



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 01:32 AM UTC

PDB ID : 3A5W / pdb_00003a5w
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 : 4-5-2 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

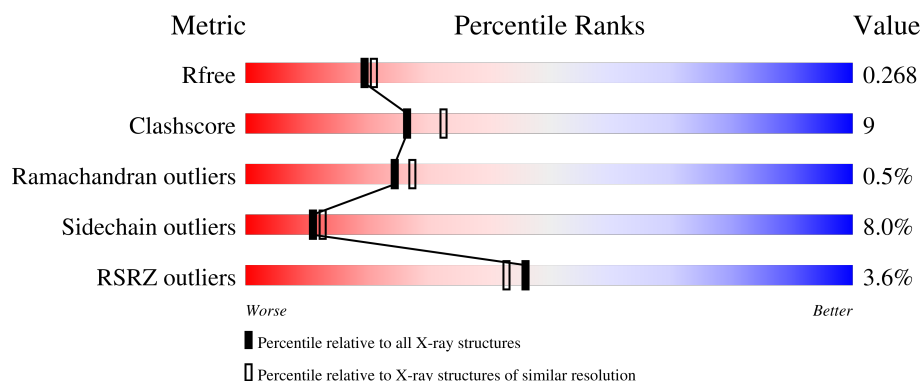
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	4% 62% 28% 6% ••
1	B	249	2% 67% 23% 8% •
1	C	249	2% 65% 27% 6% ••
1	D	249	4% 58% 34% 6% •
1	E	249	3% 59% 32% 6% •

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Mol	Chain	Length	Quality of chain
1	F	249	5% 60% 29% 7%
1	G	249	4% 61% 29% 6%
1	H	249	3% 66% 24% 7%
1	I	249	5% 57% 33% 7%
1	J	249	3% 63% 26% 8%

2 Entry composition

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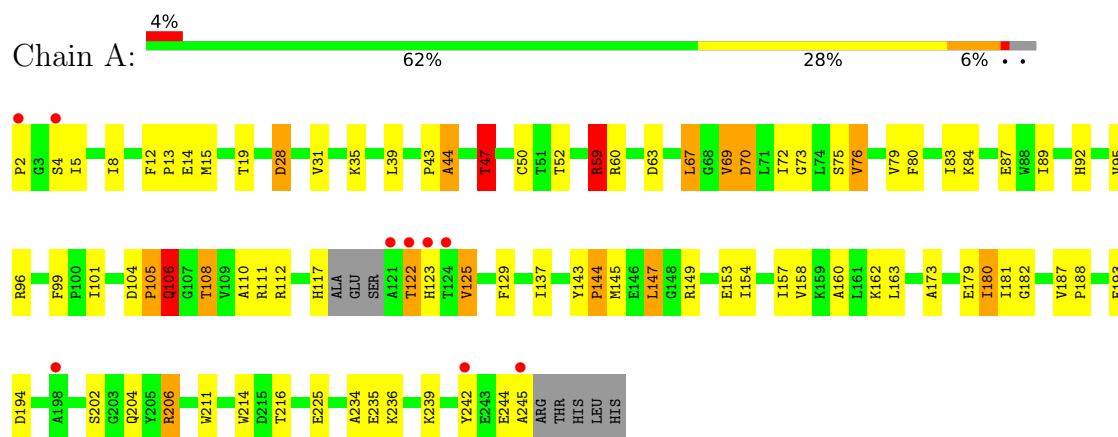
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	21	Total 21	O 21	0	0
2	F	18	Total 18	O 18	0	0
2	G	11	Total 11	O 11	0	0
2	H	15	Total 15	O 15	0	0
2	I	16	Total 16	O 16	0	0
2	J	20	Total 20	O 20	0	0

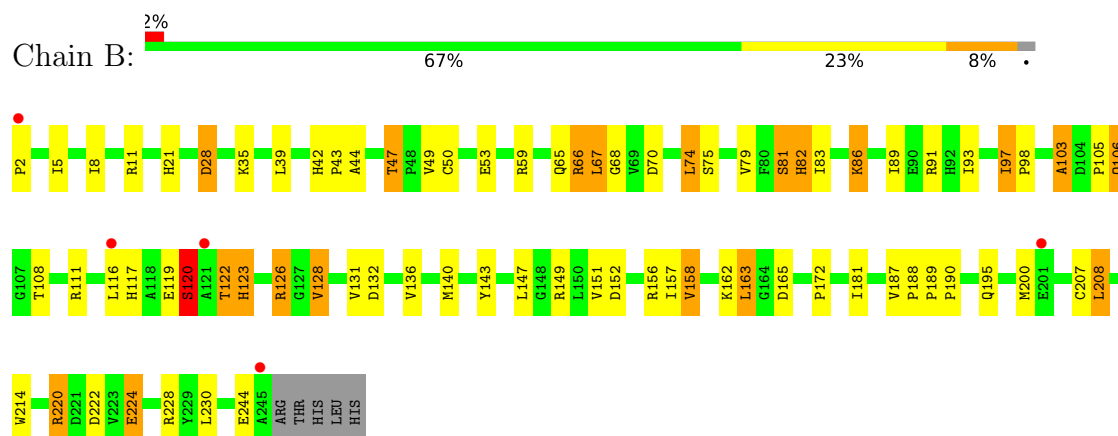
3 Residue-property plots [i](#)

