Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 02:02 PM EDT

PDB ID	:	2E2G
Title	:	Crystal structure of archaeal peroxiredoxin, thioredoxin peroxidase from Aeropyrum pernix K1 (pre-oxidation form)
Authors	:	Nakamura, T.; Yamamoto, T.; Abe, M.; Matsumura, H.; Hagihara, Y.; Goto, T.; Yamaguchi, T.; Inoue, T.
Deposited on	:	2006-11-13
Resolution	:	2.40 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:

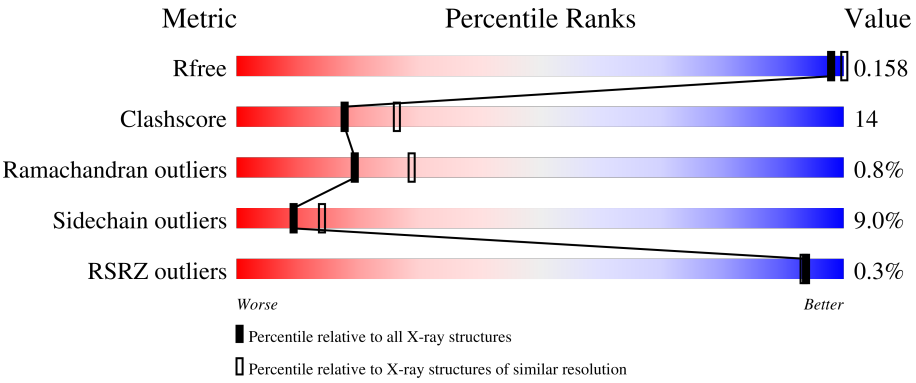
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	250	70% 21% 5%
1	B	250	64% 25% 5%
1	C	250	64% 26% 5%
1	D	250	69% 22% 5%
1	E	250	66% 22% 5% 5%

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Mol	Chain	Length	Quality of chain
1	F	250	66% 22% 5% • 5%
1	G	250	67% 23% • • 5%
1	H	250	66% 22% 5% • 5%
1	I	250	63% 29% • • 5%
1	J	250	69% 22% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19878 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	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	B	239	Total	C	N	O	S	0	0	0
			1942	1250	342	344	6			
1	C	239	Total	C	N	O	S	0	0	0
			1938	1247	340	345	6			
1	D	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	E	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	F	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	G	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	H	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	I	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	J	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	SER	CYS	engineered mutation	UNP Q9Y9L0
B	207	SER	CYS	engineered mutation	UNP Q9Y9L0
C	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
E	207	SER	CYS	engineered mutation	UNP Q9Y9L0
F	207	SER	CYS	engineered mutation	UNP Q9Y9L0
G	207	SER	CYS	engineered mutation	UNP Q9Y9L0
H	207	SER	CYS	engineered mutation	UNP Q9Y9L0
I	207	SER	CYS	engineered mutation	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	207	SER	CYS	engineered mutation	UNP Q9Y9L0

- Molecule 2 is water.

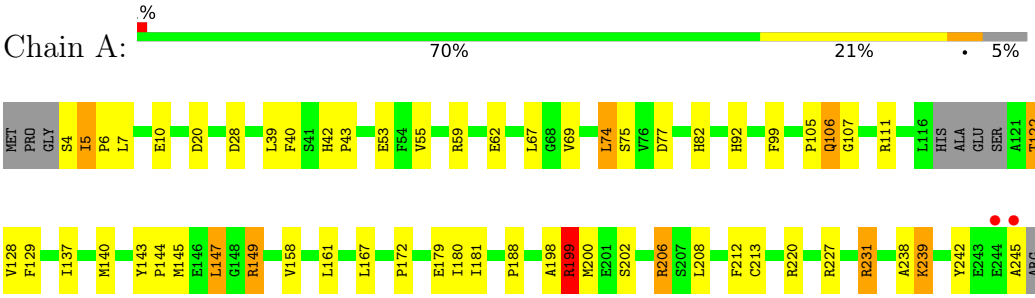
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	60	Total O 60 60	0	0
2	C	39	Total O 39 39	0	0
2	D	57	Total O 57 57	0	0
2	E	65	Total O 65 65	0	0
2	F	59	Total O 59 59	0	0
2	G	61	Total O 61 61	0	0
2	H	65	Total O 65 65	0	0
2	I	30	Total O 30 30	0	0
2	J	49	Total O 49 49	0	0

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.

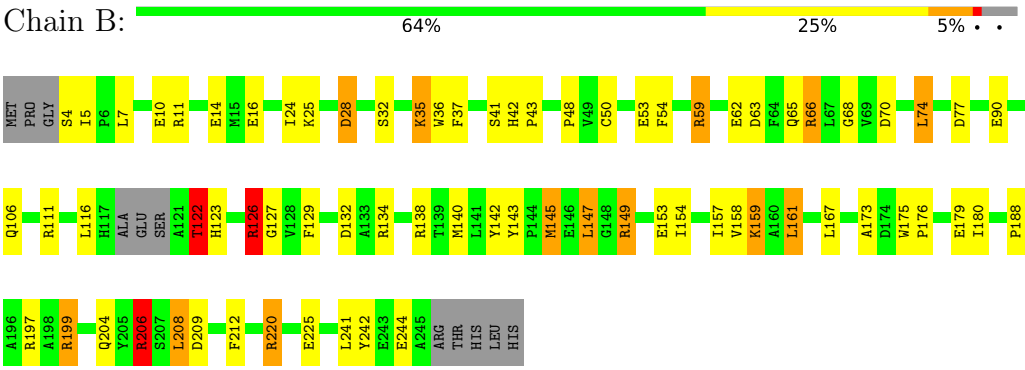
• Molecule 1: Probable peroxiredoxin

Chain A:



