



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 05:07 PM EDT

PDB ID : 3A5W
Title : Peroxiredoxin (wild type) from *Aeropyrum pernix* K1 (reduced form)
Authors : Nakamura, T.; Kado, Y.; Yamaguchi, T.; Matsumura, H.; Ishikawa, K.; Inoue, T.
Deposited on : 2009-08-12
Resolution : 2.20 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

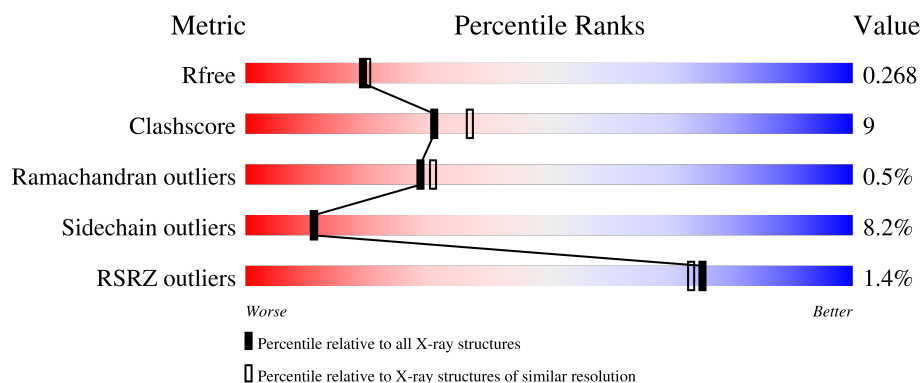
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	249	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>5%</div> <div>• •</div> </div> </div>
1	B	249	<div> <div></div> <div> <div>72%</div> <div>20%</div> <div>6%</div> <div>•</div> </div> </div>
1	C	249	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	249	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>5%</div> <div>•</div> </div> </div>
1	E	249	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>31%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	249	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>70%</div><div>22%</div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	G	249	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>67%</div><div>24%</div><div>5%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	249	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>72%</div><div>20%</div><div>5%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	I	249	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>67%</div><div>26%</div><div>5%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	J	249	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>69%</div><div>21%</div><div>7%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19832 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 Probable peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1953	1257	344	345	7			
1	B	244	Total	C	N	O	S	0	0	0
			1973	1268	347	351	7			
1	C	244	Total	C	N	O	S	0	0	0
			1973	1268	347	351	7			
1	D	244	Total	C	N	O	S	0	0	0
			1973	1268	347	351	7			
1	E	242	Total	C	N	O	S	0	0	0
			1958	1260	345	346	7			
1	F	244	Total	C	N	O	S	0	0	0
			1973	1268	347	351	7			
1	G	242	Total	C	N	O	S	0	0	0
			1958	1260	345	346	7			
1	H	243	Total	C	N	O	S	0	0	0
			1968	1265	346	350	7			
1	I	244	Total	C	N	O	S	0	0	0
			1973	1268	347	351	7			
1	J	241	Total	C	N	O	S	0	0	0
			1953	1257	344	345	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	17	Total	O	0	0
			17	17		
2	C	23	Total	O	0	0
			23	23		
2	D	20	Total	O	0	0
			20	20		

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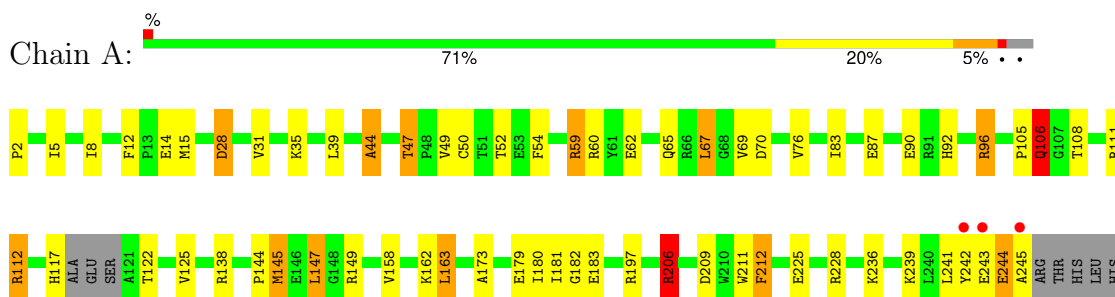
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	21	Total 21	O 21	0	0
2	F	18	Total 18	O 18	0	0
2	G	11	Total 11	O 11	0	0
2	H	15	Total 15	O 15	0	0
2	I	16	Total 16	O 16	0	0
2	J	20	Total 20	O 20	0	0

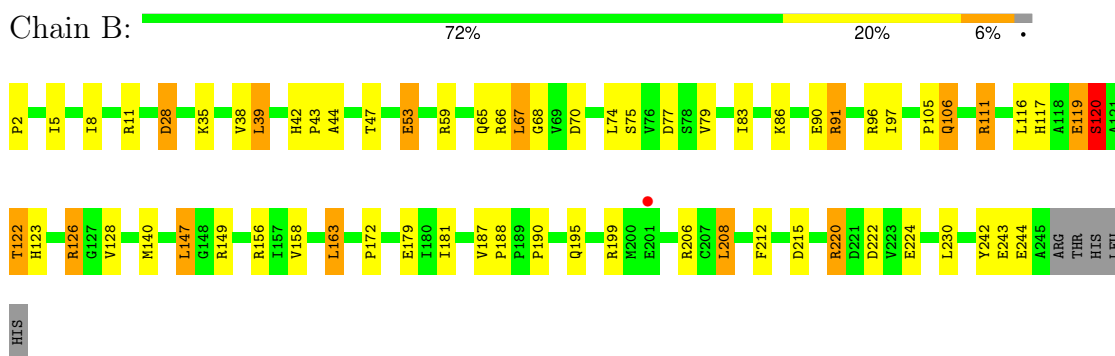
3 Residue-property plots

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.

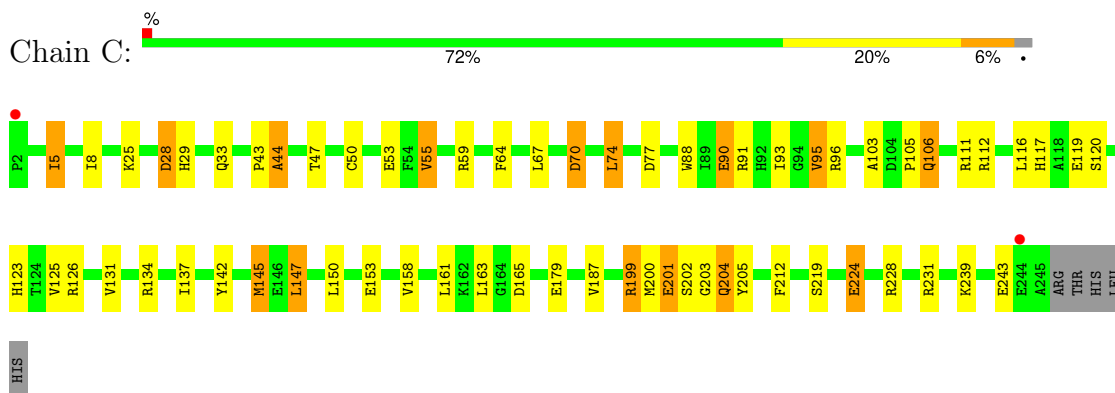
- Molecule 1: Probable peroxiredoxin



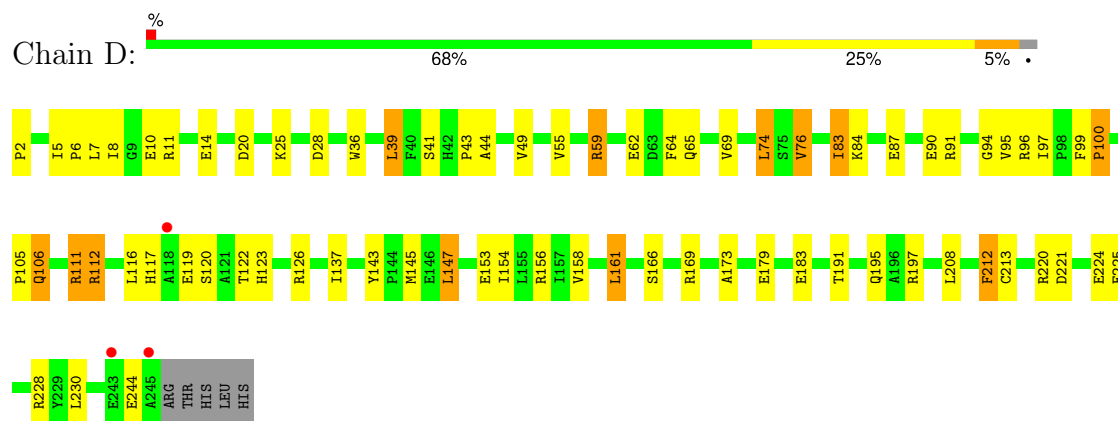
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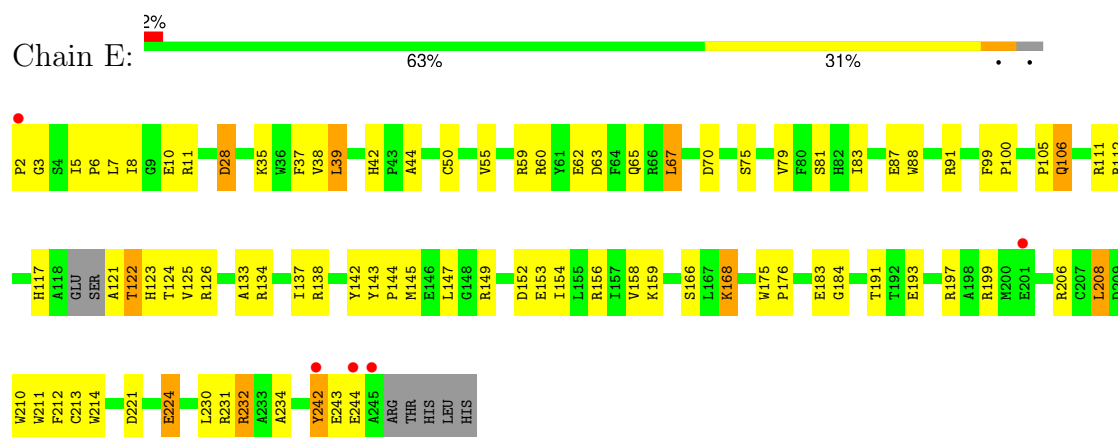
- Molecule 1: Probable peroxiredoxin