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

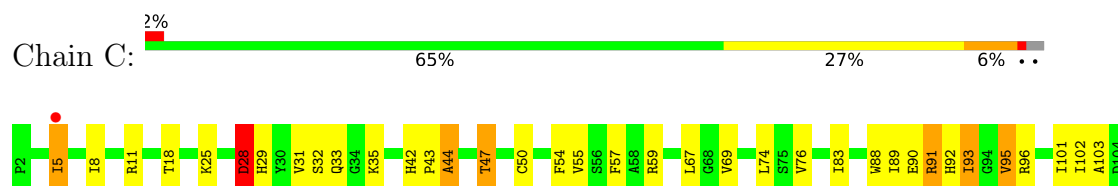
• Molecule 1: Probable peroxiredoxin

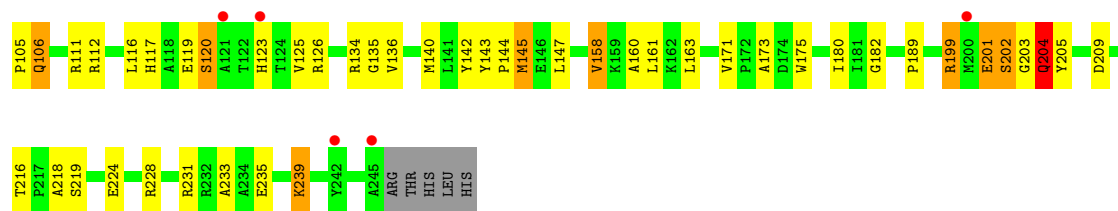


• Molecule 1: Probable peroxiredoxin

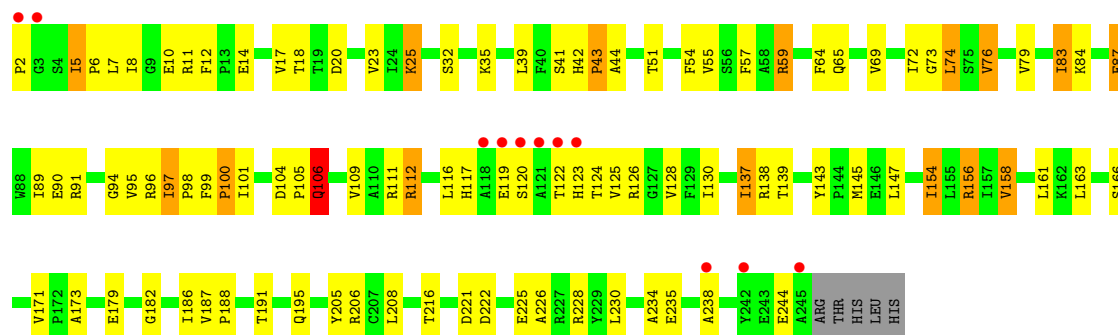


• Molecule 1: Probable peroxiredoxin

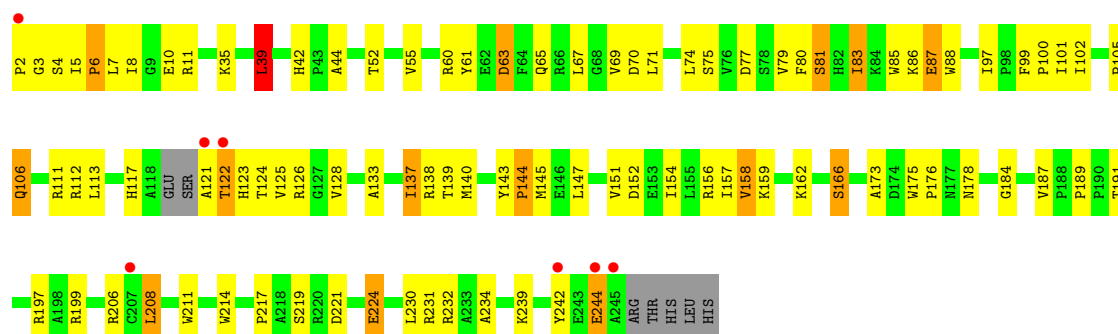




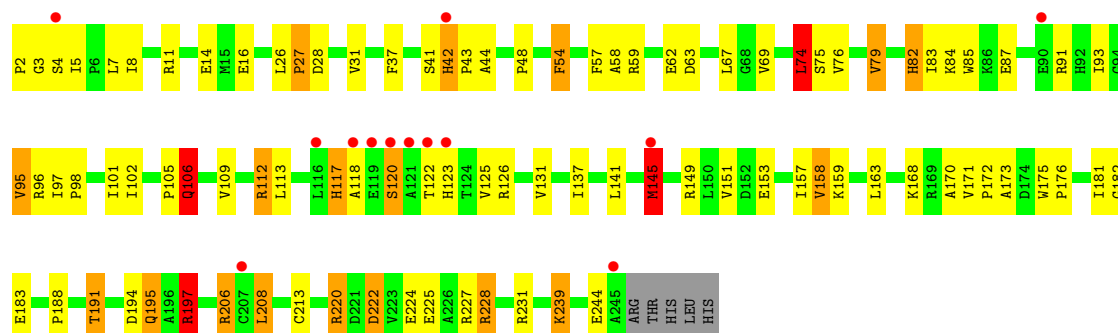
● Molecule 1: Probable peroxiredoxin



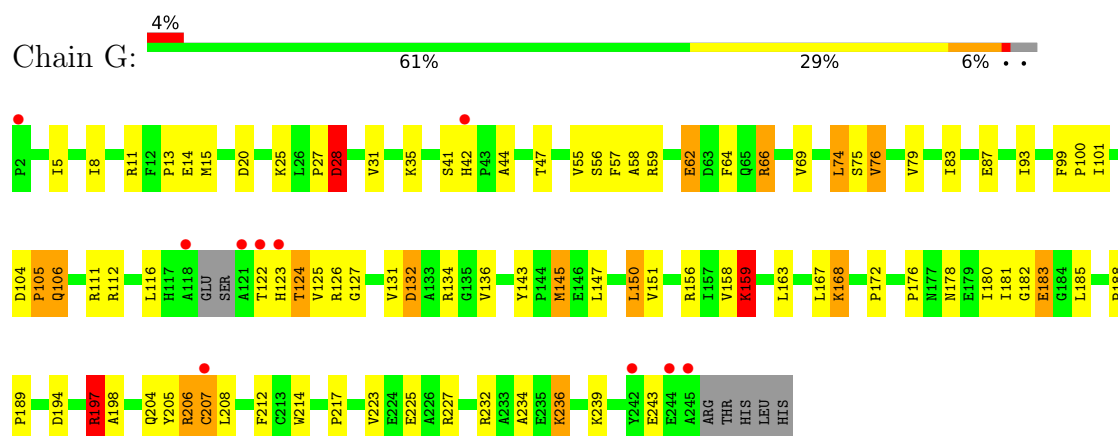
● Molecule 1: Probable peroxiredoxin



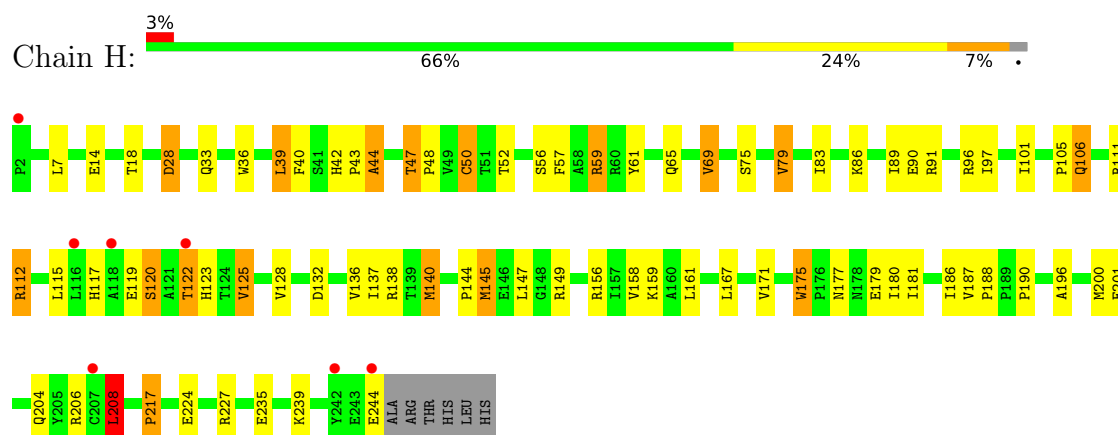
● Molecule 1: Probable peroxiredoxin



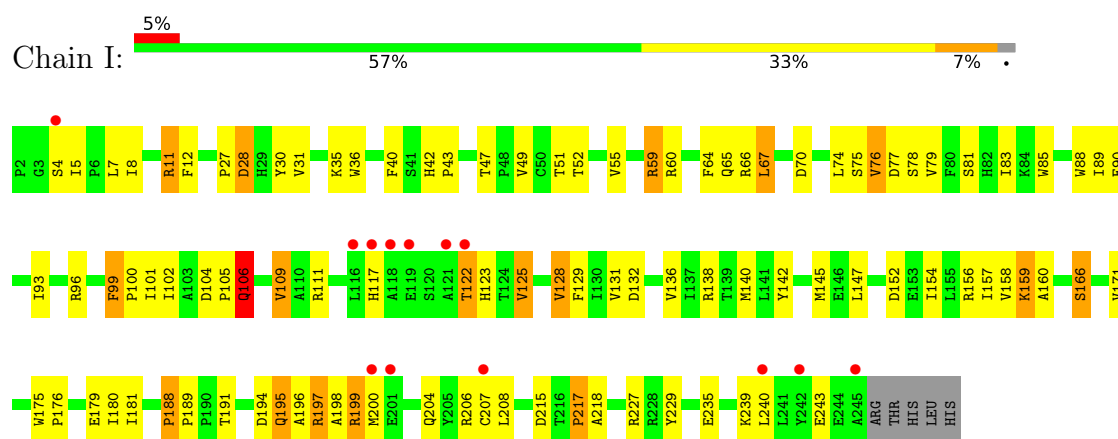
- Molecule 1: Probable peroxiredoxin



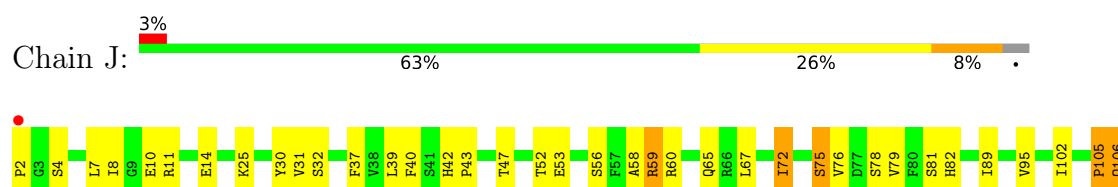
- Molecule 1: Probable peroxiredoxin

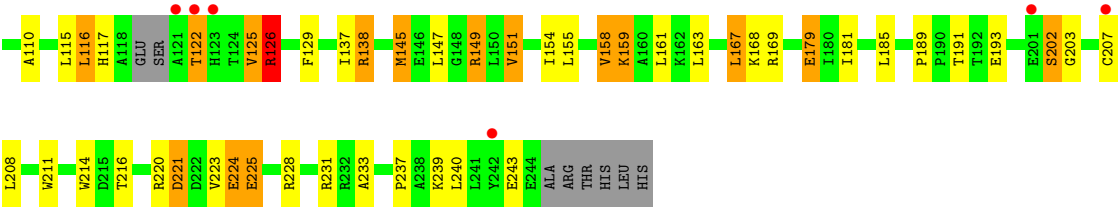


- Molecule 1: Probable peroxiredoxin



- 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 46.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (46.83-2.20) 94.3 (46.83-2.20)	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 (4.74%)	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 , 43.2	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	1.94	40/2007 (2.0%)	1.57	27/2727 (1.0%)
1	B	1.77	23/2028 (1.1%)	1.53	16/2757 (0.6%)
1	C	1.89	33/2028 (1.6%)	1.56	29/2757 (1.1%)
1	D	2.03	58/2028 (2.9%)	1.55	21/2757 (0.8%)
1	E	1.84	30/2012 (1.5%)	1.53	17/2734 (0.6%)
1	F	1.92	42/2028 (2.1%)	1.54	20/2757 (0.7%)
1	G	1.75	30/2012 (1.5%)	1.54	21/2734 (0.8%)
1	H	1.77	27/2023 (1.3%)	1.47	18/2750 (0.7%)
1	I	1.94	42/2028 (2.1%)	1.58	24/2757 (0.9%)
1	J	1.97	35/2007 (1.7%)	1.56	22/2727 (0.8%)
All	All	1.88	360/20201 (1.8%)	1.54	215/27457 (0.8%)