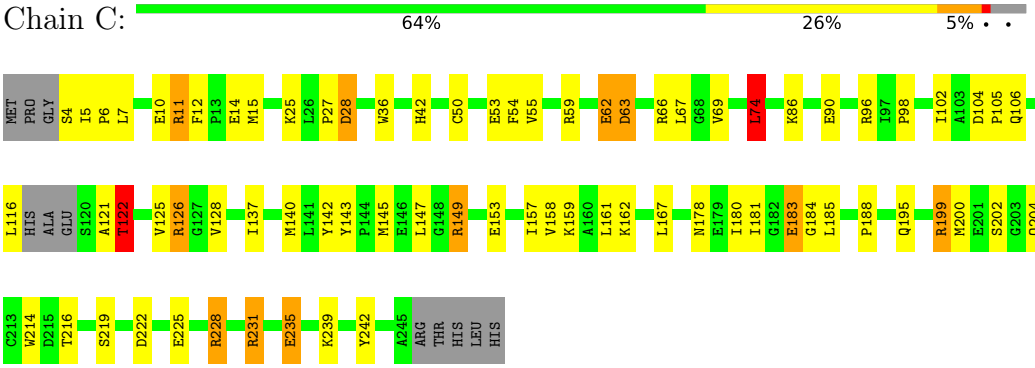
• Molecule 1: Probable peroxiredoxin

Chain B:



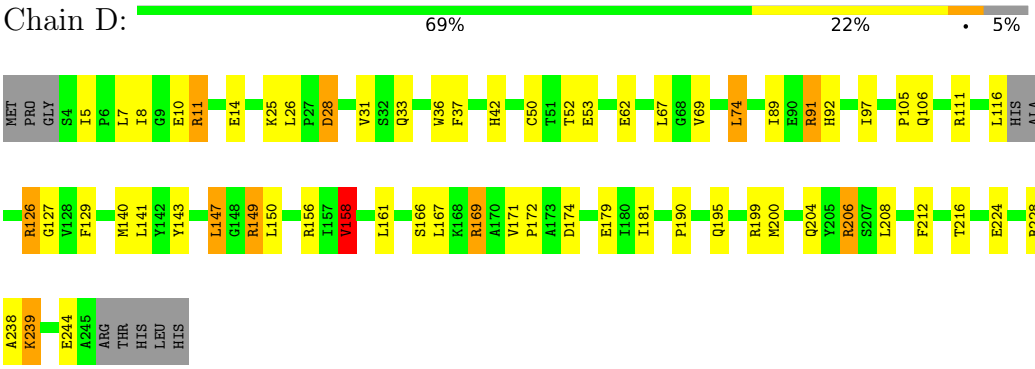
• Molecule 1: Probable peroxiredoxin

Chain C:



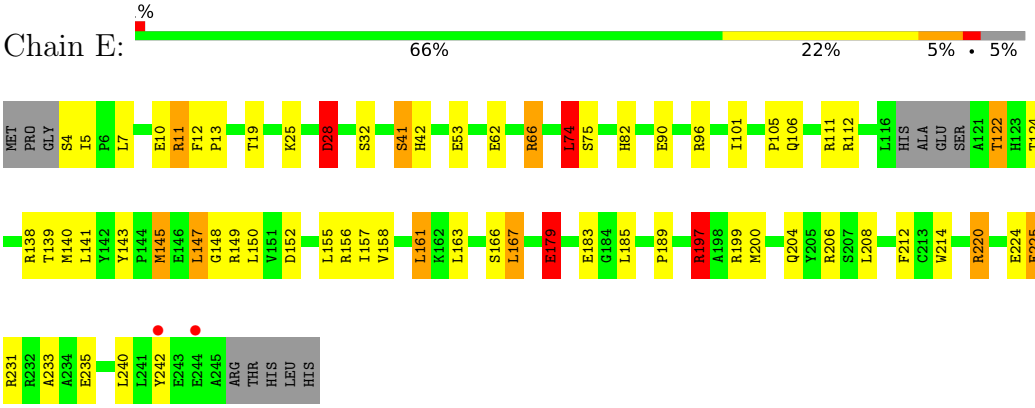
• Molecule 1: Probable peroxiredoxin

Chain D:



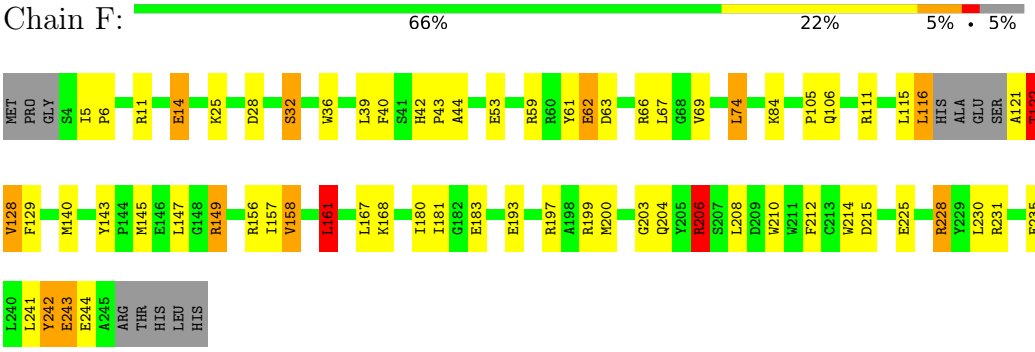
• Molecule 1: Probable peroxiredoxin

Chain E:



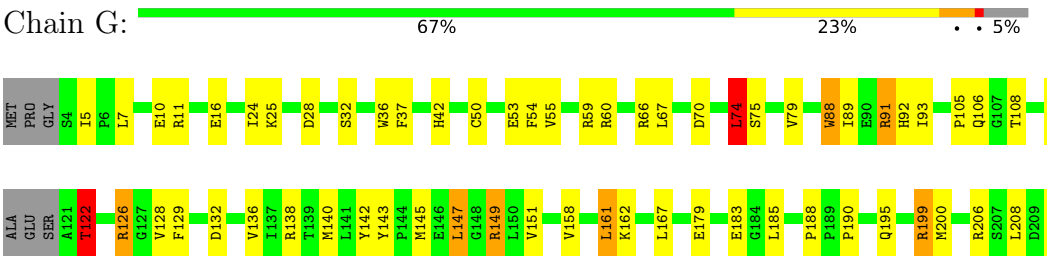
• Molecule 1: Probable peroxiredoxin

Chain F:



• Molecule 1: Probable peroxiredoxin

Chain G:

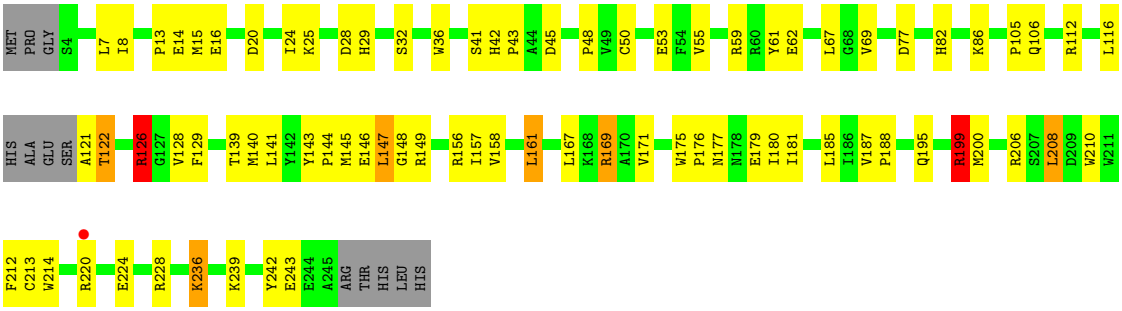


• Molecule 1: Probable peroxiredoxin

Chain H:

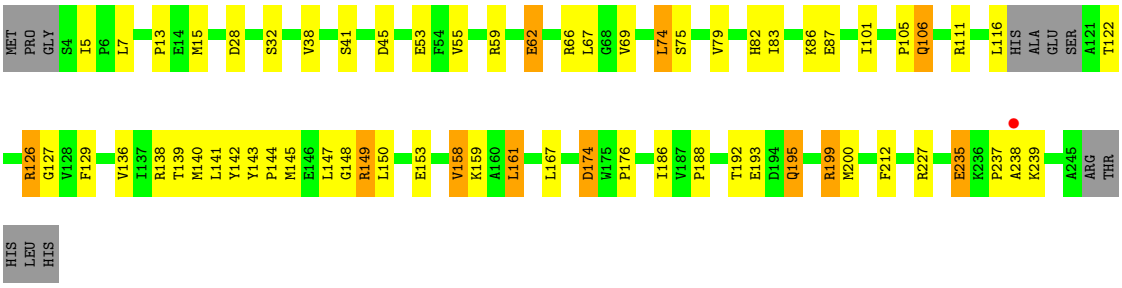
• Molecule 1: Probable peroxiredoxin

Chain I:



• Molecule 1: Probable peroxiredoxin

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.20Å 103.35Å 104.63Å 105.79° 105.19° 92.68°	Depositor
Resolution (Å)	19.99 – 2.40 49.48 – 2.39	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.99-2.40) 86.8 (49.48-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.229 0.160 , 0.158	Depositor DCC
R_{free} test set	5083 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19878	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.16	1/1984 (0.1%)	1.08	7/2696 (0.3%)
1	B	1.17	3/1995 (0.2%)	1.13	12/2711 (0.4%)
1	C	1.16	5/1990 (0.3%)	1.12	10/2704 (0.4%)
1	D	1.12	3/1984 (0.2%)	1.08	6/2696 (0.2%)
1	E	1.22	7/1984 (0.4%)	1.13	12/2696 (0.4%)
1	F	1.26	15/1984 (0.8%)	1.13	15/2696 (0.6%)
1	G	1.15	5/1984 (0.3%)	1.05	5/2696 (0.2%)
1	H	1.19	8/1984 (0.4%)	1.08	7/2696 (0.3%)
1	I	1.11	3/1984 (0.2%)	1.08	9/2696 (0.3%)
1	J	1.12	2/1984 (0.1%)	1.03	6/2696 (0.2%)
All	All	1.17	52/19857 (0.3%)	1.09	89/26983 (0.3%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	183	GLU	CD-OE2	10.14	1.36	1.25
1	H	225	GLU	CG-CD	8.59	1.64	1.51
1	F	62	GLU	CG-CD	8.18	1.64	1.51
1	F	225	GLU	CG-CD	7.85	1.63	1.51
1	E	225	GLU	CG-CD	7.60	1.63	1.51
1	C	183	GLU	CD-OE2	7.59	1.33	1.25
1	D	224	GLU	CG-CD	7.56	1.63	1.51
1	E	225	GLU	CB-CG	7.42	1.66	1.52
1	E	228	ARG	CG-CD	7.41	1.70	1.51
1	B	149	ARG	CZ-NH1	7.35	1.42	1.33
1	H	228	ARG	CG-CD	7.17	1.69	1.51
1	C	235	GLU	CB-CG	7.14	1.65	1.52
1	B	90	GLU	CG-CD	6.96	1.62	1.51
1	G	243	GLU	CG-CD	6.65	1.61	1.51
1	J	62	GLU	CG-CD	6.63	1.61	1.51
1	C	235	GLU	CG-CD	6.60	1.61	1.51
1	E	183	GLU	CD-OE2	6.46	1.32	1.25
1	C	62	GLU	CG-CD	6.46	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	197	ARG	CG-CD	6.21	1.67	1.51
1	B	179	GLU	CD-OE2	6.19	1.32	1.25
1	D	37	PHE	CE2-CZ	6.08	1.48	1.37
1	H	225	GLU	CB-CG	5.99	1.63	1.52
1	H	225	GLU	CD-OE1	5.94	1.32	1.25
1	H	62	GLU	CG-CD	5.93	1.60	1.51
1	D	158	VAL	CB-CG2	-5.83	1.40	1.52
1	F	244	GLU	CG-CD	5.75	1.60	1.51
1	E	183	GLU	CG-CD	5.65	1.60	1.51
1	G	224	GLU	CG-CD	5.62	1.60	1.51
1	E	179	GLU	CG-CD	5.58	1.60	1.51
1	F	62	GLU	CB-CG	5.58	1.62	1.52
1	A	179	GLU	CG-CD	5.55	1.60	1.51
1	I	179	GLU	CG-CD	5.49	1.60	1.51
1	F	236	LYS	CE-NZ	5.46	1.62	1.49
1	F	183	GLU	CD-OE1	5.46	1.31	1.25
1	J	235	GLU	CG-CD	5.41	1.60	1.51
1	H	193	GLU	CD-OE2	5.40	1.31	1.25
1	F	128	VAL	CB-CG1	-5.38	1.41	1.52
1	G	214	TRP	CG-CD1	5.34	1.44	1.36
1	E	228	ARG	NE-CZ	5.32	1.40	1.33
1	I	146	GLU	CG-CD	5.29	1.59	1.51
1	F	193	GLU	CG-CD	-5.28	1.44	1.51
1	F	228	ARG	NE-CZ	5.20	1.39	1.33
1	H	193	GLU	CG-CD	5.19	1.59	1.51
1	G	183	GLU	CD-OE1	5.13	1.31	1.25
1	F	228	ARG	CG-CD	5.13	1.64	1.51
1	F	239	LYS	CD-CE	5.07	1.64	1.51
1	I	236	LYS	CD-CE	5.06	1.63	1.51
1	F	243	GLU	CG-CD	5.05	1.59	1.51
1	C	90	GLU	CG-CD	5.04	1.59	1.51
1	G	183	GLU	CG-CD	5.04	1.59	1.51
1	F	235	GLU	CG-CD	5.03	1.59	1.51
1	F	62	GLU	CD-OE1	5.00	1.31	1.25