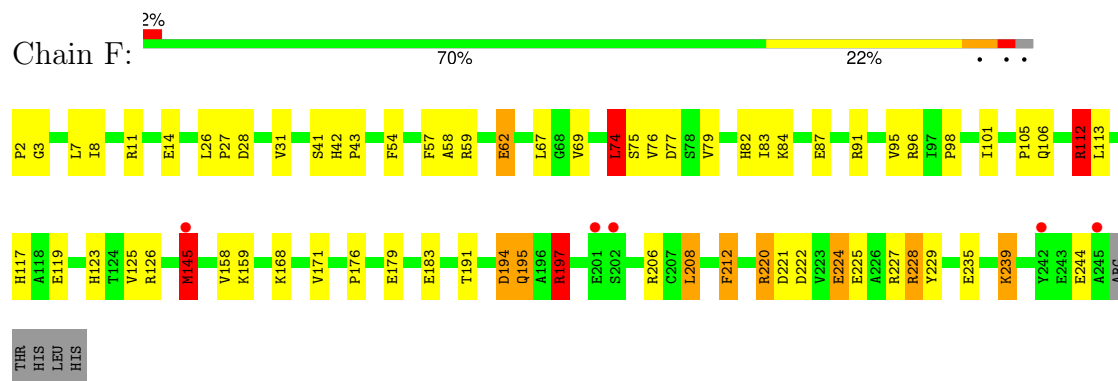
- Molecule 1: Probable peroxiredoxin



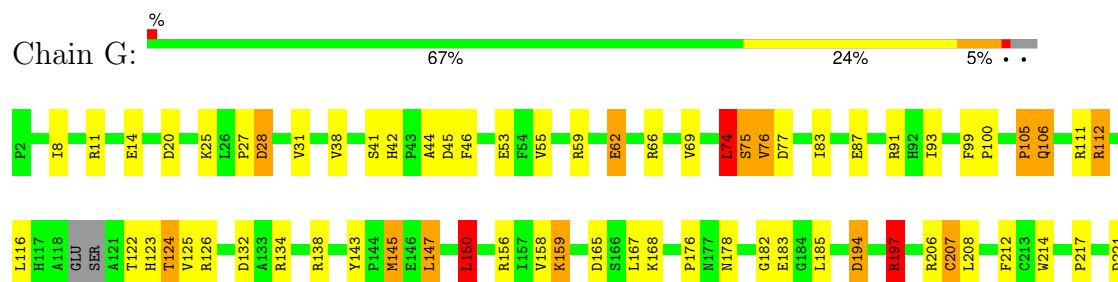
• Molecule 1: Probable peroxiredoxin

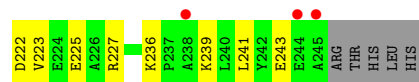


• Molecule 1: Probable peroxiredoxin

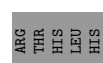
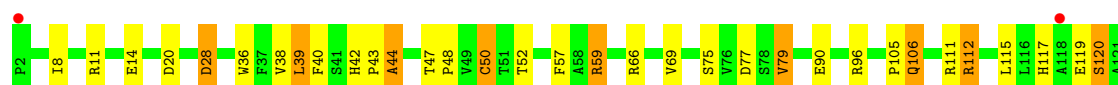
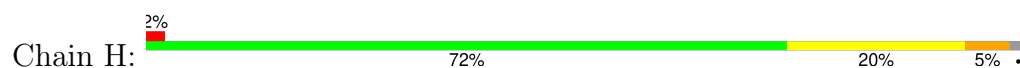


• Molecule 1: Probable peroxiredoxin

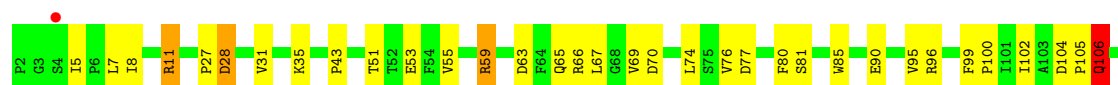




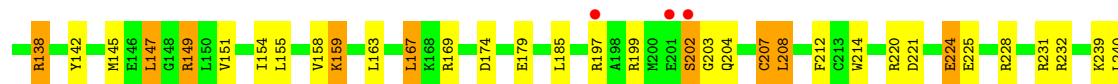
● Molecule 1: Probable peroxiredoxin



● Molecule 1: Probable peroxiredoxin



● Molecule 1: Probable peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.61Å 104.78Å 106.17Å 105.91° 104.92° 92.88°	Depositor
Resolution (Å)	46.83 – 2.20 46.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (46.83-2.20) 94.3 (46.81-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.269 0.209 , 0.268	Depositor DCC
R_{free} test set	7414 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19832	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% 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	1.58	20/2007 (1.0%)	1.19	12/2727 (0.4%)
1	B	1.47	15/2028 (0.7%)	1.25	14/2757 (0.5%)
1	C	1.54	17/2028 (0.8%)	1.25	15/2757 (0.5%)
1	D	1.68	26/2028 (1.3%)	1.24	16/2757 (0.6%)
1	E	1.52	23/2012 (1.1%)	1.24	13/2734 (0.5%)
1	F	1.54	18/2028 (0.9%)	1.21	14/2757 (0.5%)
1	G	1.39	5/2012 (0.2%)	1.22	18/2734 (0.7%)
1	H	1.42	13/2023 (0.6%)	1.17	11/2750 (0.4%)
1	I	1.59	18/2028 (0.9%)	1.22	13/2757 (0.5%)
1	J	1.57	18/2007 (0.9%)	1.30	18/2727 (0.7%)
All	All	1.53	173/20201 (0.9%)	1.23	144/27457 (0.5%)