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 (360) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	171	VAL	CA-CB	14.14	1.66	1.54
1	G	189	PRO	CA-C	11.31	1.58	1.51
1	C	175	TRP	CA-C	11.11	1.64	1.53
1	J	122	THR	CA-CB	10.66	1.70	1.53
1	I	109	VAL	CA-CB	10.12	1.66	1.54
1	D	95	VAL	CA-CB	9.52	1.65	1.54
1	J	58	ALA	CA-CB	9.37	1.68	1.53
1	D	44	ALA	CA-CB	9.30	1.69	1.53
1	J	189	PRO	CA-C	9.14	1.58	1.52
1	G	76	VAL	CA-CB	8.85	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	216	THR	CA-CB	8.80	1.64	1.53
1	A	76	VAL	CA-C	8.61	1.62	1.52
1	H	79	VAL	CA-CB	8.58	1.67	1.54
1	H	180	ILE	CA-CB	8.44	1.67	1.54
1	I	188	PRO	CA-C	8.41	1.59	1.52
1	E	125	VAL	CA-CB	8.23	1.65	1.54
1	J	37	PHE	N-CA	8.03	1.55	1.46
1	J	89	ILE	CA-CB	7.81	1.64	1.54
1	F	58	ALA	CA-CB	7.80	1.65	1.53
1	F	175	TRP	CA-C	7.77	1.61	1.53
1	A	188	PRO	CA-C	7.75	1.59	1.52
1	I	171	VAL	CA-CB	7.74	1.61	1.54
1	H	33	GLN	N-CA	7.73	1.56	1.46
1	J	169	ARG	C-O	7.64	1.33	1.23
1	D	156	ARG	N-CA	7.61	1.55	1.46
1	F	109	VAL	CA-CB	7.59	1.63	1.54
1	I	154	ILE	CA-CB	7.59	1.64	1.54
1	A	182	GLY	N-CA	7.55	1.56	1.45
1	J	43	PRO	C-O	-7.54	1.14	1.24
1	A	101	ILE	CA-C	-7.53	1.43	1.52
1	C	93	ILE	CA-CB	7.53	1.64	1.54
1	D	137	ILE	C-O	7.45	1.31	1.24
1	H	101	ILE	CA-CB	7.44	1.64	1.54
1	H	136	VAL	CA-CB	7.42	1.63	1.54
1	G	181	ILE	CA-CB	7.39	1.64	1.54
1	I	79	VAL	CA-CB	7.37	1.63	1.54
1	J	181	ILE	CA-CB	7.29	1.62	1.54
1	H	137	ILE	N-CA	7.29	1.55	1.46
1	D	101	ILE	CA-CB	7.26	1.63	1.54
1	D	171	VAL	CA-CB	7.19	1.59	1.54
1	A	95	VAL	CA-CB	7.18	1.62	1.54
1	E	221	ASP	CA-C	7.18	1.61	1.52
1	D	128	VAL	CA-CB	7.17	1.63	1.54
1	F	188	PRO	CA-C	7.14	1.58	1.52
1	G	136	VAL	CA-CB	7.14	1.62	1.54
1	E	102	ILE	CA-CB	7.14	1.62	1.54
1	I	36	TRP	N-CA	7.13	1.54	1.45
1	C	95	VAL	CA-CB	7.10	1.62	1.54
1	F	137	ILE	C-O	7.10	1.31	1.24
1	B	158	VAL	CA-CB	7.08	1.63	1.54
1	D	97	ILE	CA-C	7.08	1.58	1.53
1	A	75	SER	N-CA	7.07	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	VAL	CA-CB	7.05	1.62	1.54
1	F	206	ARG	C-O	-7.03	1.15	1.23
1	J	138	ARG	CD-NE	-7.03	1.36	1.46
1	D	187	VAL	N-CA	7.01	1.54	1.46
1	H	56	SER	CA-C	7.00	1.61	1.52
1	A	216	THR	CA-CB	6.98	1.60	1.53
1	D	173	ALA	CA-CB	6.97	1.64	1.53
1	A	123	HIS	CA-C	6.94	1.60	1.52
1	A	129	PHE	N-CA	6.89	1.54	1.46
1	J	126	ARG	CA-CB	6.89	1.61	1.52
1	J	31	VAL	CA-C	6.89	1.61	1.52
1	I	180	ILE	CA-CB	6.87	1.63	1.54
1	J	125	VAL	N-CA	6.87	1.54	1.46
1	F	63	ASP	N-CA	6.84	1.54	1.46
1	I	52	THR	CA-CB	6.83	1.64	1.53
1	J	47	THR	CA-C	6.82	1.61	1.52
1	I	122	THR	CA-C	6.81	1.59	1.52
1	F	173	ALA	CA-C	6.74	1.61	1.52
1	I	49	VAL	CA-CB	-6.73	1.45	1.54
1	A	80	PHE	N-CA	6.70	1.54	1.46
1	E	137	ILE	CG1-CD1	6.68	1.77	1.51
1	G	159	LYS	CA-C	6.68	1.61	1.52
1	E	63	ASP	CA-C	6.67	1.61	1.52
1	G	159	LYS	C-O	6.63	1.31	1.24
1	A	89	ILE	CA-C	6.61	1.60	1.52
1	D	97	ILE	CG1-CD1	6.61	1.77	1.51
1	F	227	ARG	CA-C	6.61	1.61	1.52
1	A	73	GLY	N-CA	6.60	1.50	1.44
1	I	83	ILE	CA-CB	6.58	1.62	1.54
1	J	79	VAL	CA-CB	6.57	1.62	1.54
1	D	5	ILE	CA-CB	6.57	1.62	1.54
1	C	145	MET	CG-SD	6.56	1.97	1.80
1	H	138	ARG	CA-C	6.56	1.61	1.52
1	C	83	ILE	CA-CB	6.53	1.62	1.54
1	I	196	ALA	N-CA	6.53	1.54	1.46
1	A	216	THR	C-N	6.51	1.40	1.34
1	I	47	THR	CA-CB	6.51	1.62	1.53
1	D	23	VAL	CA-CB	6.50	1.62	1.54
1	A	122	THR	CA-C	6.48	1.61	1.52
1	E	97	ILE	CA-CB	6.47	1.60	1.53
1	G	131	VAL	C-O	6.46	1.31	1.24
1	E	184	GLY	C-O	6.45	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	97	ILE	C-N	6.43	1.40	1.34
1	I	128	VAL	CA-CB	6.43	1.62	1.54
1	G	79	VAL	CA-CB	6.42	1.62	1.54
1	J	95	VAL	C-O	6.41	1.31	1.24
1	H	44	ALA	CA-CB	6.41	1.64	1.53
1	F	122	THR	CA-CB	6.40	1.63	1.53
1	C	173	ALA	C-O	6.39	1.31	1.23
1	F	145	MET	CG-SD	6.39	1.96	1.80
1	E	157	ILE	CA-CB	6.38	1.61	1.54
1	F	228	ARG	CA-C	6.36	1.61	1.52
1	B	136	VAL	CA-C	6.35	1.60	1.52
1	F	97	ILE	CA-C	6.33	1.58	1.53
1	F	95	VAL	CA-CB	6.31	1.62	1.54
1	D	43	PRO	CA-C	6.30	1.61	1.52
1	D	234	ALA	CA-C	6.30	1.61	1.52
1	G	180	ILE	CA-CB	6.28	1.63	1.54
1	E	211	TRP	CA-C	6.27	1.61	1.52
1	D	109	VAL	CA-CB	-6.25	1.46	1.54
1	F	231	ARG	N-CA	6.24	1.53	1.46
1	H	181	ILE	CA-CB	6.24	1.62	1.54
1	D	238	ALA	CA-C	6.23	1.61	1.52
1	E	178	ASN	C-O	6.22	1.31	1.23
1	A	154	ILE	CA-CB	6.22	1.62	1.54
1	B	162	LYS	N-CA	6.22	1.53	1.46
1	C	101	ILE	CA-CB	6.21	1.62	1.54
1	A	44	ALA	CA-CB	6.19	1.63	1.53
1	F	181	ILE	CA-C	6.18	1.60	1.52
1	A	99	PHE	C-O	6.18	1.30	1.24
1	E	44	ALA	CA-CB	6.18	1.64	1.53
1	H	171	VAL	CA-C	6.18	1.58	1.52
1	B	157	ILE	CA-CB	6.17	1.61	1.54
1	E	69	VAL	CA-C	6.17	1.59	1.52
1	E	86	LYS	CA-C	-6.17	1.45	1.52
1	E	39	LEU	CA-CB	6.16	1.61	1.53
1	C	136	VAL	CA-CB	6.14	1.61	1.54
1	J	233	ALA	CA-CB	6.13	1.62	1.53
1	E	133	ALA	CA-CB	6.12	1.64	1.53
1	C	44	ALA	CA-CB	6.12	1.64	1.53
1	I	78	SER	N-CA	6.10	1.53	1.45
1	F	141	LEU	N-CA	6.09	1.53	1.46
1	D	65	GLN	C-O	-6.09	1.16	1.24
1	H	177	ASN	N-CA	-6.08	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	VAL	CA-C	6.08	1.59	1.52
1	A	13	PRO	C-O	6.08	1.30	1.23
1	F	151	VAL	CA-CB	6.08	1.62	1.54
1	D	73	GLY	N-CA	6.06	1.52	1.45
1	E	71	LEU	N-CA	6.05	1.53	1.45
1	J	158	VAL	CA-CB	6.05	1.60	1.54
1	C	171	VAL	C-O	-6.05	1.17	1.23
1	A	70	ASP	N-CA	6.05	1.52	1.45
1	C	180	ILE	CA-CB	6.03	1.61	1.55
1	A	137	ILE	CA-CB	6.03	1.61	1.53
1	D	222	ASP	N-CA	6.01	1.53	1.46
1	A	89	ILE	CA-CB	5.99	1.61	1.54
1	D	76	VAL	CA-C	5.99	1.59	1.52
1	A	144	PRO	CA-C	5.98	1.60	1.52
1	I	217	PRO	CA-C	5.98	1.61	1.52
1	F	153	GLU	C-O	-5.97	1.17	1.24
1	G	234	ALA	CA-CB	-5.97	1.43	1.53
1	D	106	GLN	CA-C	5.96	1.60	1.52
1	D	89	ILE	CA-C	5.95	1.60	1.52
1	C	54	PHE	N-CA	5.95	1.53	1.46
1	D	126	ARG	CA-CB	5.95	1.60	1.52
1	F	197	ARG	C-O	-5.95	1.16	1.24
1	A	187	VAL	CA-C	5.93	1.57	1.53
1	C	140	MET	N-CA	5.93	1.53	1.46
1	D	225	GLU	N-CA	5.92	1.53	1.46
1	H	18	THR	CA-CB	5.92	1.61	1.53
1	I	93	ILE	CA-CB	5.92	1.62	1.54
1	C	102	ILE	CA-CB	5.91	1.61	1.54
1	G	44	ALA	CA-CB	5.89	1.63	1.53
1	A	157	ILE	CA-CB	5.87	1.60	1.54
1	A	110	ALA	C-O	-5.87	1.17	1.24
1	B	132	ASP	CA-CB	5.86	1.61	1.53
1	G	145	MET	CG-SD	5.86	1.95	1.80
1	A	59	ARG	N-CA	5.85	1.53	1.46
1	H	50	CYS	N-CA	5.85	1.53	1.46
1	B	93	ILE	CA-CB	5.84	1.62	1.54
1	H	180	ILE	CB-CG2	5.83	1.71	1.52
1	F	74	LEU	N-CA	5.83	1.53	1.46
1	F	157	ILE	CA-C	5.82	1.59	1.52
1	I	76	VAL	CA-C	5.82	1.61	1.52
1	D	226	ALA	CA-CB	5.82	1.62	1.53