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	206	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	C	206	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	C	126	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	E	228	ARG	NE-CZ-NH1	10.50	125.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	C	231	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	E	197	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	F	149	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	E	206	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	E	138	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	D	149	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	A	149	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	149	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	126	ARG	C-N-CA	-7.45	106.65	122.30
1	I	199	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	H	126	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	E	138	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	231	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	F	126	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	H	147	LEU	CA-CB-CG	6.81	130.97	115.30
1	I	126	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	B	74	LEU	CA-CB-CG	6.71	130.72	115.30
1	A	149	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	74	LEU	CA-CB-CG	6.60	130.48	115.30
1	B	134	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	D	174	ASP	CB-CG-OD1	6.55	124.20	118.30
1	H	227	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	C	74	LEU	CA-CB-CG	6.52	130.30	115.30
1	H	126	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	134	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	111	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	D	74	LEU	CA-CB-CG	6.45	130.12	115.30
1	I	206	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	199	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	209	ASP	CB-CG-OD2	6.34	124.00	118.30
1	E	228	ARG	CD-NE-CZ	6.32	132.45	123.60
1	I	7	LEU	CA-CB-CG	6.29	129.77	115.30
1	I	156	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	231	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	E	74	LEU	CA-CB-CG	6.15	129.44	115.30
1	I	77	ASP	CB-CG-OD2	6.10	123.79	118.30
1	H	208	LEU	CA-CB-CG	6.09	129.31	115.30
1	J	74	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	199	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	J	174	ASP	CB-CG-OD1	5.94	123.64	118.30
1	E	155	LEU	CB-CG-CD1	-5.93	100.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	122	THR	N-CA-CB	5.92	121.54	110.30
1	G	122	THR	N-CA-CB	5.86	121.43	110.30
1	G	149	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	E	122	THR	N-CA-CB	5.79	121.31	110.30
1	D	116	LEU	CA-CB-CG	5.79	128.61	115.30
1	H	74	LEU	CA-CB-CG	5.78	128.59	115.30
1	I	169	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	E	32	SER	CB-CA-C	-5.73	99.21	110.10
1	B	208	LEU	CA-CB-CG	5.72	128.46	115.30
1	H	122	THR	N-CA-CB	5.69	121.12	110.30
1	G	91	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	F	161	LEU	CA-CB-CG	5.63	128.24	115.30
1	G	126	ARG	C-N-CA	-5.60	110.55	122.30
1	J	126	ARG	C-N-CA	-5.54	110.66	122.30
1	F	149	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	I	45	ASP	CB-CG-OD1	5.48	123.23	118.30
1	F	215	ASP	CB-CG-OD1	5.47	123.22	118.30
1	E	28	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	206	ARG	CD-NE-CZ	5.45	131.24	123.60
1	E	231	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	F	236	LYS	CD-CE-NZ	5.44	124.20	111.70
1	F	111	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	122	THR	N-CA-CB	5.41	120.58	110.30
1	C	149	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	J	159	LYS	CD-CE-NZ	-5.38	99.33	111.70
1	F	74	LEU	CA-CB-CG	5.25	127.39	115.30
1	F	168	LYS	CD-CE-NZ	-5.25	99.63	111.70
1	C	63	ASP	CB-CG-OD2	5.24	123.02	118.30
1	I	45	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	122	THR	N-CA-CB	5.20	120.19	110.30
1	F	111	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	J	66	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	26	LEU	CA-CB-CG	5.18	127.20	115.30
1	F	206	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	G	74	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	161	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	149	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	122	THR	N-CA-CB	5.09	119.97	110.30
1	F	149	ARG	CB-CG-CD	5.08	124.79	111.60
1	A	231	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	F	228	ARG	CG-CD-NE	5.05	122.40	111.80
1	D	149	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	231	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1932	0	1924	58	0
1	B	1942	0	1931	69	0
1	C	1938	0	1929	63	0
1	D	1932	0	1924	48	0
1	E	1932	0	1924	63	0
1	F	1932	0	1924	55	1
1	G	1932	0	1924	64	0
1	H	1932	0	1924	60	1
1	I	1932	0	1924	54	0
1	J	1932	0	1924	44	0
2	A	57	0	0	0	0
2	B	60	0	0	2	0
2	C	39	0	0	4	0
2	D	57	0	0	4	0
2	E	65	0	0	9	0
2	F	59	0	0	6	0
2	G	61	0	0	5	0
2	H	65	0	0	6	0
2	I	30	0	0	2	0
2	J	49	0	0	1	0
All	All	19878	0	19252	524	1

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 14.