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	E	0	1

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	50	CYS	CB-SG	10.41	2.00	1.82
1	E	88	TRP	CE3-CZ3	9.00	1.53	1.38
1	I	55	VAL	CB-CG2	8.72	1.71	1.52
1	D	119	GLU	CD-OE2	8.45	1.34	1.25
1	J	224	GLU	CB-CG	8.37	1.68	1.52
1	B	243	GLU	CG-CD	8.23	1.64	1.51
1	D	183	GLU	CD-OE2	8.18	1.34	1.25
1	J	243	GLU	CG-CD	8.14	1.64	1.51
1	F	179	GLU	CD-OE1	8.07	1.34	1.25
1	E	243	GLU	CG-CD	8.07	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	183	GLU	CD-OE2	8.02	1.34	1.25
1	D	44	ALA	CA-CB	7.91	1.69	1.52
1	I	179	GLU	CG-CD	7.82	1.63	1.51
1	D	143	TYR	CE2-CZ	7.71	1.48	1.38
1	A	225	GLU	CG-CD	7.69	1.63	1.51
1	F	225	GLU	CG-CD	7.52	1.63	1.51
1	D	179	GLU	CG-CD	7.37	1.63	1.51
1	J	58	ALA	CA-CB	7.36	1.68	1.52
1	H	38	VAL	CB-CG1	7.33	1.68	1.52
1	A	212	PHE	CE2-CZ	7.18	1.50	1.37
1	I	183	GLU	CD-OE2	7.12	1.33	1.25
1	E	55	VAL	CB-CG1	7.11	1.67	1.52
1	I	235	GLU	CG-CD	7.06	1.62	1.51
1	H	213	CYS	CB-SG	6.98	1.94	1.82
1	D	49	VAL	CB-CG2	6.87	1.67	1.52
1	A	182	GLY	N-CA	6.85	1.56	1.46
1	E	62	GLU	CG-CD	6.81	1.62	1.51
1	I	243	GLU	CG-CD	6.80	1.62	1.51
1	D	224	GLU	CB-CG	6.78	1.65	1.52
1	A	243	GLU	CG-CD	6.76	1.62	1.51
1	B	179	GLU	CG-CD	6.75	1.62	1.51
1	F	62	GLU	CG-CD	6.70	1.62	1.51
1	B	179	GLU	CD-OE2	6.66	1.32	1.25
1	G	38	VAL	CB-CG1	6.62	1.66	1.52
1	J	220	ARG	CG-CD	6.61	1.68	1.51
1	J	138	ARG	CG-CD	6.58	1.68	1.51
1	A	90	GLU	CG-CD	6.57	1.61	1.51
1	I	152	ASP	CB-CG	6.52	1.65	1.51
1	D	213	CYS	CB-SG	6.51	1.93	1.82
1	I	80	PHE	CE1-CZ	6.44	1.49	1.37
1	F	225	GLU	CB-CG	6.43	1.64	1.52
1	I	225	GLU	CG-CD	6.43	1.61	1.51
1	E	153	GLU	CB-CG	6.42	1.64	1.52
1	F	229	TYR	CD1-CE1	6.42	1.49	1.39
1	J	122	THR	CA-CB	6.41	1.70	1.53
1	A	179	GLU	CG-CD	6.39	1.61	1.51
1	F	119	GLU	CD-OE2	6.39	1.32	1.25
1	A	211	TRP	CE3-CZ3	6.35	1.49	1.38
1	H	183	GLU	CD-OE2	6.32	1.32	1.25
1	F	235	GLU	CG-CD	6.32	1.61	1.51
1	D	55	VAL	CB-CG2	6.26	1.66	1.52
1	E	50	CYS	CB-SG	6.24	1.92	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	58	ALA	CA-CB	6.18	1.65	1.52
1	J	32	SER	CB-OG	-6.18	1.34	1.42
1	D	65	GLN	CG-CD	6.18	1.65	1.51
1	C	153	GLU	CB-CG	6.17	1.63	1.52
1	C	145	MET	CG-SD	6.15	1.97	1.81
1	I	53	GLU	CB-CG	6.14	1.63	1.52
1	H	180	ILE	CB-CG2	6.11	1.71	1.52
1	B	179	GLU	CB-CG	6.11	1.63	1.52
1	F	235	GLU	CD-OE2	6.05	1.32	1.25
1	I	95	VAL	CB-CG1	6.02	1.65	1.52
1	B	90	GLU	CG-CD	6.01	1.60	1.51
1	J	142	TYR	CE2-CZ	6.00	1.46	1.38
1	C	53	GLU	CD-OE1	6.00	1.32	1.25
1	F	145	MET	CG-SD	5.99	1.96	1.81
1	F	212	PHE	CB-CG	5.99	1.61	1.51
1	G	53	GLU	CB-CG	5.98	1.63	1.52
1	H	183	GLU	CG-CD	5.98	1.60	1.51
1	J	243	GLU	CB-CG	5.97	1.63	1.52
1	D	153	GLU	CG-CD	5.95	1.60	1.51
1	A	225	GLU	CD-OE2	5.94	1.32	1.25
1	B	90	GLU	CB-CG	5.93	1.63	1.52
1	A	62	GLU	CB-CG	5.92	1.63	1.52
1	J	138	ARG	CD-NE	-5.91	1.36	1.46
1	E	142	TYR	CE2-CZ	5.90	1.46	1.38
1	D	99	PHE	CE1-CZ	5.89	1.48	1.37
1	B	38	VAL	CB-CG1	5.87	1.65	1.52
1	D	119	GLU	CG-CD	5.86	1.60	1.51
1	H	79	VAL	CA-CB	5.86	1.67	1.54
1	C	55	VAL	CB-CG1	5.81	1.65	1.52
1	F	224	GLU	CD-OE1	5.80	1.32	1.25
1	H	158	VAL	CB-CG1	5.78	1.65	1.52
1	C	219	SER	CB-OG	-5.77	1.34	1.42
1	F	224	GLU	CD-OE2	5.76	1.31	1.25
1	A	209	ASP	CB-CG	5.74	1.63	1.51
1	A	12	PHE	CE1-CZ	5.72	1.48	1.37
1	F	171	VAL	CA-CB	5.70	1.66	1.54
1	D	173	ALA	CA-CB	5.69	1.64	1.52
1	J	53	GLU	CB-CG	5.69	1.62	1.52
1	A	62	GLU	CG-CD	5.67	1.60	1.51
1	H	149	ARG	CZ-NH1	-5.65	1.25	1.33
1	E	133	ALA	CA-CB	5.64	1.64	1.52
1	D	225	GLU	CB-CG	5.63	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	GLU	CG-CD	5.63	1.60	1.51
1	I	109	VAL	CA-CB	5.61	1.66	1.54
1	E	184	GLY	C-O	5.61	1.32	1.23
1	C	179	GLU	CD-OE2	5.60	1.31	1.25
1	E	242	TYR	CE2-CZ	5.60	1.45	1.38
1	G	76	VAL	CA-CB	5.59	1.66	1.54
1	E	193	GLU	CD-OE1	5.58	1.31	1.25
1	H	183	GLU	CD-OE1	5.56	1.31	1.25
1	F	183	GLU	CG-CD	5.56	1.60	1.51
1	E	138	ARG	CG-CD	5.55	1.65	1.51
1	E	210	TRP	CB-CG	5.55	1.60	1.50
1	D	212	PHE	CE2-CZ	5.54	1.47	1.37
1	C	243	GLU	CG-CD	5.54	1.60	1.51
1	A	179	GLU	CB-CG	5.53	1.62	1.52
1	A	183	GLU	CD-OE2	5.53	1.31	1.25
1	H	44	ALA	CA-CB	5.53	1.64	1.52
1	B	77	ASP	CB-CG	5.51	1.63	1.51
1	D	36	TRP	CE3-CZ3	5.50	1.47	1.38
1	E	168	LYS	CD-CE	5.50	1.65	1.51
1	C	44	ALA	CA-CB	5.49	1.64	1.52
1	G	145	MET	CG-SD	5.48	1.95	1.81
1	E	44	ALA	CA-CB	5.48	1.64	1.52
1	B	243	GLU	CB-CG	5.46	1.62	1.52
1	C	90	GLU	CB-CG	5.39	1.62	1.52
1	A	65	GLN	CG-CD	5.39	1.63	1.51
1	A	49	VAL	CB-CG2	5.38	1.64	1.52
1	J	77	ASP	CB-CG	5.38	1.63	1.51
1	A	44	ALA	CA-CB	5.37	1.63	1.52
1	I	156	ARG	CG-CD	5.37	1.65	1.51
1	C	179	GLU	CD-OE1	5.36	1.31	1.25
1	A	54	PHE	CE1-CZ	-5.36	1.27	1.37
1	D	83	ILE	CB-CG2	5.34	1.69	1.52
1	E	221	ASP	CB-CG	5.34	1.62	1.51
1	B	119	GLU	CG-CD	5.34	1.59	1.51
1	J	197	ARG	CB-CG	5.32	1.67	1.52
1	I	69	VAL	CB-CG2	5.32	1.64	1.52
1	J	30	TYR	CB-CG	5.31	1.59	1.51
1	B	242	TYR	CD1-CE1	5.30	1.47	1.39
1	E	38	VAL	CB-CG2	5.30	1.64	1.52
1	B	53	GLU	CB-CG	5.29	1.62	1.52
1	A	212	PHE	CB-CG	5.28	1.60	1.51
1	F	57	PHE	CE2-CZ	5.28	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	49	VAL	CB-CG2	5.28	1.64	1.52
1	H	180	ILE	CA-CB	5.27	1.67	1.54
1	I	146	GLU	CB-CG	5.25	1.62	1.52
1	I	206	ARG	CB-CG	5.23	1.66	1.52
1	J	159	LYS	CE-NZ	5.23	1.62	1.49
1	I	179	GLU	CB-CG	5.22	1.62	1.52
1	H	57	PHE	CE2-CZ	5.22	1.47	1.37
1	E	125	VAL	CB-CG1	5.19	1.63	1.52
1	E	125	VAL	CA-CB	5.19	1.65	1.54
1	C	131	VAL	CB-CG2	5.18	1.63	1.52
1	A	52	THR	CB-CG2	5.18	1.69	1.52
1	J	12	PHE	CE2-CZ	5.17	1.47	1.37
1	I	119	GLU	CD-OE1	5.17	1.31	1.25
1	J	169	ARG	C-O	5.16	1.33	1.23
1	B	68	GLY	N-CA	5.16	1.53	1.46
1	G	44	ALA	CA-CB	5.14	1.63	1.52
1	C	137	ILE	CB-CG2	5.14	1.68	1.52
1	D	64	PHE	CB-CG	5.14	1.60	1.51
1	H	50	CYS	CB-SG	5.13	1.91	1.82
1	C	187	VAL	CB-CG2	5.12	1.63	1.52
1	D	225	GLU	CG-CD	5.12	1.59	1.51
1	E	211	TRP	CE3-CZ3	5.12	1.47	1.38
1	E	37	PHE	CE2-CZ	5.11	1.47	1.37
1	D	100	PRO	CB-CG	5.11	1.75	1.50
1	D	62	GLU	CG-CD	5.10	1.59	1.51
1	C	179	GLU	CB-CG	5.07	1.61	1.52
1	B	179	GLU	CD-OE1	5.07	1.31	1.25
1	E	234	ALA	CA-CB	5.06	1.63	1.52
1	B	91	ARG	CG-CD	5.05	1.64	1.51
1	D	76	VAL	CB-CG1	-5.05	1.42	1.52
1	D	197	ARG	CG-CD	5.05	1.64	1.51
1	D	95	VAL	CA-CB	5.03	1.65	1.54
1	C	64	PHE	CE1-CZ	5.02	1.46	1.37
1	C	88	TRP	CE3-CZ3	5.01	1.47	1.38
1	I	235	GLU	CD-OE1	5.01	1.31	1.25
1	D	76	VAL	CB-CG2	-5.00	1.42	1.52
1	F	77	ASP	CB-CG	5.00	1.62	1.51