1	B	68	GLY	N-CA	5.80	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	VAL	CA-CB	5.79	1.63	1.54
1	I	188	PRO	C-N	5.79	1.38	1.33
1	G	156	ARG	N-CA	5.78	1.53	1.46
1	G	56	SER	CA-C	5.78	1.60	1.52
1	G	101	ILE	CA-CB	5.78	1.61	1.54
1	G	5	ILE	CA-CB	5.77	1.61	1.55
1	B	131	VAL	N-CA	5.77	1.53	1.46
1	A	147	LEU	C-O	-5.76	1.17	1.24
1	I	101	ILE	CA-CB	5.76	1.61	1.54
1	J	102	ILE	CA-CB	5.75	1.61	1.54
1	B	123	HIS	CA-C	5.74	1.59	1.52
1	H	175	TRP	N-CA	5.74	1.52	1.45
1	G	132	ASP	CA-C	5.73	1.60	1.53
1	C	88	TRP	CA-C	5.73	1.59	1.52
1	E	234	ALA	CA-CB	5.73	1.63	1.53
1	F	191	THR	CA-C	5.72	1.60	1.52
1	D	173	ALA	C-O	5.70	1.30	1.23
1	C	31	VAL	CA-C	5.70	1.59	1.52
1	C	102	ILE	C-O	5.69	1.30	1.24
1	D	187	VAL	CA-C	5.69	1.57	1.53
1	J	137	ILE	CA-CB	5.69	1.60	1.53
1	J	168	LYS	CA-C	5.69	1.60	1.53
1	F	44	ALA	CA-CB	5.67	1.62	1.53
1	C	50	CYS	CB-SG	5.67	2.00	1.81
1	G	197	ARG	N-CA	5.67	1.53	1.46
1	I	131	VAL	N-CA	5.66	1.53	1.46
1	F	102	ILE	CA-CB	5.65	1.60	1.54
1	A	104	ASP	CA-C	5.65	1.59	1.53
1	F	79	VAL	CA-CB	5.64	1.62	1.54
1	D	79	VAL	CA-CB	5.64	1.61	1.54
1	I	55	VAL	CB-CG2	5.64	1.71	1.52
1	H	217	PRO	CA-C	5.64	1.58	1.52
1	E	139	THR	N-CA	5.62	1.52	1.46
1	G	35	LYS	CA-C	5.62	1.60	1.52
1	D	57	PHE	C-O	5.62	1.30	1.24
1	D	99	PHE	CA-CB	5.61	1.61	1.54
1	H	188	PRO	CA-C	5.61	1.57	1.52
1	J	52	THR	CA-CB	5.61	1.62	1.53
1	J	53	GLU	C-O	-5.61	1.17	1.24
1	D	205	TYR	N-CA	5.60	1.53	1.45
1	A	225	GLU	N-CA	5.60	1.53	1.46
1	F	172	PRO	C-O	5.60	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	11	ARG	CA-C	5.60	1.59	1.52
1	B	103	ALA	CA-CB	-5.59	1.46	1.53
1	D	98	PRO	N-CA	5.59	1.51	1.47
1	I	197	ARG	N-CA	-5.58	1.39	1.46
1	E	158	VAL	CA-CB	5.58	1.61	1.54
1	C	18	THR	CA-CB	5.58	1.60	1.53
1	G	205	TYR	CA-C	-5.57	1.45	1.52
1	B	98	PRO	CA-C	5.57	1.58	1.52
1	I	75	SER	CA-C	5.56	1.60	1.52
1	C	204	GLN	CA-C	5.55	1.60	1.52
1	C	89	ILE	CG1-CD1	5.55	1.73	1.51
1	A	19	THR	CA-CB	5.55	1.62	1.53
1	D	130	ILE	CA-CB	5.53	1.60	1.54
1	B	165	ASP	C-O	-5.53	1.17	1.24
1	E	52	THR	CA-CB	5.53	1.62	1.53
1	I	125	VAL	CA-C	5.52	1.59	1.52
1	G	151	VAL	CA-CB	5.51	1.61	1.54
1	D	139	THR	N-CA	5.51	1.53	1.46
1	D	216	THR	CA-CB	-5.51	1.47	1.53
1	I	40	PHE	N-CA	5.50	1.52	1.46
1	B	89	ILE	CA-CB	5.48	1.61	1.54
1	C	218	ALA	C-O	-5.48	1.17	1.23
1	D	138	ARG	CA-C	5.47	1.59	1.52
1	E	162	LYS	C-O	-5.46	1.17	1.24
1	D	12	PHE	CA-CB	5.45	1.61	1.53
1	A	211	TRP	CA-C	5.45	1.59	1.52
1	I	79	VAL	CA-C	-5.44	1.45	1.52
1	E	137	ILE	N-CA	5.43	1.53	1.46
1	I	64	PHE	CA-C	5.43	1.59	1.52
1	J	237	PRO	N-CA	5.42	1.53	1.47
1	B	97	ILE	CA-C	5.42	1.57	1.53
1	A	153	GLU	C-O	5.42	1.30	1.24
1	D	188	PRO	CA-C	5.42	1.57	1.52
1	G	172	PRO	C-O	5.42	1.30	1.23
1	I	136	VAL	CA-C	5.42	1.59	1.52
1	E	144	PRO	CA-C	5.41	1.58	1.53
1	G	64	PHE	CA-C	5.41	1.59	1.52
1	E	6	PRO	CA-C	5.41	1.59	1.52
1	G	212	PHE	C-O	-5.41	1.16	1.23
1	J	76	VAL	CA-CB	5.40	1.60	1.54
1	I	166	SER	CA-C	-5.40	1.45	1.52
1	D	137	ILE	N-CA	5.40	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	189	PRO	CA-C	5.39	1.54	1.51
1	D	186	ILE	N-CA	5.38	1.52	1.46
1	D	35	LYS	CA-C	-5.38	1.46	1.52
1	E	85	TRP	N-CA	5.38	1.52	1.46
1	A	47	THR	CA-C	5.37	1.57	1.52
1	J	76	VAL	N-CA	5.37	1.52	1.46
1	C	69	VAL	N-CA	5.36	1.52	1.46
1	F	4	SER	CA-C	5.36	1.59	1.52
1	I	152	ASP	CB-CG	5.36	1.65	1.52
1	F	170	ALA	CA-C	5.35	1.60	1.53
1	F	5	ILE	CA-C	5.34	1.58	1.52
1	I	30	TYR	CA-CB	5.34	1.62	1.53
1	B	152	ASP	N-CA	5.34	1.52	1.46
1	J	220	ARG	CG-CD	5.34	1.68	1.52
1	D	104	ASP	C-O	5.33	1.28	1.23
1	A	234	ALA	CA-C	5.32	1.60	1.52
1	A	43	PRO	CA-C	5.32	1.60	1.52
1	J	138	ARG	CG-CD	5.32	1.68	1.52
1	I	157	ILE	C-O	-5.31	1.18	1.24
1	F	225	GLU	CA-CB	5.29	1.61	1.53
1	D	65	GLN	CG-CD	5.28	1.65	1.52
1	G	57	PHE	CA-C	5.27	1.59	1.52
1	D	17	VAL	CA-C	5.26	1.58	1.52
1	E	217	PRO	CA-C	5.26	1.58	1.52
1	B	128	VAL	CA-C	5.25	1.59	1.52
1	F	222	ASP	C-O	-5.25	1.18	1.24
1	D	18	THR	CA-CB	5.24	1.60	1.53
1	H	57	PHE	CA-C	5.24	1.59	1.52
1	F	158	VAL	CA-CB	5.23	1.60	1.54
1	G	198	ALA	CA-CB	5.23	1.62	1.53
1	I	227	ARG	N-CA	5.23	1.52	1.46
1	F	82	HIS	CA-C	-5.22	1.46	1.52
1	J	211	TRP	CA-C	5.20	1.60	1.52
1	J	224	GLU	CB-CG	5.20	1.68	1.52
1	D	64	PHE	CA-C	5.20	1.59	1.52
1	C	135	GLY	N-CA	5.19	1.53	1.45
1	C	182	GLY	N-CA	5.19	1.52	1.45
1	H	208	LEU	CA-C	5.18	1.59	1.52
1	J	161	LEU	CA-C	5.18	1.59	1.52
1	I	42	HIS	CA-CB	5.17	1.61	1.53
1	D	100	PRO	CB-CG	5.17	1.75	1.49
1	H	91	ARG	C-O	-5.17	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	125	VAL	CA-C	5.16	1.59	1.52
1	E	138	ARG	C-O	5.16	1.30	1.23
1	I	4	SER	CA-C	5.15	1.59	1.52
1	H	97	ILE	CA-C	5.14	1.58	1.52
1	A	160	ALA	CA-C	5.13	1.59	1.52
1	E	173	ALA	CA-C	5.13	1.59	1.52
1	D	182	GLY	N-CA	5.12	1.52	1.45
1	A	52	THR	CB-CG2	5.12	1.69	1.52
1	F	183	GLU	CA-CB	5.11	1.61	1.53
1	D	83	ILE	CB-CG2	5.11	1.69	1.52
1	I	218	ALA	CA-C	5.11	1.59	1.52
1	D	51	THR	CA-CB	5.11	1.61	1.53
1	C	89	ILE	CA-CB	5.11	1.60	1.54
1	D	55	VAL	CA-C	5.11	1.59	1.52
1	B	49	VAL	N-CA	5.10	1.52	1.46
1	B	47	THR	CA-CB	5.10	1.63	1.54
1	F	93	ILE	N-CA	5.10	1.52	1.46
1	H	144	PRO	CA-C	5.10	1.58	1.52
1	F	57	PHE	N-CA	5.10	1.52	1.46
1	A	214	TRP	C-O	-5.09	1.17	1.23
1	C	76	VAL	CA-CB	5.09	1.60	1.54
1	F	213	CYS	N-CA	5.09	1.51	1.45
1	J	78	SER	CA-C	-5.09	1.46	1.53
1	I	55	VAL	CA-CB	-5.09	1.48	1.54
1	D	54	PHE	CA-C	-5.08	1.46	1.52
1	B	50	CYS	N-CA	5.07	1.52	1.46
1	C	158	VAL	CA-CB	5.07	1.60	1.54
1	C	28	ASP	N-CA	5.07	1.52	1.46
1	A	111	ARG	N-CA	5.06	1.52	1.46
1	D	25	LYS	CA-C	5.06	1.59	1.52
1	C	171	VAL	CA-CB	5.06	1.58	1.54
1	H	69	VAL	CA-CB	5.06	1.60	1.54
1	D	119	GLU	CD-OE2	5.05	1.34	1.25
1	I	158	VAL	CA-CB	5.05	1.60	1.54
1	I	160	ALA	CA-CB	5.05	1.61	1.53
1	F	131	VAL	N-CA	5.05	1.52	1.46
1	D	72	ILE	CA-CB	5.05	1.61	1.54
1	G	232	ARG	N-CA	5.04	1.52	1.46
1	H	65	GLN	N-CA	5.04	1.52	1.46
1	I	181	ILE	CA-CB	5.04	1.60	1.54
1	C	35	LYS	N-CA	5.04	1.52	1.46
1	J	72	ILE	N-CA	5.04	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	88	TRP	CE3-CZ3	5.03	1.53	1.38
1	H	149	ARG	CZ-NH1	-5.03	1.25	1.32
1	G	58	ALA	N-CA	5.03	1.52	1.46
1	J	191	THR	CA-CB	-5.02	1.45	1.53
1	B	74	LEU	N-CA	-5.02	1.40	1.46
1	B	81	SER	N-CA	5.02	1.52	1.46
1	D	158	VAL	CA-C	-5.02	1.47	1.52
1	F	117	HIS	N-CA	5.02	1.51	1.45
1	G	183	GLU	N-CA	5.02	1.52	1.46
1	J	225	GLU	CA-C	5.02	1.59	1.52
1	F	182	GLY	N-CA	5.02	1.52	1.45
1	G	188	PRO	CA-C	5.02	1.56	1.52
1	E	219	SER	C-O	5.01	1.29	1.23
1	C	57	PHE	CA-C	5.00	1.59	1.52