All (524) 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:F:206:ARG:HG3	1:F:206:ARG:HH11	1.10	1.15
1:A:123:HIS:HA	1:A:145:MET:HE1	1.33	1.10
1:I:129:PHE:CE2	1:I:140:MET:HE3	1.88	1.08
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.18	1.07
1:E:220:ARG:HG2	1:E:220:ARG:HH11	0.96	1.06
1:I:105:PRO:O	1:I:106:GLN:HB2	1.54	1.05
1:C:105:PRO:O	1:C:106:GLN:HB3	1.56	1.05
1:H:129:PHE:CE2	1:H:140:MET:HE2	1.93	1.02
1:B:59:ARG:HH11	1:B:59:ARG:HG2	1.28	0.98
1:J:105:PRO:O	1:J:106:GLN:HB2	1.58	0.97
1:A:105:PRO:O	1:A:106:GLN:HB2	1.58	0.97
1:G:105:PRO:O	1:G:106:GLN:HB2	1.59	0.97
1:E:220:ARG:HG2	1:E:220:ARG:NH1	1.68	0.96
1:H:235:GLU:HG3	2:H:255:HOH:O	1.65	0.95
1:H:126:ARG:HD2	1:H:145:MET:HA	1.48	0.95
1:H:129:PHE:HE2	1:H:140:MET:CE	1.82	0.93
1:B:111:ARG:HH21	1:F:106:GLN:HE21	1.08	0.93
1:E:220:ARG:HH11	1:E:220:ARG:CG	1.82	0.93
1:H:11:ARG:HD3	2:H:280:HOH:O	1.71	0.91
1:H:106:GLN:O	1:H:111:ARG:NH2	2.05	0.90
1:A:231:ARG:HG2	2:F:269:HOH:O	1.69	0.90
1:H:105:PRO:O	1:H:106:GLN:HB2	1.74	0.87
1:C:11:ARG:HG2	1:C:11:ARG:HH11	1.38	0.86
1:H:200:MET:HE3	1:H:210:TRP:HA	1.58	0.86
1:E:126:ARG:HD3	1:E:143:TYR:O	1.76	0.85
1:D:42:HIS:CE1	1:D:149:ARG:NH2	2.43	0.85
1:B:59:ARG:HG2	1:B:59:ARG:NH1	1.87	0.85
1:D:206:ARG:CG	1:D:206:ARG:HH11	1.90	0.84
1:H:199:ARG:HD3	2:H:259:HOH:O	1.76	0.84
1:E:11:ARG:HG3	1:E:11:ARG:HH11	1.44	0.83
1:H:129:PHE:CE2	1:H:140:MET:CE	2.59	0.83
1:F:206:ARG:HG3	1:F:206:ARG:NH1	1.87	0.83
1:A:111:ARG:HH21	1:D:106:GLN:HE21	1.27	0.82
1:F:11:ARG:NH1	1:F:14:GLU:OE2	2.12	0.82
1:A:180:ILE:HG22	1:A:181:ILE:HG23	1.62	0.82
1:B:4:SER:HG	1:E:4:SER:N	1.78	0.81
1:G:42:HIS:NE2	1:G:54:PHE:HE1	1.78	0.81
1:F:105:PRO:O	1:F:106:GLN:HB2	1.79	0.81
1:B:93:ILE:HG22	1:B:95:VAL:HG23	1.61	0.80
1:J:5:ILE:HD12	1:J:140:MET:HE1	1.62	0.80
1:F:129:PHE:CE2	1:F:140:MET:HE2	2.15	0.80
1:A:123:HIS:CA	1:A:145:MET:HE1	2.09	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:LYS:HD3	1:D:28:ASP:OD2	1.82	0.79
1:E:11:ARG:HH11	1:E:11:ARG:CG	1.95	0.79
1:F:129:PHE:CE2	1:F:140:MET:CE	2.65	0.79
1:H:200:MET:CE	1:H:210:TRP:HA	2.12	0.78
1:B:59:ARG:HH11	1:B:59:ARG:CG	1.95	0.78
1:C:111:ARG:HH21	1:G:106:GLN:HE21	1.32	0.78
1:F:129:PHE:HE2	1:F:140:MET:CE	1.97	0.77
1:I:129:PHE:CE2	1:I:140:MET:CE	2.67	0.77
1:H:126:ARG:HD3	1:H:143:TYR:O	1.83	0.77
1:H:194:ASP:OD1	1:H:197:ARG:NH2	2.18	0.77
1:G:7:LEU:HB2	1:G:10:GLU:OE2	1.83	0.77
1:H:129:PHE:HE2	1:H:140:MET:HE2	1.37	0.77
1:G:179:GLU:OE1	1:H:59:ARG:HD3	1.85	0.76
1:A:42:HIS:CE1	1:A:149:ARG:NH2	2.52	0.76
1:A:129:PHE:CE2	1:A:140:MET:CE	2.69	0.76
1:F:25:LYS:HD3	1:F:28:ASP:OD2	1.84	0.76
1:A:238:ALA:O	1:A:239:LYS:HB2	1.83	0.76
1:E:105:PRO:O	1:E:106:GLN:HB2	1.86	0.76
1:D:169:ARG:HG2	1:D:169:ARG:HH11	1.50	0.75
1:B:5:ILE:HG12	1:E:5:ILE:CG1	2.16	0.75
1:B:111:ARG:NH2	1:F:106:GLN:HE21	1.84	0.75
1:D:105:PRO:O	1:D:106:GLN:HB2	1.85	0.75
1:B:220:ARG:HH11	1:B:220:ARG:HB3	1.50	0.75
1:F:42:HIS:CE1	1:F:149:ARG:HH22	2.04	0.74
1:D:228:ARG:HD3	2:D:271:HOH:O	1.87	0.74
1:B:5:ILE:HG12	1:E:5:ILE:HG12	1.70	0.74
1:C:5:ILE:HG12	1:D:5:ILE:HG12	1.68	0.74
1:F:129:PHE:HE2	1:F:140:MET:HE2	1.49	0.73
1:H:126:ARG:HD2	1:H:145:MET:CA	2.19	0.73