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	138	ARG	NE-CZ-NH2	-15.63	112.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	138	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	G	208	LEU	CA-CB-CG	10.66	139.81	115.30
1	E	134	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	E	149	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	E	208	LEU	CA-CB-CG	8.61	135.09	115.30
1	C	74	LEU	CB-CG-CD2	8.55	125.53	111.00
1	B	199	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	H	77	ASP	CB-CG-OD1	-8.37	110.77	118.30
1	F	208	LEU	CA-CB-CG	8.26	134.29	115.30
1	D	169	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	J	96	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	B	91	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	E	134	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	I	134	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	E	59	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	I	197	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	C	59	ARG	NE-CZ-NH1	-7.71	116.45	120.30
1	B	111	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	H	208	LEU	CA-CB-CG	7.57	132.71	115.30
1	J	174	ASP	CB-CG-OD2	7.51	125.06	118.30
1	G	197	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	67	LEU	C-N-CA	-7.40	106.75	122.30
1	J	96	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	J	232	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	C	145	MET	CB-CG-SD	7.26	134.19	112.40
1	G	165	ASP	CB-CG-OD1	7.13	124.72	118.30
1	H	149	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	C	163	LEU	CB-CG-CD1	-7.13	98.87	111.00
1	C	165	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	138	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	F	74	LEU	CA-CB-CG	7.00	131.41	115.30
1	F	227	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	H	228	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	C	70	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	147	LEU	CA-CB-CG	6.88	131.11	115.30
1	J	138	ARG	CG-CD-NE	-6.84	97.43	111.80
1	D	126	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	147	LEU	CA-CB-CG	6.81	130.96	115.30
1	J	149	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	B	74	LEU	CA-CB-CG	6.59	130.47	115.30
1	C	70	ASP	CB-CG-OD1	6.57	124.21	118.30
1	I	194	ASP	CB-CG-OD2	-6.54	112.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	D	74	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	197	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	G	222	ASP	CB-CG-OD1	6.44	124.09	118.30
1	F	112	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	J	199	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	F	197	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	111	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	I	141	LEU	CA-CB-CG	6.38	129.97	115.30
1	E	59	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	D	220	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	126	ARG	CG-CD-NE	-6.22	98.73	111.80
1	C	74	LEU	CA-CB-CG	6.19	129.53	115.30
1	A	206	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	G	138	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	H	20	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	96	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	77	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	138	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	D	39	LEU	CA-CB-CG	6.06	129.23	115.30
1	B	39	LEU	CA-CB-CG	6.05	129.23	115.30
1	J	149	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	J	32	SER	CB-CA-C	-6.01	98.68	110.10
1	D	197	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	E	149	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	C	126	ARG	CG-CD-NE	-5.97	99.26	111.80
1	C	95	VAL	CB-CA-C	-5.97	100.06	111.40
1	C	219	SER	CB-CA-C	-5.96	98.78	110.10
1	B	77	ASP	CB-CG-OD2	5.96	123.66	118.30
1	D	161	LEU	CA-CB-CG	5.95	128.98	115.30
1	J	147	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	111	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	215	ASP	CB-CG-OD1	5.92	123.63	118.30
1	H	77	ASP	CB-CG-OD2	5.92	123.63	118.30
1	F	126	ARG	CG-CD-NE	-5.91	99.40	111.80
1	D	147	LEU	CB-CG-CD2	5.90	121.03	111.00
1	F	112	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	228	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	74	LEU	CB-CG-CD2	5.87	120.98	111.00
1	A	163	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	145	MET	CA-CB-CG	5.83	123.20	113.30
1	I	132	ASP	CB-CG-OD1	5.81	123.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	ARG	CG-CD-NE	5.80	123.98	111.80
1	I	134	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	G	207	CYS	CA-CB-SG	5.75	124.36	114.00
1	E	232	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	F	145	MET	CB-CG-SD	5.75	129.64	112.40
1	J	207	CYS	CA-CB-SG	-5.73	103.69	114.00
1	G	156	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	241	LEU	CA-CB-CG	5.61	128.20	115.30
1	G	74	LEU	CA-CB-CG	5.59	128.15	115.30
1	F	221	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	C	150	LEU	CB-CG-CD1	-5.54	101.59	111.00
1	E	67	LEU	CA-CB-CG	5.52	128.00	115.30
1	G	150	LEU	CA-CB-CG	5.52	128.00	115.30
1	D	91	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	J	232	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	C	200	MET	CG-SD-CE	5.48	108.97	100.20
1	I	109	VAL	CB-CA-C	5.47	121.79	111.40
1	H	241	LEU	CA-CB-CG	5.46	127.86	115.30
1	B	206	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	I	163	LEU	CA-CB-CG	5.45	127.83	115.30
1	G	194	ASP	CB-CG-OD1	5.43	123.19	118.30
1	I	215	ASP	CB-CG-OD2	5.38	123.15	118.30
1	G	105	PRO	N-CA-C	-5.37	98.14	112.10
1	G	147	LEU	CA-CB-CG	5.34	127.58	115.30
1	H	66	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	147	LEU	CA-CB-CG	5.31	127.52	115.30
1	I	63	ASP	CB-CG-OD2	5.29	123.07	118.30
1	G	221	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	F	228	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	H	194	ASP	CB-CG-OD1	5.27	123.04	118.30
1	I	199	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	F	197	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	G	77	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	J	116	LEU	CA-CB-CG	5.21	127.29	115.30
1	E	213	CYS	CA-CB-SG	5.18	123.33	114.00
1	G	77	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	91	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	G	207	CYS	N-CA-CB	-5.16	101.31	110.60
1	J	60	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	J	208	LEU	CA-CB-CG	5.16	127.17	115.30
1	G	112	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	G	241	LEU	CA-CB-CG	5.15	127.14	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	LEU	CA-CB-CG	5.14	127.12	115.30
1	D	111	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	F	228	ARG	CG-CD-NE	5.12	122.55	111.80
1	E	39	LEU	CA-CB-CG	5.11	127.05	115.30
1	F	194	ASP	CB-CG-OD1	5.10	122.89	118.30
1	I	152	ASP	CB-CG-OD1	5.09	122.89	118.30
1	B	96	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	F	77	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	149	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	H	232	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	H	227	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	I	126	ARG	CG-CD-NE	-5.05	101.19	111.80
1	D	221	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	A	228	ARG	CG-CD-NE	5.03	122.36	111.80
1	E	28	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	J	138	ARG	CD-NE-CZ	5.03	130.64	123.60
1	D	39	LEU	CB-CG-CD2	5.01	119.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	121	ALA	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	1953	0	1942	48	0
1	B	1973	0	1957	39	0
1	C	1973	0	1959	30	0
1	D	1973	0	1959	44	0
1	E	1958	0	1945	36	0
1	F	1973	0	1957	38	0
1	G	1958	0	1945	42	0
1	H	1968	0	1952	41	0
1	I	1973	0	1957	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1953	0	1940	36	0
2	A	16	0	0	1	0
2	B	17	0	0	2	0
2	C	23	0	0	5	0
2	D	20	0	0	0	0
2	E	21	0	0	3	0
2	F	18	0	0	0	0
2	G	11	0	0	0	0
2	H	15	0	0	2	0
2	I	16	0	0	4	0
2	J	20	0	0	3	0
All	All	19832	0	19513	356	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 9.