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	LEU	N-CA-C	-10.12	97.64	110.19
1	I	99	PHE	CA-C-N	9.53	129.47	119.85
1	I	99	PHE	C-N-CA	9.53	129.47	119.85
1	G	104	ASP	CA-C-N	-9.21	111.28	120.31
1	G	104	ASP	C-N-CA	-9.21	111.28	120.31
1	E	189	PRO	N-CA-C	9.21	119.31	110.47
1	G	105	PRO	N-CA-C	-8.84	98.14	111.57
1	F	42	HIS	CA-C-N	8.83	128.42	119.24
1	F	42	HIS	C-N-CA	8.83	128.42	119.24
1	A	143	TYR	CA-C-N	-8.38	109.36	119.84
1	A	143	TYR	C-N-CA	-8.38	109.36	119.84
1	I	208	LEU	N-CA-C	-8.23	103.75	113.88
1	E	166	SER	N-CA-C	8.08	119.72	111.07
1	E	77	ASP	N-CA-C	8.05	120.32	110.41
1	C	202	SER	N-CA-C	-7.96	102.54	111.14
1	C	216	THR	CA-C-N	-7.95	111.78	121.00
1	C	216	THR	C-N-CA	-7.95	111.78	121.00
1	C	91	ARG	N-CA-C	7.88	120.64	111.02
1	J	151	VAL	N-CA-C	7.85	118.63	110.62
1	A	105	PRO	N-CA-C	-7.66	99.21	111.38
1	J	65	GLN	N-CA-C	7.53	119.13	111.07
1	J	221	ASP	N-CA-C	7.52	119.11	111.07
1	B	67	LEU	CA-C-N	-7.48	106.75	121.41
1	B	67	LEU	C-N-CA	-7.48	106.75	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	VAL	CB-CA-C	-7.47	100.06	110.96
1	J	138	ARG	NE-CZ-NH2	-7.46	112.48	119.20
1	I	109	VAL	CB-CA-C	7.46	121.79	112.02
1	D	5	ILE	CA-C-N	-7.38	113.12	120.21
1	D	5	ILE	C-N-CA	-7.38	113.12	120.21
1	G	204	GLN	N-CA-C	7.30	121.45	112.54
1	H	206	ARG	N-CA-C	-7.25	99.76	110.48
1	C	145	MET	CB-CG-SD	7.16	134.19	112.70
1	D	99	PHE	CA-C-N	-7.09	113.50	120.52
1	D	99	PHE	C-N-CA	-7.09	113.50	120.52
1	J	4	SER	N-CA-C	7.08	121.72	107.41
1	A	12	PHE	CA-C-N	-7.00	112.76	119.76
1	A	12	PHE	C-N-CA	-7.00	112.76	119.76
1	G	236	LYS	CA-C-N	-6.92	112.65	119.78
1	G	236	LYS	C-N-CA	-6.92	112.65	119.78
1	I	88	TRP	N-CA-C	6.90	119.39	111.11
1	I	75	SER	N-CA-C	6.90	118.58	108.86
1	D	109	VAL	CB-CA-C	-6.86	103.03	112.02
1	A	180	ILE	N-CA-C	-6.79	105.22	111.67
1	A	79	VAL	N-CA-CB	6.78	118.95	110.47
1	G	208	LEU	CA-CB-CG	6.72	139.81	116.30
1	I	79	VAL	N-CA-CB	6.64	119.58	110.54
1	C	171	VAL	CA-C-N	6.63	127.01	119.92
1	C	171	VAL	C-N-CA	6.63	127.01	119.92
1	J	138	ARG	CG-CD-NE	-6.62	97.43	112.00
1	A	111	ARG	N-CA-C	6.62	119.06	111.11
1	J	122	THR	CB-CA-C	6.59	120.78	109.24
1	C	44	ALA	N-CA-C	6.56	118.49	108.52
1	I	189	PRO	O-C-N	6.56	124.33	121.31
1	C	160	ALA	N-CA-C	6.52	119.22	111.33
1	C	42	HIS	CB-CA-C	6.48	119.72	109.55
1	B	200	MET	N-CA-C	6.46	118.32	111.28
1	E	187	VAL	CA-C-N	-6.45	113.73	120.38
1	E	187	VAL	C-N-CA	-6.45	113.73	120.38
1	G	47	THR	CA-C-N	6.37	125.80	118.85
1	G	47	THR	C-N-CA	6.37	125.80	118.85
1	I	198	ALA	N-CA-C	-6.36	104.27	111.14
1	I	47	THR	CA-C-N	6.34	125.76	118.85
1	I	47	THR	C-N-CA	6.34	125.76	118.85
1	H	83	ILE	N-CA-C	6.34	116.51	110.42
1	G	28	ASP	N-CA-C	6.30	118.95	111.71
1	H	47	THR	CA-C-N	6.29	127.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	47	THR	C-N-CA	6.29	127.70	119.84
1	G	44	ALA	N-CA-C	6.27	117.93	108.46
1	F	120	SER	N-CA-C	6.27	119.47	108.75
1	B	207	CYS	N-CA-C	6.24	118.87	108.13
1	A	234	ALA	N-CA-C	6.24	120.15	112.54
1	C	239	LYS	N-CA-C	6.22	119.27	108.76
1	H	200	MET	N-CA-C	6.21	118.05	111.28
1	D	143	TYR	CA-C-N	-6.21	112.08	119.84
1	D	143	TYR	C-N-CA	-6.21	112.08	119.84
1	C	163	LEU	N-CA-C	6.16	117.69	110.97
1	B	189	PRO	O-C-N	6.16	124.04	121.15
1	C	219	SER	CB-CA-C	-6.14	98.78	109.64
1	C	42	HIS	CA-C-N	-6.12	112.70	119.19
1	C	42	HIS	C-N-CA	-6.12	112.70	119.19
1	I	194	ASP	CA-C-N	6.10	128.73	120.44
1	I	194	ASP	C-N-CA	6.10	128.73	120.44
1	J	129	PHE	CA-C-N	-6.09	115.63	123.19
1	J	129	PHE	C-N-CA	-6.09	115.63	123.19
1	G	189	PRO	N-CA-C	6.09	116.32	110.47
1	J	32	SER	CB-CA-C	-6.07	98.68	110.46
1	J	223	VAL	N-CA-C	6.07	116.81	110.62
1	D	91	ARG	N-CA-C	6.07	117.90	111.28
1	G	151	VAL	N-CA-C	6.05	116.79	110.62
1	B	126	ARG	CG-CD-NE	-6.03	98.73	112.00
1	A	63	ASP	N-CA-C	6.03	117.52	111.07
1	D	235	GLU	N-CA-C	6.02	119.33	109.76
1	B	21	HIS	N-CA-C	-6.00	105.92	113.72
1	B	214	TRP	N-CA-C	5.96	118.13	109.07
1	D	221	ASP	CA-C-N	5.94	128.56	120.54
1	D	221	ASP	C-N-CA	5.94	128.56	120.54
1	E	87	GLU	N-CA-C	5.93	118.22	111.11
1	B	82	HIS	N-CA-CB	5.86	118.74	110.12
1	H	91	ARG	N-CA-C	5.85	117.66	111.28
1	B	108	THR	N-CA-C	5.83	117.31	111.07
1	F	163	LEU	N-CA-C	5.81	117.42	111.14
1	H	86	LYS	N-CA-C	5.81	118.36	111.33
1	C	126	ARG	CG-CD-NE	-5.79	99.26	112.00
1	E	113	LEU	N-CA-C	5.76	120.31	113.28
1	J	159	LYS	N-CA-C	5.76	118.03	111.11
1	A	193	GLU	N-CA-C	5.76	117.56	111.28
1	F	28	ASP	N-CA-C	5.76	117.56	111.28