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.52	0.72
1:A:123:HIS:HA	1:A:145:MET:CE	2.18	0.72
1:C:228:ARG:NE	2:C:287:HOH:O	2.08	0.72
1:H:208:LEU:HD22	1:H:214:TRP:HZ3	1.55	0.72
1:D:42:HIS:CE1	1:D:149:ARG:HH21	2.08	0.72
1:E:62:GLU:HG3	1:E:66:ARG:HH22	1.55	0.71
1:J:149:ARG:NH1	2:J:299:HOH:O	2.23	0.71
1:A:42:HIS:CE1	1:A:149:ARG:HH22	2.09	0.71
1:B:127:GLY:H	1:B:149:ARG:HH12	1.39	0.71
1:D:169:ARG:HG2	1:D:169:ARG:NH1	2.05	0.71
1:J:188:PRO:O	1:J:199:ARG:NH2	2.22	0.71
2:C:260:HOH:O	1:D:231:ARG:HG3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ARG:HD2	1:E:145:MET:HA	1.71	0.70
1:H:228:ARG:HD3	2:H:258:HOH:O	1.91	0.70
1:B:206:ARG:HG3	1:B:206:ARG:HH11	1.56	0.70
1:E:228:ARG:NH1	2:E:308:HOH:O	2.25	0.70
1:B:5:ILE:CD1	1:E:5:ILE:HG12	2.22	0.70
1:F:42:HIS:CE1	1:F:149:ARG:NH2	2.60	0.70
1:F:197:ARG:HH11	1:F:197:ARG:HG3	1.56	0.69
1:E:41:SER:HB3	1:E:74:LEU:HD12	1.72	0.69
1:G:5:ILE:HG12	1:H:5:ILE:HG12	1.72	0.69
1:E:225:GLU:HG3	2:E:293:HOH:O	1.93	0.69
1:G:126:ARG:HD2	1:G:145:MET:HA	1.75	0.69
1:G:53:GLU:OE1	1:G:126:ARG:NH2	2.26	0.69
1:F:206:ARG:HH11	1:F:206:ARG:CG	1.99	0.69
1:E:200:MET:HE2	1:E:200:MET:HA	1.76	0.68
1:J:126:ARG:HD3	1:J:143:TYR:O	1.94	0.68
1:A:67:LEU:HD13	1:A:158:VAL:HG22	1.74	0.68
1:C:105:PRO:O	1:C:106:GLN:CB	2.35	0.68
1:C:122:THR:HA	1:C:125:VAL:HG23	1.76	0.68
1:B:53:GLU:OE2	1:B:149:ARG:HG3	1.94	0.68
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.05	0.68
1:C:11:ARG:HH11	1:C:11:ARG:CG	2.05	0.68
1:B:111:ARG:HH21	1:F:106:GLN:NE2	1.89	0.67
1:D:244:GLU:O	1:D:244:GLU:HG2	1.95	0.67
1:I:105:PRO:O	1:I:106:GLN:CB	2.35	0.67
1:C:42:HIS:CE1	1:C:149:ARG:NH2	2.63	0.67
1:E:220:ARG:NH1	1:E:220:ARG:CG	2.46	0.66
1:A:206:ARG:HG3	1:A:206:ARG:NH1	1.93	0.66
1:I:42:HIS:CE1	1:I:149:ARG:NH2	2.64	0.66
1:I:121:ALA:O	1:I:122:THR:HG22	1.96	0.66
1:F:126:ARG:HD3	1:F:143:TYR:O	1.96	0.66
1:E:62:GLU:HG3	1:E:66:ARG:NH2	2.11	0.66
1:H:105:PRO:O	1:H:106:GLN:CB	2.44	0.66
1:J:105:PRO:O	1:J:106:GLN:CB	2.36	0.66
1:A:5:ILE:HG12	1:F:5:ILE:HG12	1.77	0.65
1:F:200:MET:HE3	1:F:210:TRP:HA	1.78	0.65
1:C:106:GLN:O	1:C:111:ARG:NH2	2.27	0.65
1:D:129:PHE:CE2	1:D:140:MET:HE2	2.31	0.65
1:A:106:GLN:HE21	1:D:111:ARG:HH21	1.43	0.65
1:C:67:LEU:O	1:C:162:LYS:HE2	1.97	0.65
1:B:105:PRO:O	1:B:106:GLN:HB2	1.95	0.65
1:D:53:GLU:OE1	1:D:126:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ILE:CG1	1:E:5:ILE:HG12	2.27	0.65
1:A:123:HIS:CB	1:A:145:MET:CE	2.74	0.64
1:C:128:VAL:O	1:C:140:MET:HA	1.97	0.64
1:G:16:GLU:OE2	1:G:25:LYS:HD3	1.98	0.64
1:A:126:ARG:HD3	1:A:143:TYR:O	1.97	0.64
1:I:67:LEU:HD13	1:I:158:VAL:HG23	1.79	0.64
1:B:126:ARG:HD3	1:B:143:TYR:O	1.98	0.64
1:C:106:GLN:HE21	1:G:111:ARG:HH21	1.45	0.64
1:G:126:ARG:HD3	1:G:143:TYR:O	1.97	0.64
1:H:62:GLU:OE1	1:H:62:GLU:HA	1.98	0.63
1:F:129:PHE:CE2	1:F:140:MET:HE3	2.32	0.63
1:A:123:HIS:HB3	1:A:145:MET:CE	2.29	0.63
1:E:143:TYR:HD2	1:E:147:LEU:HD13	1.64	0.62
1:C:225:GLU:HA	1:C:228:ARG:HH11	1.64	0.62
1:D:11:ARG:NH1	1:D:14:GLU:OE2	2.31	0.62
1:G:208:LEU:HD13	1:G:214:TRP:CZ3	2.34	0.62
1:B:159:LYS:NZ	1:B:225:GLU:OE2	2.30	0.62
1:F:200:MET:CE	1:F:210:TRP:HA	2.30	0.62
1:G:25:LYS:NZ	1:G:28:ASP:OD2	2.32	0.61