All (356) 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:E:137:ILE:CG1	1:E:137:ILE:CD1	1.77	1.62
1:D:97:ILE:CD1	1:D:97:ILE:CG1	1.77	1.56
1:D:100:PRO:CG	1:D:100:PRO:CB	1.75	1.40
2:C:268:HOH:O	1:E:83:ILE:HD11	1.42	1.14
1:I:11:ARG:HH11	1:I:11:ARG:HG2	1.11	1.09
1:A:59:ARG:HG2	1:A:59:ARG:HH11	0.94	1.07
1:A:105:PRO:O	1:A:106:GLN:CB	2.03	1.06
1:D:59:ARG:NH1	1:D:59:ARG:HG3	1.59	1.04
1:E:105:PRO:O	1:E:106:GLN:HB2	1.55	1.04
1:A:59:ARG:HG2	1:A:59:ARG:NH1	1.64	1.02
1:D:41:SER:HB2	1:D:74:LEU:HD12	1.42	1.00
1:F:105:PRO:O	1:F:106:GLN:HB2	1.55	1.00
1:I:105:PRO:O	1:I:106:GLN:HB2	1.62	0.99
1:J:105:PRO:O	1:J:106:GLN:HB2	1.61	0.98
1:D:59:ARG:HH11	1:D:59:ARG:CG	1.74	0.98
1:J:59:ARG:HG3	1:J:59:ARG:HH11	1.27	0.97
1:H:90:GLU:OE2	1:H:96:ARG:HG2	1.64	0.97
1:A:59:ARG:HH11	1:A:59:ARG:CG	1.76	0.97
1:D:59:ARG:HG3	1:D:59:ARG:HH11	0.80	0.97
1:A:105:PRO:O	1:A:106:GLN:HB3	1.65	0.95
1:B:106:GLN:O	1:B:111:ARG:NH2	2.01	0.93
1:C:228:ARG:HD3	2:C:262:HOH:O	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HD13	1:D:5:ILE:HD11	1.50	0.92
1:B:119:GLU:O	1:B:120:SER:HB3	1.69	0.92
1:J:224:GLU:OE2	1:J:231:ARG:NH2	2.03	0.91
1:G:69:VAL:HG21	1:G:158:VAL:HG11	1.52	0.89
1:I:11:ARG:HG2	1:I:11:ARG:NH1	1.83	0.88
1:G:8:ILE:H	1:H:117:HIS:HD2	1.19	0.87
1:A:117:HIS:HB2	1:A:125:VAL:HG11	1.55	0.87
1:E:8:ILE:H	1:F:117:HIS:HD2	1.17	0.86
1:C:8:ILE:H	1:D:117:HIS:HD2	1.21	0.85
1:C:5:ILE:HD13	1:D:5:ILE:CD1	2.05	0.85
1:A:117:HIS:HD2	1:B:8:ILE:H	1.25	0.85
1:C:5:ILE:CD1	1:D:5:ILE:HD11	2.06	0.85
1:I:59:ARG:HG3	1:J:179:GLU:OE1	1.77	0.84
1:A:76:VAL:HB	2:J:265:HOH:O	1.75	0.84
1:F:239:LYS:HE2	1:F:239:LYS:O	1.78	0.82
1:G:105:PRO:O	1:G:106:GLN:CB	2.26	0.82
1:C:117:HIS:HD2	1:D:8:ILE:H	1.26	0.82
1:G:105:PRO:O	1:G:106:GLN:HB3	1.80	0.81
1:H:122:THR:HG22	1:H:123:HIS:CD2	2.16	0.80
1:J:154:ILE:O	1:J:158:VAL:HG22	1.81	0.80
1:H:105:PRO:O	1:H:106:GLN:HB2	1.81	0.80
1:E:224:GLU:OE2	1:E:231:ARG:NH2	2.14	0.80
1:I:140:MET:CE	1:I:142:TYR:OH	2.30	0.79
1:G:185:LEU:O	1:G:214:TRP:HB2	1.83	0.77
1:E:42:HIS:CE1	1:E:75:SER:HB3	2.20	0.77
1:A:2:PRO:HB3	2:B:267:HOH:O	1.86	0.76
1:D:76:VAL:O	1:D:105:PRO:HA	1.86	0.76
1:F:112:ARG:HG2	1:F:112:ARG:HH11	1.49	0.76
1:J:105:PRO:O	1:J:106:GLN:CB	2.31	0.75
1:A:105:PRO:O	1:A:106:GLN:HB2	1.87	0.75
1:J:59:ARG:HG3	1:J:59:ARG:NH1	1.97	0.75
1:I:140:MET:HE1	1:I:142:TYR:OH	1.87	0.73
1:C:67:LEU:HD13	1:C:158:VAL:HG23	1.68	0.73
1:G:206:ARG:O	1:G:207:CYS:HB2	1.89	0.73
1:C:43:PRO:HG3	1:C:145:MET:HG2	1.71	0.73
1:I:66:ARG:HG2	1:I:66:ARG:HH11	1.52	0.73
1:D:106:GLN:O	1:D:111:ARG:NH2	2.21	0.73
1:I:11:ARG:HH11	1:I:11:ARG:CG	1.99	0.73
1:C:224:GLU:OE1	1:C:231:ARG:NH2	2.22	0.72
1:D:112:ARG:HG3	1:D:112:ARG:HH11	1.53	0.72
1:F:69:VAL:HG21	1:F:158:VAL:HG11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:SER:HB2	1:G:74:LEU:HD12	1.72	0.72
1:D:112:ARG:HH11	1:D:112:ARG:CG	2.04	0.71
1:H:122:THR:HG23	1:I:105:PRO:HG2	1.72	0.71
1:A:69:VAL:HG21	1:A:158:VAL:HG21	1.71	0.71
1:H:115:LEU:O	1:H:125:VAL:HG13	1.90	0.70
1:F:67:LEU:HD21	1:F:159:LYS:HG2	1.74	0.70
2:C:268:HOH:O	1:E:83:ILE:CD1	2.15	0.70
1:E:112:ARG:HG2	1:E:112:ARG:HH11	1.57	0.69
1:H:106:GLN:O	1:H:111:ARG:NH2	2.25	0.69
1:J:42:HIS:CE1	1:J:75:SER:HB3	2.27	0.69
1:I:5:ILE:HG23	2:I:263:HOH:O	1.91	0.68
1:F:239:LYS:O	1:F:239:LYS:CE	2.41	0.68
1:E:126:ARG:HB2	1:E:143:TYR:O	1.92	0.68
1:A:8:ILE:H	1:B:117:HIS:HD2	1.39	0.68
1:H:59:ARG:HH11	1:H:59:ARG:HB2	1.57	0.68
1:J:224:GLU:OE1	1:J:228:ARG:NH1	2.26	0.68
1:B:67:LEU:HD13	1:B:158:VAL:HG23	1.76	0.67
1:A:5:ILE:O	1:B:2:PRO:HB3	1.95	0.67
1:D:106:GLN:OE1	1:D:106:GLN:HA	1.96	0.66
1:I:117:HIS:HD2	1:J:8:ILE:H	1.42	0.66
1:A:117:HIS:HB2	1:A:125:VAL:CG1	2.26	0.65
1:F:117:HIS:HB2	1:F:125:VAL:CG1	2.27	0.65
1:A:14:GLU:O	1:A:112:ARG:NH2	2.30	0.65
1:B:91:ARG:HD3	2:B:262:HOH:O	1.97	0.64
1:I:7:LEU:HD13	1:J:117:HIS:HA	1.79	0.64
1:J:155:LEU:HA	1:J:158:VAL:CG2	2.27	0.64
1:I:28:ASP:OD1	1:I:28:ASP:N	2.31	0.64
1:E:35:LYS:HE2	2:E:271:HOH:O	1.98	0.64
1:E:117:HIS:HD2	1:F:8:ILE:H	1.46	0.64
1:F:220:ARG:O	1:F:224:GLU:HG3	1.98	0.64
1:I:90:GLU:OE1	1:I:96:ARG:HG3	1.98	0.64
1:A:67:LEU:O	1:A:162:LYS:HE3	1.99	0.63
1:G:124:THR:HG23	1:G:125:VAL:O	1.98	0.63
1:H:44:ALA:O	1:H:47:THR:OG1	2.16	0.63
1:F:191:THR:H	1:F:195:GLN:NE2	1.96	0.63
1:G:150:LEU:HD22	2:H:259:HOH:O	1.99	0.62
1:H:39:LEU:C	1:H:39:LEU:HD12	2.20	0.62
1:H:105:PRO:O	1:H:106:GLN:CB	2.47	0.62
1:I:188:PRO:O	1:I:199:ARG:NH2	2.32	0.62
1:C:117:HIS:CD2	1:D:8:ILE:H	2.14	0.61
1:B:35:LYS:HD3	1:B:70:ASP:OD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ARG:HG2	1:E:112:ARG:NH1	2.15	0.61
1:G:8:ILE:H	1:H:117:HIS:CD2	2.10	0.61
1:D:106:GLN:HE22	1:E:111:ARG:HH21	1.49	0.61
1:G:69:VAL:CG2	1:G:158:VAL:HG11	2.28	0.61
1:B:244:GLU:O	1:B:244:GLU:HG2	2.01	0.61
1:B:105:PRO:O	1:B:106:GLN:HB2	2.01	0.60
1:A:122:THR:HA	1:J:106:GLN:HG3	1.83	0.60
1:A:47:THR:HG23	2:A:252:HOH:O	2.02	0.60
1:D:43:PRO:HB3	1:D:123:HIS:CD2	2.36	0.60
1:F:105:PRO:O	1:F:106:GLN:CB	2.37	0.60
1:H:106:GLN:HE22	1:I:111:ARG:HH21	1.50	0.60
1:I:35:LYS:HD3	1:I:70:ASP:OD2	2.02	0.60
1:I:77:ASP:OD2	2:I:258:HOH:O	2.16	0.60
1:C:93:ILE:HG22	1:C:95:VAL:HG23	1.84	0.59
1:G:55:VAL:O	1:G:59:ARG:HG2	2.01	0.59
1:E:144:PRO:HD2	1:E:147:LEU:HB3	1.85	0.59
1:F:194:ASP:OD1	1:F:197:ARG:NH2	2.36	0.59
1:D:14:GLU:HG2	1:D:25:LYS:HE2	1.85	0.59