1	H	204	GLN	N-CA-C	5.75	119.56	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	189	PRO	CA-C-N	-5.74	114.06	119.85
1	J	189	PRO	C-N-CA	-5.74	114.06	119.85
1	F	126	ARG	CG-CD-NE	-5.73	99.40	112.00
1	J	105	PRO	N-CA-C	-5.71	102.30	111.38
1	F	118	ALA	N-CA-C	5.71	119.06	111.75
1	D	42	HIS	CB-CA-C	5.70	118.01	109.63
1	J	149	ARG	CB-CG-CD	5.70	124.41	111.30
1	G	127	GLY	N-CA-C	5.69	119.28	111.54
1	B	86	LYS	N-CA-C	5.68	118.24	111.71
1	B	66	ARG	N-CA-C	5.66	117.45	111.28
1	J	56	SER	N-CA-C	5.66	117.13	111.07
1	A	59	ARG	N-CA-C	5.66	118.18	111.33
1	F	145	MET	CB-CG-SD	5.65	129.64	112.70
1	G	159	LYS	N-CA-C	5.64	117.12	110.97
1	E	4	SER	N-CA-C	5.64	118.43	107.71
1	A	108	THR	N-CA-C	5.64	117.10	111.07
1	J	30	TYR	N-CA-C	-5.61	106.11	113.12
1	E	83	ILE	N-CA-C	-5.61	105.06	110.72
1	I	188	PRO	CB-CA-C	5.59	117.74	110.92
1	E	128	VAL	CB-CA-C	-5.58	102.89	110.42
1	C	143	TYR	N-CA-C	-5.57	102.60	110.29
1	A	235	GLU	CB-CA-C	-5.53	100.82	109.84
1	D	87	GLU	N-CA-C	5.53	118.02	111.33
1	I	60	ARG	N-CA-C	-5.53	106.12	112.92
1	C	189	PRO	N-CA-C	5.53	117.44	110.70
1	A	4	SER	N-CA-C	5.52	118.62	109.46
1	D	32	SER	N-CA-C	5.51	119.50	112.34
1	A	194	ASP	N-CA-C	5.50	116.96	111.07
1	F	85	TRP	N-CA-C	5.50	116.95	111.07
1	F	48	PRO	N-CA-C	5.49	120.75	113.40
1	C	92	HIS	N-CA-C	5.49	120.08	112.45
1	F	97	ILE	CA-C-O	5.49	122.19	119.12
1	D	106	GLN	N-CA-CB	-5.48	102.63	110.80
1	H	7	LEU	N-CA-C	5.48	118.33	109.40
1	C	233	ALA	N-CA-C	5.47	116.93	111.07
1	J	179	GLU	N-CA-C	5.46	118.15	111.82
1	D	228	ARG	CG-CD-NE	5.45	123.98	112.00
1	H	89	ILE	N-CA-C	5.44	116.08	110.36
1	C	209	ASP	N-CA-C	-5.44	99.87	108.14
1	G	207	CYS	N-CA-CB	-5.43	101.31	110.49
1	D	109	VAL	N-CA-C	5.42	115.63	110.53
1	I	89	ILE	N-CA-C	5.42	116.15	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	163	LEU	N-CA-C	5.40	117.92	111.71
1	I	78	SER	N-CA-C	5.39	117.83	110.55
1	D	206	ARG	CB-CA-C	5.39	118.52	109.89
1	E	208	LEU	CA-CB-CG	5.37	135.09	116.30
1	C	32	SER	CA-CB-OG	-5.36	100.38	111.10
1	A	160	ALA	N-CA-C	5.35	117.87	111.71
1	C	47	THR	CA-C-N	5.35	124.68	118.85
1	C	47	THR	C-N-CA	5.35	124.68	118.85
1	D	154	ILE	N-CA-C	5.33	116.06	110.62
1	F	54	PHE	CA-C-N	5.33	127.39	120.56
1	F	54	PHE	C-N-CA	5.33	127.39	120.56
1	I	12	PHE	CA-C-N	5.33	126.50	119.84
1	I	12	PHE	C-N-CA	5.33	126.50	119.84
1	C	144	PRO	CA-C-N	5.32	127.67	120.38
1	C	144	PRO	C-N-CA	5.32	127.67	120.38
1	A	187	VAL	CA-C-N	-5.29	114.93	120.38
1	A	187	VAL	C-N-CA	-5.29	114.93	120.38
1	H	61	TYR	N-CA-C	5.29	117.46	111.11
1	A	84	LYS	N-CA-C	-5.29	105.60	111.36
1	I	67	LEU	N-CA-C	-5.28	106.88	113.38
1	J	189	PRO	N-CA-C	5.28	116.23	110.58
1	B	81	SER	CA-C-N	-5.28	113.21	120.28
1	B	81	SER	C-N-CA	-5.28	113.21	120.28
1	F	149	ARG	CB-CG-CD	5.25	123.37	111.30
1	F	106	GLN	N-CA-CB	-5.24	108.86	114.10
1	B	143	TYR	N-CA-C	-5.24	103.58	110.39
1	E	187	VAL	CB-CA-C	-5.23	106.08	110.94
1	E	61	TYR	N-CA-C	5.21	116.64	111.07
1	E	151	VAL	N-CA-C	5.21	117.56	111.05
1	I	79	VAL	CB-CA-C	-5.19	105.13	112.14
1	F	27	PRO	CA-C-N	5.19	127.23	120.28
1	F	27	PRO	C-N-CA	5.19	127.23	120.28
1	H	149	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	H	187	VAL	CA-C-N	-5.17	115.05	120.38
1	H	187	VAL	C-N-CA	-5.17	115.05	120.38
1	E	80	PHE	CA-C-N	5.16	127.20	120.28
1	E	80	PHE	C-N-CA	5.16	127.20	120.28
1	H	186	ILE	N-CA-C	5.16	116.02	108.58
1	H	235	GLU	N-CA-C	5.16	118.36	110.20
1	I	229	TYR	N-CA-C	-5.16	105.65	111.28
1	J	193	GLU	N-CA-C	5.16	117.57	111.33
1	F	208	LEU	CA-CB-CG	5.14	134.29	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	206	ARG	CA-C-N	-5.13	111.74	121.54
1	G	206	ARG	C-N-CA	-5.13	111.74	121.54
1	H	65	GLN	CA-C-N	5.12	127.66	120.28
1	H	65	GLN	C-N-CA	5.12	127.66	120.28
1	I	206	ARG	CB-CG-CD	5.12	123.09	111.30
1	D	163	LEU	N-CA-C	5.12	116.55	111.07
1	C	28	ASP	N-CA-C	5.12	116.86	111.28
1	A	99	PHE	N-CA-C	-5.11	101.23	109.82
1	A	149	ARG	CB-CG-CD	5.11	123.06	111.30
1	J	82	HIS	N-CA-CB	5.11	117.42	110.01
1	A	105	PRO	CA-C-N	-5.11	111.78	121.54
1	A	105	PRO	C-N-CA	-5.11	111.78	121.54
1	E	81	SER	N-CA-C	5.11	116.85	111.28
1	F	37	PHE	N-CA-C	5.09	117.54	109.50
1	G	132	ASP	N-CA-C	5.09	117.37	110.35
1	A	193	GLU	N-CA-CB	-5.08	102.65	110.12
1	I	47	THR	CB-CA-C	5.06	116.42	108.63
1	C	59	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	D	124	THR	CB-CA-C	-5.03	100.62	109.62
1	A	72	ILE	CA-C-N	-5.02	117.96	122.43
1	A	72	ILE	C-N-CA	-5.02	117.96	122.43
1	G	168	LYS	N-CA-C	5.02	118.32	111.39
1	F	228	ARG	N-CA-C	5.01	116.75	111.28

