HB2	1:J:48:CYS:SG	2.60	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:D:88:ARG:CG	1:D:93:LEU:O	2.69	0.41
1:J:37:LEU:HG	1:J:39:PHE:HE1	1.86	0.41
1:J:110:ARG:HA	1:J:110:ARG:HE	1.85	0.41
1:J:135:ILE:C	1:J:136:ARG:HG2	2.44	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:I:109:SER:OG	1:I:115:LEU:HB2	2.20	0.41
1:F:93:LEU:CD1	1:F:96:VAL:HG13	2.51	0.41
1:H:38:ALA:HB1	1:H:147:ARG:NH2	2.35	0.41
1:H:128:ILE:HG12	1:H:156:VAL:HG22	2.02	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:G:4:GLU:HB3	1:G:7:LYS:CG	2.51	0.41
1:I:10:PRO:O	1:I:112:TYR:OH	2.25	0.41
1:D:44:PHE:CE1	1:D:86:LEU:CD2	3.04	0.41
1:D:126:LEU:HB3	1:D:139:THR:HB	2.03	0.41
1:D:153:LEU:O	1:D:156:VAL:HG22	2.21	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:F:155:LEU:O	1:F:159:PHE:CD2	2.73	0.41
1:B:50:THR:HG1	1:A:171:CYS:CB	2.31	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:D:89:LYS:HG3	1:D:90:ASP:N	2.36	0.41
1:E:29:LYS:HB3	1:E:30:TYR:CE1	2.56	0.41
1:E:37:LEU:HD23	1:E:112:TYR:HE2	1.86	0.41
1:F:130:ASP:OD1	1:F:134:ILE:N	2.50	0.41
1:F:164:LYS:C	1:F:166:GLY:N	2.79	0.41
1:B:78:TYR:HB3	1:C:44:PHE:CD2	2.56	0.40
1:B:103:ASP:O	1:B:103:ASP:OD1	2.39	0.40
1:A:5:VAL:HG13	1:A:135:ILE:O	2.21	0.40
1:G:80:LEU:HD12	1:G:102:ALA:HB2	2.04	0.40
1:F:-2:PHE:CD1	1:F:1:MET:SD	3.14	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:H:124:ARG:HG3	1:H:143:LEU:HD23	2.03	0.40
1:A:81:LEU:O	1:A:85:ASN:OD1	2.39	0.40
1:G:103:ASP:OD1	1:G:105:ASN:OD1	2.38	0.40
1:D:39:PHE:HD1	1:D:39:PHE:N	2.19	0.40
1:D:108:LEU:O	1:D:111:ASP:N	2.54	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:C:15:THR:HG22	1:C:24:GLU:OE2	2.20	0.40
1:A:2:VAL:HA	1:A:111:ASP:O	2.21	0.40
1:I:44:PHE:H	1:I:83:TRP:CD1	2.39	0.40
1:I:116:ILE:HD11	1:I:143:LEU:HD11	2.03	0.40
1:E:48:CYS:HB3	1:E:50:THR:HG23	2.03	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:J:124:ARG:HD3	1:J:147:ARG:HH21	1.87	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: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:J:168:VAL:HG22	1:J:169:LEU:H	1.86	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
1:B:16:ALA:HB3	1:B:25:ILE:CG1	2.51	0.40
1:B:169:LEU:O	1:B:170:PRO:C	2.53	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

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%)	21	58
1	B	171/217 (79%)	161 (94%)	7 (4%)	3 (2%)	6	32
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%)	21	58
1	G	173/217 (80%)	162 (94%)	9 (5%)	2 (1%)	10	42
1	H	176/217 (81%)	166 (94%)	9 (5%)	1 (1%)	21	58
1	I	175/217 (81%)	164 (94%)	10 (6%)	1 (1%)	21	58
1	J	173/217 (80%)	153 (88%)	16 (9%)	4 (2%)	5	27
All	All	1723/2170 (79%)	1605 (93%)	105 (6%)	13 (1%)	16	53