1:F:59:ARG:NH1	1:F:59:ARG:HG2	2.19	0.58
1:H:105:PRO:HG2	1:I:122:THR:HB	1.85	0.58
1:J:202:SER:OG	1:J:203:GLY:N	2.36	0.58
1:B:65:GLN:O	1:B:67:LEU:O	2.21	0.58
1:E:10:GLU:OE2	1:F:2:PRO:HG2	2.04	0.57
1:H:43:PRO:HG3	1:H:145:MET:SD	2.44	0.57
1:H:119:GLU:O	1:H:120:SER:HB2	2.05	0.57
1:C:117:HIS:HB2	1:C:125:VAL:CG1	2.34	0.57
1:J:159:LYS:NZ	1:J:225:GLU:OE2	2.34	0.57
1:C:106:GLN:O	1:C:111:ARG:NH2	2.38	0.57
1:E:145:MET:HG2	2:E:266:HOH:O	2.05	0.57
1:G:8:ILE:N	1:H:117:HIS:HD2	1.99	0.56
1:I:5:ILE:CG2	2:I:263:HOH:O	2.49	0.56
1:A:242:TYR:HD1	1:B:208:LEU:CD1	2.19	0.56
1:G:223:VAL:CG1	1:G:227:ARG:NH1	2.68	0.56
1:B:128:VAL:O	1:B:140:MET:HA	2.06	0.55
1:C:8:ILE:N	1:D:117:HIS:HD2	1.97	0.55
1:J:240:LEU:O	1:J:243:GLU:HB2	2.06	0.55
1:H:224:GLU:HG2	2:H:263:HOH:O	2.06	0.55
1:I:59:ARG:HH11	1:I:59:ARG:CG	2.19	0.55
1:H:39:LEU:HD12	1:H:40:PHE:N	2.21	0.55
1:H:69:VAL:HG21	1:H:158:VAL:HG11	1.87	0.55
1:B:172:PRO:HG3	1:B:181:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:MET:HE2	1:I:142:TYR:OH	2.05	0.55
1:D:41:SER:CB	1:D:74:LEU:HD12	2.27	0.55
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.42	0.55
1:D:59:ARG:NH1	1:D:59:ARG:CG	2.45	0.55
1:A:76:VAL:CB	2:J:265:HOH:O	2.45	0.54
1:G:83:ILE:O	1:G:87:GLU:HG3	2.06	0.54
1:A:117:HIS:HD2	1:B:8:ILE:N	2.02	0.54
1:A:105:PRO:HG2	1:J:122:THR:HB	1.90	0.54
1:D:69:VAL:HG21	1:D:158:VAL:HG11	1.90	0.54
1:J:7:LEU:O	1:J:10:GLU:HB2	2.08	0.54
1:G:28:ASP:OD1	1:G:28:ASP:N	2.41	0.54
2:I:251:HOH:O	1:J:138:ARG:HD2	2.08	0.53
1:I:8:ILE:H	1:J:117:HIS:HD2	1.55	0.53
1:B:44:ALA:O	1:B:47:THR:OG1	2.25	0.53
1:F:59:ARG:HG2	1:F:59:ARG:HH11	1.73	0.53
1:I:105:PRO:O	1:I:106:GLN:CB	2.45	0.53
1:F:42:HIS:CE1	1:F:75:SER:HB3	2.44	0.53
1:G:122:THR:OG1	1:G:123:HIS:CD2	2.62	0.53
1:E:105:PRO:O	1:E:106:GLN:CB	2.38	0.52
1:J:126:ARG:HB3	1:J:149:ARG:CZ	2.39	0.52
1:A:5:ILE:HD13	1:B:5:ILE:HD13	1.91	0.52
1:E:7:LEU:HD21	1:F:3:GLY:HA3	1.92	0.52
1:A:76:VAL:CG2	2:J:265:HOH:O	2.58	0.52
1:C:117:HIS:HB2	1:C:125:VAL:HG11	1.91	0.52
1:H:167:LEU:HD13	1:H:217:PRO:HG2	1.91	0.52
1:C:5:ILE:HG12	1:C:142:TYR:OH	2.10	0.52
1:C:199:ARG:HD2	2:C:260:HOH:O	2.09	0.52
1:F:96:ARG:O	1:F:98:PRO:HD3	2.09	0.52
1:G:176:PRO:HG2	1:G:227:ARG:HG3	1.92	0.52
1:G:93:ILE:HD11	1:H:208:LEU:HD21	1.92	0.52
1:J:39:LEU:HD13	1:J:72:ILE:HG23	1.92	0.52
1:E:8:ILE:H	1:F:117:HIS:CD2	2.10	0.52
1:E:242:TYR:OH	1:F:206:ARG:HG2	2.09	0.52
1:A:242:TYR:HD1	1:B:208:LEU:HD13	1.74	0.51
1:C:90:GLU:OE1	1:C:96:ARG:NH2	2.41	0.51
1:I:191:THR:H	1:I:195:GLN:NE2	2.08	0.51
1:I:27:PRO:O	1:I:31:VAL:HG23	2.10	0.51
1:I:99:PHE:HB2	1:I:100:PRO:HD2	1.93	0.51
1:A:242:TYR:CD1	1:B:208:LEU:CD1	2.94	0.51
1:D:41:SER:HB2	1:D:74:LEU:CD1	2.29	0.51
1:A:242:TYR:CD1	1:B:208:LEU:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:ASP:OD1	1:G:197:ARG:NH2	2.40	0.51
1:J:59:ARG:HH11	1:J:59:ARG:CG	2.12	0.51
1:I:67:LEU:HD21	1:I:159:LYS:HG2	1.91	0.51
1:C:8:ILE:H	1:D:117:HIS:CD2	2.13	0.51
1:H:117:HIS:HB2	1:H:125:VAL:HG11	1.93	0.51
1:J:14:GLU:OE2	1:J:25:LYS:NZ	2.32	0.51
1:F:54:PHE:HE2	1:F:101:ILE:HD11	1.75	0.50
1:F:117:HIS:HB2	1:F:125:VAL:HG11	1.92	0.50
1:G:62:GLU:HG3	1:G:66:ARG:NH2	2.26	0.50
1:G:42:HIS:CE1	1:G:75:SER:HB3	2.47	0.50
1:D:122:THR:HB	1:E:105:PRO:HG2	1.94	0.50
1:I:65:GLN:HA	1:I:65:GLN:OE1	2.12	0.50
1:I:66:ARG:HG2	1:I:66:ARG:NH1	2.22	0.50
1:G:59:ARG:HG3	1:H:179:GLU:OE1	2.12	0.50
1:I:51:THR:HG1	1:I:85:TRP:HZ2	1.58	0.50
1:F:123:HIS:HB2	1:F:145:MET:HE1	1.94	0.50
1:E:152:ASP:OD1	1:E:232:ARG:NH2	2.45	0.49
1:I:66:ARG:NH1	1:I:66:ARG:CG	2.76	0.49
1:B:28:ASP:OD1	1:B:28:ASP:N	2.38	0.49
1:I:240:LEU:HB2	1:I:243:GLU:HG3	1.95	0.49
1:J:39:LEU:HD12	1:J:40:PHE:N	2.28	0.49
1:B:220:ARG:CG	1:B:220:ARG:HH11	2.25	0.49
1:C:29:HIS:O	1:C:33:GLN:NE2	2.35	0.49
1:D:83:ILE:O	1:D:87:GLU:HG3	2.13	0.49
1:F:41:SER:HB2	1:F:74:LEU:HD12	1.95	0.49
1:G:99:PHE:HB2	1:G:100:PRO:HD2	1.94	0.49
1:I:66:ARG:HH11	1:I:66:ARG:CG	2.21	0.49
1:J:67:LEU:HD21	1:J:159:LYS:HD3	1.94	0.49
1:B:126:ARG:HB3	1:B:149:ARG:CZ	2.42	0.49
1:F:83:ILE:O	1:F:87:GLU:HG3	2.13	0.49
1:B:86:LYS:HD3	1:B:97:ILE:HB	1.94	0.49
1:E:137:ILE:CD1	1:E:137:ILE:CB	2.81	0.49
1:F:82:HIS:CD2	1:F:101:ILE:HG22	2.48	0.48
1:E:65:GLN:NE2	2:E:271:HOH:O	2.45	0.48
1:D:7:LEU:HD12	1:D:10:GLU:OE2	2.13	0.48
1:I:74:LEU:HD12	1:I:102:ILE:HB	1.94	0.48
1:D:156:ARG:HD3	1:D:230:LEU:HD21	1.96	0.48
1:H:122:THR:HG22	1:H:123:HIS:CG	2.48	0.48
1:G:236:LYS:HG2	1:H:227:ARG:NH2	2.28	0.48
1:H:48:PRO:O	1:H:52:THR:HG23	2.14	0.48
1:I:59:ARG:HG3	1:I:59:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:116:LEU:H	1:J:116:LEU:HD22	1.79	0.47
1:I:43:PRO:O	1:I:123:HIS:HB3	2.15	0.47
1:B:122:THR:CG2	1:B:123:HIS:CD2	2.98	0.47
1:C:55:VAL:HG13	1:C:95:VAL:HG21	1.96	0.47
1:H:59:ARG:HB2	1:H:59:ARG:NH1	2.27	0.47
1:I:76:VAL:O	1:I:105:PRO:HA	2.14	0.47
1:J:110:ALA:HA	1:J:115:LEU:HD12	1.96	0.47
1:B:190:PRO:HB3	1:B:195:GLN:HB3	1.96	0.47
1:D:112:ARG:CG	1:D:112:ARG:NH1	2.70	0.47
1:G:243:GLU:OE2	1:G:243:GLU:HA	2.14	0.47
1:I:215:ASP:OD2	1:I:217:PRO:HD3	2.14	0.47
1:A:47:THR:CG2	1:A:50:CYS:SG	3.02	0.47
1:E:83:ILE:O	1:E:87:GLU:HG3	2.14	0.47
1:I:132:ASP:HB3	1:I:138:ARG:HG3	1.97	0.47
1:E:206:ARG:HD2	1:E:214:TRP:CH2	2.50	0.46
1:F:59:ARG:HH11	1:F:59:ARG:CG	2.28	0.46
1:A:69:VAL:CG2	1:A:158:VAL:HG21	2.42	0.46
1:H:28:ASP:OD1	1:H:28:ASP:N	2.47	0.46
1:I:59:ARG:HH11	1:I:59:ARG:HB3	1.79	0.46