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	49	0
1	B	1973	0	1957	41	0
1	C	1973	0	1959	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1973	0	1959	44	0
1	E	1958	0	1945	39	0
1	F	1973	0	1957	38	0
1	G	1958	0	1945	42	0
1	H	1968	0	1952	40	0
1	I	1973	0	1957	54	0
1	J	1953	0	1940	37	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	364	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 (364) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:140:MET:HE2	1:I:142:TYR:OH	1.67	0.94
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
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:I:129:PHE:CE2	1:I:140:MET:HE3	2.14	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	0.78
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:C:120:SER:HB3	1:C:145:MET:HE1	1.68	0.75
1:J:59:ARG:HG3	1:J:59:ARG:NH1	1.97	0.75
1:C:67:LEU:HD13	1:C:158:VAL:HG23	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:129:PHE:HE2	1:I:140:MET:HE3	1.54	0.72
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:H:39:LEU:C	1:H:39:LEU:HD12	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:J:14:GLU:OE2	1:J:25:LYS:NZ	2.32	0.60
1:C:93:ILE:HG22	1:C:95:VAL:HG23	1.84	0.59
1:B:244:GLU:O	1:B:244:GLU:HG2	2.01	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:13:PRO:HB2	1:G:15:MET:HE3	1.93	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: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:C:103:ALA:C	1:C:105:PRO:HD3	2.38	0.48
1:F:82:HIS:CD2	1:F:101:ILE:HG22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:8:ILE:HG13	1:E:140:MET:HE2	1.96	0.48
1:H:122:THR:HG22	1:H:123:HIS:CG	2.48	0.48
1:B:66:ARG:C	1:B:67:LEU:O	2.51	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
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:D:74:LEU:HD13	1:D:74:LEU:C	2.40	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:A:39:LEU:C	1:A:39:LEU:HD23	2.40	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:104:ASP:CG	1:I:104:ASP:O	2.58	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:G:74:LEU:HD13	1:G:74:LEU:C	2.40	0.46
1:G:132:ASP:OD1	1:G:132:ASP:C	2.59	0.46
1:B:79:VAL:O	1:B:83:ILE:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:25:LYS:HD3	1:C:28:ASP:CG	2.43	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
1:A:83:ILE:O	1:A:87:GLU:HG3	2.16	0.44
1:E:39:LEU:C	1:E:39:LEU:HD12	2.42	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: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:J:145:MET:HE3	1:J:145:MET:HB3	1.66	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:LYS:HE2	1:E:244:GLU:CD	2.45	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: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:D:191:THR:H	1:D:195:GLN:HE22	1.68	0.41
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:A:202:SER:C	1:A:204:GLN:N	2.78	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: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:F:120:SER:CB	1:F:145:MET:HE1	2.49	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:81:SER:O	1:B:82:HIS:C	2.61	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:B:103:ALA:C	1:B:105:PRO:HD3	2.46	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: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
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:G:206:ARG:O	1:G:207:CYS:CB	2.55	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%)	16	16
1	B	242/249 (97%)	226 (93%)	15 (6%)	1 (0%)	30	34
1	C	242/249 (97%)	233 (96%)	8 (3%)	1 (0%)	30	34
1	D	242/249 (97%)	229 (95%)	12 (5%)	1 (0%)	30	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	238/249 (96%)	226 (95%)	11 (5%)	1 (0%)	30	34
1	F	242/249 (97%)	228 (94%)	14 (6%)	0	100	100
1	G	238/249 (96%)	225 (94%)	11 (5%)	2 (1%)	16	16
1	H	241/249 (97%)	230 (95%)	9 (4%)	2 (1%)	16	16
1	I	242/249 (97%)	234 (97%)	7 (3%)	1 (0%)	30	34
1	J	237/249 (95%)	225 (95%)	10 (4%)	2 (1%)	16	16
All	All	2401/2490 (96%)	2278 (95%)	110 (5%)	13 (0%)	24	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	SER
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%)	191 (92%)	17 (8%)	10	12
1	B	210/215 (98%)	195 (93%)	15 (7%)	13	16
1	C	210/215 (98%)	194 (92%)	16 (8%)	12	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	210/215 (98%)	196 (93%)	14 (7%)	15	17
1	E	208/215 (97%)	190 (91%)	18 (9%)	9	10
1	F	210/215 (98%)	190 (90%)	20 (10%)	8	8
1	G	208/215 (97%)	190 (91%)	18 (9%)	9	10
1	H	210/215 (98%)	194 (92%)	16 (8%)	12	14
1	I	210/215 (98%)	190 (90%)	20 (10%)	8	8
1	J	208/215 (97%)	194 (93%)	14 (7%)	15	17
All	All	2092/2150 (97%)	1924 (92%)	168 (8%)	11	13