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 ⓘ

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%)	136 (92%)	11 (8%)	12	33
1	B	145/184 (79%)	137 (94%)	8 (6%)	19	42
1	C	144/184 (78%)	140 (97%)	4 (3%)	38	59
1	D	142/184 (77%)	135 (95%)	7 (5%)	22	44
1	E	150/184 (82%)	146 (97%)	4 (3%)	39	60
1	F	142/184 (77%)	132 (93%)	10 (7%)	14	36
1	G	147/184 (80%)	142 (97%)	5 (3%)	32	54
1	H	150/184 (82%)	142 (95%)	8 (5%)	20	42
1	I	149/184 (81%)	145 (97%)	4 (3%)	39	60
1	J	147/184 (80%)	141 (96%)	6 (4%)	27	49
All	All	1463/1840 (80%)	1396 (95%)	67 (5%)	24	46

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	46	PHE
1	H	71	PHE
1	H	96	VAL
1	H	141	ASN
1	H	145	VAL
1	H	153	LEU
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	121	ILE
1	B	127	PHE
1	B	128	ILE
1	C	-2	PHE
1	C	89	LYS
1	C	93	LEU
1	C	98	VAL
1	A	-2	PHE
1	A	8	GLN
1	A	12	PHE
1	A	34	TYR
1	A	35	VAL
1	A	37	LEU
1	A	39	PHE
1	A	46	PHE
1	A	127	PHE
1	A	128	ILE
1	A	143	LEU
1	G	39	PHE
1	G	55	PHE
1	G	98	VAL
1	G	126	LEU
1	G	127	PHE
1	I	116	ILE
1	I	123	LEU
1	I	143	LEU
1	I	154	ARG
1	D	-2	PHE
1	D	39	PHE
1	D	46	PHE

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Mol	Chain	Res	Type
1	D	69	VAL
1	D	93	LEU
1	D	112	TYR
1	D	149	VAL
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	40	VAL
1	J	129	ILE
1	J	145	VAL
1	F	-2	PHE
1	F	12	PHE
1	F	34	TYR
1	F	39	PHE
1	F	62	PHE
1	F	93	LEU
1	F	101	LEU
1	F	127	PHE
1	F	149	VAL
1	F	153	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	85	ASN
1	C	106	HIS
1	A	106	HIS
1	G	65	GLN
1	G	141	ASN
1	D	8	GLN
1	D	160	GLN
1	E	106	HIS
1	J	85	ASN
1	F	160	GLN
1	F	165	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	175/217 (80%)	-0.20	3 (1%) 69 56	313, 374, 442, 476	0
1	B	173/217 (79%)	-0.05	4 (2%) 61 50	311, 364, 413, 508	0
1	C	172/217 (79%)	-0.41	0 100 100	307, 370, 441, 493	0
1	D	170/217 (78%)	-0.24	1 (0%) 85 73	314, 361, 444, 598	0
1	E	178/217 (82%)	-0.41	0 100 100	302, 350, 391, 445	0
1	F	170/217 (78%)	-0.05	4 (2%) 59 49	266, 319, 375, 482	0
1	G	175/217 (80%)	-0.18	3 (1%) 69 56	239, 304, 378, 411	0
1	H	178/217 (82%)	-0.31	0 100 100	259, 302, 368, 462	0
1	I	177/217 (81%)	-0.35	4 (2%) 61 50	274, 332, 396, 413	0
1	J	175/217 (80%)	-0.29	1 (0%) 85 73	306, 356, 422, 578	0
All	All	1743/2170 (80%)	-0.25	20 (1%) 78 63	239, 348, 416, 598	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	144	SER	5.4
1	F	100	LEU	4.6
1	F	71	PHE	4.4
1	A	72	ALA	3.7
1	B	98	VAL	3.5
1	I	35	VAL	3.2
1	A	80	LEU	3.2
1	I	37	LEU	3.0
1	J	37	LEU	2.8
1	A	169	LEU	2.8
1	G	81	LEU	2.8
1	B	129	ILE	2.3
1	D	100	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	35	VAL	2.3
1	G	38	ALA	2.2
1	F	20	GLY	2.2
1	F	144	SER	2.2
1	I	70	LEU	2.1
1	B	42	LEU	2.0
1	I	36	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.