1:G:159:LYS:NZ	1:G:225:GLU:OE2	2.41	0.46
1:I:179:GLU:CB	1:J:59:ARG:HH12	2.29	0.46
1:D:154:ILE:O	1:D:158:VAL:HG23	2.15	0.46
1:H:156:ARG:HD2	1:H:175:TRP:O	2.16	0.46
1:A:106:GLN:OE1	1:A:106:GLN:HA	2.16	0.46
1:F:27:PRO:O	1:F:31:VAL:HG23	2.16	0.46
1:B:66:ARG:C	1:B:67:LEU:O	2.51	0.45
1:B:79:VAL:O	1:B:83:ILE:HG13	2.15	0.45
1:H:42:HIS:CE1	1:H:75:SER:HB3	2.51	0.45
1:F:117:HIS:CG	1:F:125:VAL:HG11	2.52	0.45
1:G:167:LEU:HD13	1:G:217:PRO:HG2	1.98	0.45
1:A:180:ILE:HG22	1:A:181:ILE:HG23	1.99	0.45
1:H:43:PRO:HD2	1:H:50:CYS:SG	2.56	0.45
1:J:72:ILE:HG23	1:J:72:ILE:O	2.16	0.45
1:E:3:GLY:HA3	1:F:7:LEU:HD21	1.98	0.45
1:G:178:ASN:O	1:G:182:GLY:HA2	2.17	0.45
1:A:35:LYS:HD2	1:A:70:ASP:OD2	2.16	0.44
1:G:14:GLU:OE1	1:G:25:LYS:HE2	2.17	0.44
1:J:115:LEU:O	1:J:125:VAL:HG22	2.17	0.44
1:C:5:ILE:HD13	1:D:5:ILE:HD13	1.96	0.44
1:D:20:ASP:OD1	1:D:20:ASP:N	2.51	0.44
1:I:11:ARG:NH1	1:I:11:ARG:CG	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ILE:O	1:A:87:GLU:HG3	2.16	0.44
1:E:156:ARG:HD3	1:E:230:LEU:HD21	1.99	0.44
1:I:59:ARG:NH1	1:J:179:GLU:OE1	2.50	0.44
1:J:8:ILE:HD13	1:J:8:ILE:HG21	1.79	0.44
1:E:67:LEU:HD11	1:E:159:LYS:HD3	2.00	0.44
1:C:103:ALA:C	1:C:105:PRO:HD3	2.38	0.44
1:H:69:VAL:CG2	1:H:158:VAL:HG11	2.47	0.44
1:B:105:PRO:O	1:B:106:GLN:CB	2.65	0.44
1:B:220:ARG:O	1:B:224:GLU:HB2	2.17	0.43
1:A:206:ARG:HE	1:A:206:ARG:HB2	1.66	0.43
1:D:84:LYS:HB3	1:D:84:LYS:HE3	1.84	0.43
1:I:106:GLN:O	1:I:111:ARG:NH2	2.52	0.43
1:A:59:ARG:NH1	1:A:59:ARG:CG	2.46	0.43
1:B:156:ARG:HD3	1:B:230:LEU:HD21	2.01	0.43
1:C:44:ALA:O	1:C:47:THR:OG1	2.33	0.43
1:F:113:LEU:HD23	1:F:113:LEU:HA	1.73	0.43
1:A:28:ASP:OD1	1:A:28:ASP:N	2.51	0.43
1:A:47:THR:HG22	1:A:50:CYS:SG	2.59	0.42
1:D:123:HIS:CD2	1:D:123:HIS:O	2.72	0.42
1:F:43:PRO:O	1:F:123:HIS:ND1	2.52	0.42
1:I:59:ARG:HG3	1:I:59:ARG:HH11	1.82	0.42
1:D:74:LEU:HD13	1:D:74:LEU:C	2.40	0.42
1:D:191:THR:H	1:D:195:GLN:NE2	2.17	0.42
1:E:99:PHE:HB2	1:E:100:PRO:HD2	2.01	0.42
1:A:2:PRO:HA	1:B:5:ILE:O	2.20	0.42
1:A:8:ILE:H	1:B:117:HIS:CD2	2.28	0.42
1:A:47:THR:HG21	1:A:50:CYS:SG	2.60	0.42
1:B:163:LEU:HD21	1:B:222:ASP:HB3	2.00	0.42
1:E:175:TRP:CG	1:E:176:PRO:HA	2.54	0.42
1:E:60:ARG:O	1:E:63:ASP:HB2	2.19	0.42
1:I:175:TRP:CG	1:I:176:PRO:HA	2.54	0.42
1:J:185:LEU:O	1:J:214:TRP:HB2	2.20	0.42
1:H:8:ILE:N	1:H:140:MET:HE2	2.35	0.42
1:G:105:PRO:O	1:G:106:GLN:HB2	2.16	0.42
1:A:117:HIS:CB	1:A:125:VAL:HG11	2.37	0.42
1:F:159:LYS:HE3	1:F:222:ASP:HA	2.01	0.42
1:H:128:VAL:O	1:H:140:MET:HA	2.20	0.42
1:I:59:ARG:HA	1:I:59:ARG:HD2	1.84	0.42
1:E:154:ILE:O	1:E:158:VAL:HG22	2.20	0.42
1:I:104:ASP:O	1:I:104:ASP:CG	2.58	0.42
1:D:191:THR:H	1:D:195:GLN:HE22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLU:HG3	1:D:8:ILE:HG22	2.02	0.41
1:I:240:LEU:HA	1:I:240:LEU:HD23	1.72	0.41
1:A:92:HIS:O	1:A:245:ALA:HB1	2.20	0.41
1:I:51:THR:OG1	1:I:85:TRP:HZ2	2.02	0.41
1:I:156:ARG:HD2	1:I:175:TRP:O	2.20	0.41
1:C:25:LYS:HD3	1:C:28:ASP:OD2	2.21	0.41
1:D:116:LEU:HD23	1:D:116:LEU:HA	1.92	0.41
1:E:8:ILE:N	1:F:117:HIS:HD2	1.99	0.41
1:F:84:LYS:HA	1:F:84:LYS:HD2	1.91	0.41
1:G:59:ARG:CD	1:H:179:GLU:OE1	2.68	0.41
1:G:59:ARG:HD3	1:H:179:GLU:OE1	2.19	0.41
1:H:190:PRO:HG2	1:H:196:ALA:HA	2.02	0.41
1:F:14:GLU:HA	1:F:26:LEU:O	2.20	0.41
1:G:126:ARG:HB2	1:G:143:TYR:O	2.20	0.41
1:H:36:TRP:CD2	1:H:132:ASP:HA	2.56	0.41
1:A:39:LEU:C	1:A:39:LEU:HD23	2.40	0.41
1:C:28:ASP:N	1:C:28:ASP:OD1	2.53	0.41
1:D:6:PRO:HB2	1:D:137:ILE:CD1	2.51	0.41
1:G:20:ASP:OD1	1:G:20:ASP:N	2.54	0.41
1:I:59:ARG:HH11	1:I:59:ARG:CB	2.34	0.41
1:D:90:GLU:O	1:D:94:GLY:HA2	2.21	0.41
1:G:74:LEU:HD13	1:G:74:LEU:C	2.40	0.41
1:G:132:ASP:OD1	1:G:132:ASP:C	2.59	0.41
1:G:223:VAL:HG11	1:G:227:ARG:HH12	1.85	0.41
1:I:59:ARG:CG	1:I:59:ARG:NH1	2.80	0.41
1:C:202:SER:OG	1:C:203:GLY:N	2.53	0.41
1:G:45:ASP:O	1:G:46:PHE:HB2	2.21	0.41
1:J:163:LEU:O	1:J:167:LEU:HB2	2.20	0.41
1:A:60:ARG:HG3	1:A:60:ARG:HH11	1.86	0.41
1:A:117:HIS:CD2	1:B:8:ILE:H	2.17	0.41
1:A:173:ALA:HB2	1:B:53:GLU:HG2	2.02	0.41
1:C:43:PRO:O	1:C:123:HIS:HB3	2.21	0.41
2:C:263:HOH:O	1:D:2:PRO:HB3	2.20	0.41
1:A:44:ALA:O	1:A:47:THR:HB	2.21	0.40
1:A:244:GLU:OE2	1:A:244:GLU:N	2.54	0.40
1:B:43:PRO:CB	1:B:123:HIS:HB3	2.51	0.40
1:E:122:THR:CG2	1:E:123:HIS:CD2	3.03	0.40
1:G:206:ARG:O	1:G:207:CYS:CB	2.55	0.40
1:G:223:VAL:CG1	1:G:227:ARG:HH12	2.34	0.40
1:H:14:GLU:O	1:H:112:ARG:NH2	2.54	0.40
1:B:187:VAL:HA	1:B:188:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ILE:HG13	1:E:6:PRO:O	2.21	0.40
1:F:42:HIS:NE2	1:F:75:SER:HB3	2.37	0.40
1:H:42:HIS:HA	1:H:43:PRO:HD3	1.98	0.40
1:C:204:GLN:HG2	1:C:205:TYR:CE1	2.57	0.40
1:G:27:PRO:O	1:G:31:VAL:HG23	2.22	0.40
1:J:60:ARG:HD3	1:J:151:VAL:HG12	2.03	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	237/249 (95%)	222 (94%)	13 (6%)	2 (1%)	19	19
1	B	242/249 (97%)	226 (93%)	15 (6%)	1 (0%)	34	37
1	C	242/249 (97%)	233 (96%)	8 (3%)	1 (0%)	34	37
1	D	242/249 (97%)	229 (95%)	12 (5%)	1 (0%)	34	37
1	E	238/249 (96%)	226 (95%)	11 (5%)	1 (0%)	34	37
1	F	242/249 (97%)	228 (94%)	14 (6%)	0	100	100
1	G	238/249 (96%)	225 (94%)	11 (5%)	2 (1%)	19	19
1	H	241/249 (97%)	230 (95%)	9 (4%)	2 (1%)	19	19
1	I	242/249 (97%)	234 (97%)	7 (3%)	1 (0%)	34	37
1	J	237/249 (95%)	225 (95%)	10 (4%)	2 (1%)	19	19
All	All	2401/2490 (96%)	2278 (95%)	110 (5%)	13 (0%)	29	31