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
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	125	VAL
1	A	144	PRO
1	A	145	MET
1	A	147	LEU
1	A	163	LEU
1	A	179	GLU
1	A	206	ARG
1	A	236	LYS
1	A	239	LYS
1	B	11	ARG
1	B	28	ASP
1	B	39	LEU
1	B	59	ARG
1	B	74	LEU
1	B	106	GLN
1	B	116	LEU
1	B	120	SER
1	B	122	THR
1	B	147	LEU
1	B	163	LEU

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Mol	Chain	Res	Type
1	B	208	LEU
1	B	220	ARG
1	B	224	GLU
1	B	228	ARG
1	C	5	ILE
1	C	28	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
1	C	199	ARG
1	C	201	GLU
1	C	204	GLN
1	C	235	GLU
1	C	239	LYS
1	D	11	ARG
1	D	39	LEU
1	D	59	ARG
1	D	74	LEU
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	179	GLU
1	D	208	LEU
1	D	244	GLU
1	E	2	PRO
1	E	11	ARG
1	E	39	LEU
1	E	55	VAL
1	E	70	ASP
1	E	74	LEU
1	E	79	VAL
1	E	81	SER

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Mol	Chain	Res	Type
1	E	101	ILE
1	E	122	THR
1	E	124	THR
1	E	166	SER
1	E	191	THR
1	E	197	ARG
1	E	199	ARG
1	E	208	LEU
1	E	224	GLU
1	E	244	GLU
1	F	11	ARG
1	F	16	GLU
1	F	62	GLU
1	F	74	LEU
1	F	76	VAL
1	F	79	VAL
1	F	91	ARG
1	F	95	VAL
1	F	106	GLN
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	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	66	ARG
1	G	74	LEU
1	G	76	VAL
1	G	111	ARG
1	G	112	ARG
1	G	116	LEU
1	G	124	THR
1	G	134	ARG
1	G	145	MET

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Mol	Chain	Res	Type
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	H	28	ASP
1	H	39	LEU
1	H	59	ARG
1	H	79	VAL
1	H	112	ARG
1	H	122	THR
1	H	125	VAL
1	H	140	MET
1	H	145	MET
1	H	147	LEU
1	H	159	LYS
1	H	161	LEU
1	H	201	GLU
1	H	208	LEU
1	H	239	LYS
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	128	VAL
1	I	145	MET
1	I	147	LEU
1	I	159	LYS
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	235	GLU
1	I	239	LYS

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Mol	Chain	Res	Type
1	J	2	PRO
1	J	11	ARG
1	J	59	ARG
1	J	75	SER
1	J	81	SER
1	J	116	LEU
1	J	126	ARG
1	J	145	MET
1	J	147	LEU
1	J	167	LEU
1	J	207	CYS
1	J	208	LEU
1	J	221	ASP
1	J	239	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	B	117	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	117	HIS
1	E	123	HIS
1	F	106	GLN
1	F	117	HIS
1	F	195	GLN
1	G	123	HIS
1	H	65	GLN
1	H	106	GLN
1	H	117	HIS
1	H	195	GLN
1	I	117	HIS
1	I	195	GLN
1	J	65	GLN
1	J	92	HIS
1	J	117	HIS
1	J	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	241/249 (96%)	0.13	9 (3%) 45 42	18, 28, 50, 61	0
1	B	244/249 (97%)	0.10	5 (2%) 65 62	18, 30, 52, 64	0
1	C	244/249 (97%)	-0.05	6 (2%) 58 55	15, 27, 51, 66	0
1	D	244/249 (97%)	0.06	11 (4%) 38 35	15, 26, 48, 63	0
1	E	242/249 (97%)	0.06	7 (2%) 53 50	16, 28, 47, 64	0
1	F	244/249 (97%)	0.28	13 (5%) 32 29	20, 31, 53, 70	0
1	G	242/249 (97%)	0.27	10 (4%) 41 38	21, 33, 53, 73	0
1	H	243/249 (97%)	0.19	7 (2%) 53 50	19, 32, 56, 68	0
1	I	244/249 (97%)	0.19	13 (5%) 32 29	16, 29, 53, 58	0
1	J	241/249 (96%)	0.11	7 (2%) 53 50	18, 28, 49, 64	0
All	All	2429/2490 (97%)	0.13	88 (3%) 46 43	15, 29, 52, 73	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	121	ALA	4.2
1	F	245	ALA	4.0
1	A	121	ALA	3.9
1	A	245	ALA	3.7
1	I	4	SER	3.7
1	I	245	ALA	3.6
1	E	242	TYR	3.6
1	F	4	SER	3.6
1	E	122	THR	3.5
1	J	122	THR	3.5
1	F	121	ALA	3.4
1	E	2	PRO	3.4
1	C	121	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	242	TYR	3.4
1	G	118	ALA	3.4
1	B	245	ALA	3.3
1	G	121	ALA	3.3
1	C	5	ILE	3.3
1	I	119	GLU	3.3
1	I	200	MET	3.2
1	D	245	ALA	3.2
1	J	207	CYS	3.2
1	J	2	PRO	3.2
1	E	245	ALA	3.2
1	H	242	TYR	3.1
1	G	245	ALA	3.0
1	H	118	ALA	3.0
1	A	122	THR	3.0
1	E	121	ALA	3.0
1	H	2	PRO	3.0
1	D	119	GLU	2.9
1	B	121	ALA	2.9
1	D	120	SER	2.9
1	F	119	GLU	2.9
1	F	145	MET	2.9
1	I	118	ALA	2.8
1	J	201	GLU	2.8
1	F	207	CYS	2.8
1	C	200	MET	2.8
1	I	207	CYS	2.7
1	A	123	HIS	2.7
1	F	122	THR	2.7
1	H	244	GLU	2.7
1	I	121	ALA	2.6
1	D	118	ALA	2.6
1	D	122	THR	2.5
1	I	242	TYR	2.5
1	H	116	LEU	2.5
1	D	2	PRO	2.5
1	G	122	THR	2.5
1	B	201	GLU	2.5
1	J	242	TYR	2.5
1	F	116	LEU	2.5
1	D	238	ALA	2.5
1	F	120	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	207	CYS	2.3
1	J	123	HIS	2.3
1	C	242	TYR	2.3
1	E	207	CYS	2.3
1	G	2	PRO	2.3
1	D	121	ALA	2.3
1	H	122	THR	2.3
1	D	123	HIS	2.3
1	F	42	HIS	2.3
1	A	124	THR	2.2
1	F	123	HIS	2.2
1	G	42	HIS	2.2
1	G	242	TYR	2.2
1	F	90	GLU	2.2
1	G	123	HIS	2.2
1	I	117	HIS	2.2
1	G	207	CYS	2.2
1	A	198	ALA	2.2
1	E	244	GLU	2.2
1	A	4	SER	2.2
1	B	2	PRO	2.1
1	C	123	HIS	2.1
1	B	116	LEU	2.1
1	I	240	LEU	2.1
1	G	244	GLU	2.1
1	D	3	GLY	2.1
1	I	122	THR	2.1
1	I	201	GLU	2.1
1	D	242	TYR	2.1
1	C	245	ALA	2.0
1	I	116	LEU	2.0
1	A	2	PRO	2.0
1	F	118	ALA	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.