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	SER

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Mol	Chain	Res	Type
1	D	120	SER
1	C	201	GLU
1	G	106	GLN
1	H	106	GLN
1	H	120	SER
1	E	106	GLN
1	G	239	LYS
1	I	106	GLN
1	A	106	GLN
1	J	202	SER
1	J	106	GLN
1	A	31	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	208/215 (97%)	190 (91%)	18 (9%)	10	10
1	B	210/215 (98%)	197 (94%)	13 (6%)	18	21
1	C	210/215 (98%)	192 (91%)	18 (9%)	10	10
1	D	210/215 (98%)	196 (93%)	14 (7%)	16	18
1	E	208/215 (97%)	190 (91%)	18 (9%)	10	10
1	F	210/215 (98%)	190 (90%)	20 (10%)	8	8
1	G	208/215 (97%)	188 (90%)	20 (10%)	8	8
1	H	210/215 (98%)	198 (94%)	12 (6%)	20	24
1	I	210/215 (98%)	191 (91%)	19 (9%)	9	9
1	J	208/215 (97%)	189 (91%)	19 (9%)	9	9
All	All	2092/2150 (97%)	1921 (92%)	171 (8%)	11	11

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET

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Mol	Chain	Res	Type
1	A	28	ASP
1	A	47	THR
1	A	59	ARG
1	A	67	LEU
1	A	96	ARG
1	A	106	GLN
1	A	108	THR
1	A	112	ARG
1	A	144	PRO
1	A	145	MET
1	A	147	LEU
1	A	163	LEU
1	A	206	ARG
1	A	212	PHE
1	A	236	LYS
1	A	239	LYS
1	A	244	GLU
1	B	11	ARG
1	B	28	ASP
1	B	39	LEU
1	B	59	ARG
1	B	106	GLN
1	B	116	LEU
1	B	120	SER
1	B	122	THR
1	B	147	LEU
1	B	163	LEU
1	B	208	LEU
1	B	212	PHE
1	B	220	ARG
1	C	5	ILE
1	C	28	ASP
1	C	70	ASP
1	C	74	LEU
1	C	91	ARG
1	C	106	GLN
1	C	112	ARG
1	C	116	LEU
1	C	120	SER
1	C	134	ARG
1	C	147	LEU
1	C	161	LEU

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Mol	Chain	Res	Type
1	C	199	ARG
1	C	201	GLU
1	C	204	GLN
1	C	212	PHE
1	C	224	GLU
1	C	239	LYS
1	D	11	ARG
1	D	28	ASP
1	D	39	LEU
1	D	59	ARG
1	D	96	ARG
1	D	106	GLN
1	D	112	ARG
1	D	145	MET
1	D	147	LEU
1	D	161	LEU
1	D	166	SER
1	D	208	LEU
1	D	212	PHE
1	D	244	GLU
1	E	2	PRO
1	E	11	ARG
1	E	28	ASP
1	E	39	LEU
1	E	70	ASP
1	E	79	VAL
1	E	81	SER
1	E	122	THR
1	E	124	THR
1	E	166	SER
1	E	168	LYS
1	E	191	THR
1	E	197	ARG
1	E	199	ARG
1	E	208	LEU
1	E	212	PHE
1	E	224	GLU
1	E	244	GLU
1	F	11	ARG
1	F	28	ASP
1	F	62	GLU
1	F	74	LEU

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Mol	Chain	Res	Type
1	F	76	VAL
1	F	79	VAL
1	F	91	ARG
1	F	95	VAL
1	F	112	ARG
1	F	145	MET
1	F	168	LYS
1	F	176	PRO
1	F	195	GLN
1	F	197	ARG
1	F	208	LEU
1	F	212	PHE
1	F	220	ARG
1	F	228	ARG
1	F	239	LYS
1	F	244	GLU
1	G	11	ARG
1	G	28	ASP
1	G	62	GLU
1	G	74	LEU
1	G	75	SER
1	G	76	VAL
1	G	91	ARG
1	G	111	ARG
1	G	112	ARG
1	G	116	LEU
1	G	124	THR
1	G	134	ARG
1	G	145	MET
1	G	147	LEU
1	G	150	LEU
1	G	159	LYS
1	G	168	LYS
1	G	183	GLU
1	G	197	ARG
1	G	212	PHE
1	H	11	ARG
1	H	28	ASP
1	H	39	LEU
1	H	59	ARG
1	H	79	VAL
1	H	112	ARG

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Mol	Chain	Res	Type
1	H	145	MET
1	H	147	LEU
1	H	161	LEU
1	H	212	PHE
1	H	227	ARG
1	H	244	GLU
1	I	11	ARG
1	I	28	ASP
1	I	59	ARG
1	I	81	SER
1	I	106	GLN
1	I	109	VAL
1	I	125	VAL
1	I	145	MET
1	I	147	LEU
1	I	166	SER
1	I	195	GLN
1	I	197	ARG
1	I	199	ARG
1	I	200	MET
1	I	204	GLN
1	I	207	CYS
1	I	212	PHE
1	I	235	GLU
1	I	239	LYS
1	J	2	PRO
1	J	11	ARG
1	J	28	ASP
1	J	59	ARG
1	J	75	SER
1	J	81	SER
1	J	116	LEU
1	J	117	HIS
1	J	126	ARG
1	J	145	MET
1	J	147	LEU
1	J	167	LEU
1	J	204	GLN
1	J	207	CYS
1	J	208	LEU
1	J	212	PHE
1	J	221	ASP

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Mol	Chain	Res	Type
1	J	239	LYS
1	J	242	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	204	GLN
1	B	117	HIS
1	C	92	HIS
1	C	117	HIS
1	C	195	GLN
1	D	117	HIS
1	D	123	HIS
1	D	195	GLN
1	D	204	GLN
1	E	92	HIS
1	E	117	HIS
1	E	123	HIS
1	F	92	HIS
1	F	106	GLN
1	F	117	HIS
1	F	195	GLN
1	G	92	HIS
1	G	123	HIS
1	H	106	GLN
1	H	117	HIS
1	H	195	GLN
1	I	117	HIS
1	I	195	GLN
1	J	92	HIS
1	J	117	HIS
1	J	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	241/249 (96%)	-0.25	3 (1%) 79 77	18, 28, 50, 61	0
1	B	244/249 (97%)	-0.33	1 (0%) 92 91	18, 30, 52, 64	0
1	C	244/249 (97%)	-0.42	2 (0%) 86 85	15, 27, 51, 66	0
1	D	244/249 (97%)	-0.30	3 (1%) 79 77	15, 26, 48, 63	0
1	E	242/249 (97%)	-0.42	5 (2%) 63 61	16, 28, 47, 64	0
1	F	244/249 (97%)	-0.21	5 (2%) 65 63	20, 31, 53, 70	0
1	G	242/249 (97%)	-0.31	3 (1%) 79 77	21, 33, 53, 73	0
1	H	243/249 (97%)	-0.35	5 (2%) 63 61	19, 32, 56, 68	0
1	I	244/249 (97%)	-0.29	3 (1%) 79 77	16, 29, 53, 58	0
1	J	241/249 (96%)	-0.40	4 (1%) 70 68	18, 28, 49, 64	0
All	All	2429/2490 (97%)	-0.33	34 (1%) 75 73	15, 29, 52, 73	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	245	ALA	4.0
1	H	118	ALA	3.8
1	A	245	ALA	3.4
1	H	238	ALA	3.4
1	I	245	ALA	3.3
1	C	2	PRO	3.3
1	I	4	SER	3.2
1	H	2	PRO	3.1
1	E	2	PRO	2.9
1	C	244	GLU	2.8
1	G	245	ALA	2.8
1	E	242	TYR	2.8
1	D	245	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	242	TYR	2.7
1	J	2	PRO	2.6
1	E	201	GLU	2.6
1	F	202	SER	2.6
1	B	201	GLU	2.6
1	D	243	GLU	2.5
1	A	243	GLU	2.5
1	E	245	ALA	2.4
1	G	238	ALA	2.4
1	F	201	GLU	2.3
1	G	244	GLU	2.3
1	D	118	ALA	2.3
1	E	244	GLU	2.2
1	H	239	LYS	2.2
1	J	201	GLU	2.1
1	J	202	SER	2.1
1	J	197	ARG	2.1
1	I	119	GLU	2.1
1	F	145	MET	2.1
1	F	242	TYR	2.1
1	H	243	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.