1:G:208:LEU:HD13	1:G:214:TRP:HZ3	1.64	0.61
1:J:200:MET:CE	1:J:200:MET:HA	2.31	0.61
1:J:86:LYS:HE3	1:J:101:ILE:CD1	2.31	0.61
1:D:67:LEU:HD13	1:D:158:VAL:HG22	1.81	0.61
1:G:188:PRO:O	1:G:199:ARG:NH2	2.33	0.61
1:H:208:LEU:CD2	1:H:214:TRP:HZ3	2.12	0.61
1:C:206:ARG:HH11	1:C:206:ARG:HG3	1.64	0.61
1:F:59:ARG:NE	2:F:293:HOH:O	2.34	0.61
1:G:42:HIS:ND1	1:G:50:CYS:SG	2.68	0.61
1:I:14:GLU:OE1	1:I:25:LYS:HE2	2.01	0.61
1:J:129:PHE:CE2	1:J:140:MET:HE2	2.35	0.61
1:G:55:VAL:O	1:G:59:ARG:HG3	2.01	0.61
1:I:129:PHE:CD2	1:I:140:MET:HE3	2.35	0.61
1:A:123:HIS:CA	1:A:145:MET:CE	2.79	0.60
1:F:59:ARG:NH2	1:F:241:LEU:HD21	2.16	0.60
1:A:172:PRO:HG3	1:A:181:ILE:HD11	1.82	0.60
1:C:14:GLU:OE1	1:C:28:ASP:OD1	2.20	0.60
1:I:188:PRO:O	1:I:199:ARG:NH2	2.34	0.60
1:C:231:ARG:O	1:C:235:GLU:HG2	2.01	0.60
1:E:235:GLU:CG	2:E:264:HOH:O	2.50	0.60
1:I:42:HIS:ND1	1:I:50:CYS:SG	2.72	0.60
1:D:206:ARG:HH11	1:D:206:ARG:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ARG:NH1	1:H:179:GLU:HG2	2.17	0.60
1:B:153:GLU:OE1	1:E:150:LEU:HD22	2.02	0.60
1:G:42:HIS:HB3	1:G:50:CYS:SG	2.41	0.60
1:C:126:ARG:HD2	1:C:145:MET:HA	1.84	0.59
1:E:11:ARG:HD3	2:E:263:HOH:O	2.01	0.59
1:C:42:HIS:CE1	1:C:149:ARG:HH21	2.21	0.59
1:B:7:LEU:O	1:B:10:GLU:HB2	2.03	0.59
1:I:208:LEU:HD22	1:I:214:TRP:HZ3	1.68	0.59
1:G:7:LEU:HD22	2:H:288:HOH:O	2.03	0.59
1:I:129:PHE:HE2	1:I:140:MET:HE3	1.64	0.59
1:A:55:VAL:O	1:A:59:ARG:HG3	2.03	0.59
1:J:129:PHE:CE2	1:J:140:MET:CE	2.85	0.59
1:F:39:LEU:C	1:F:39:LEU:HD23	2.23	0.59
1:F:105:PRO:O	1:F:106:GLN:CB	2.44	0.59
1:I:208:LEU:HD22	1:I:214:TRP:CZ3	2.38	0.59
1:B:5:ILE:HD11	1:E:5:ILE:HG12	1.84	0.58
1:H:48:PRO:O	1:H:52:THR:HG23	2.03	0.58
1:I:228:ARG:HD3	2:I:259:HOH:O	2.01	0.58
1:J:86:LYS:HE3	1:J:101:ILE:HD12	1.86	0.58
1:B:143:TYR:CD2	1:B:147:LEU:HD13	2.39	0.58
1:D:228:ARG:HD2	2:D:285:HOH:O	2.03	0.58
1:D:42:HIS:CE1	1:D:149:ARG:HH22	2.20	0.58
1:B:7:LEU:HB2	1:B:10:GLU:OE2	2.03	0.58
1:G:5:ILE:HD12	1:G:140:MET:HE1	1.86	0.57
1:J:129:PHE:HE2	1:J:140:MET:CE	2.17	0.57
1:A:128:VAL:O	1:A:140:MET:HA	2.03	0.57
1:E:220:ARG:O	1:E:224:GLU:HG3	2.04	0.57
1:B:140:MET:CE	1:B:142:TYR:OH	2.52	0.57
1:B:206:ARG:HG3	1:B:206:ARG:NH1	2.19	0.57
1:E:90:GLU:OE2	1:E:96:ARG:HG3	2.04	0.57
1:I:13:PRO:HB2	1:I:15:MET:HE3	1.87	0.57
1:A:227:ARG:HH21	1:F:236:LYS:NZ	2.03	0.57
1:J:38:VAL:HG23	1:J:69:VAL:CG1	2.35	0.57
1:A:198:ALA:O	1:A:202:SER:HB3	2.05	0.57
1:G:88:TRP:HZ2	1:H:209:ASP:HB2	1.70	0.56
1:J:238:ALA:O	1:J:239:LYS:HB2	2.04	0.56
1:H:132:ASP:OD2	1:H:138:ARG:HD3	2.05	0.56
1:G:105:PRO:O	1:G:106:GLN:CB	2.40	0.56
1:D:91:ARG:HG2	1:D:92:HIS:CD2	2.40	0.56
1:C:115:LEU:HD22	1:C:126:ARG:O	2.06	0.56
1:G:190:PRO:HB3	1:G:195:GLN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:HE	1:E:179:GLU:HG2	1.70	0.56
1:B:53:GLU:OE1	1:B:126:ARG:NH2	2.39	0.56
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.41	0.55
1:B:42:HIS:ND1	1:B:50:CYS:SG	2.79	0.55
1:B:63:ASP:OD1	1:B:66:ARG:NH1	2.39	0.55
1:F:129:PHE:CD2	1:F:140:MET:HE3	2.41	0.55
1:H:86:LYS:HE3	1:H:101:ILE:HD12	1.88	0.55
1:D:36:TRP:HB2	1:D:69:VAL:HG22	1.88	0.55
1:G:74:LEU:HD13	1:G:75:SER:N	2.22	0.55
1:B:123:HIS:HA	1:B:145:MET:HE2	1.88	0.55
1:C:180:ILE:HG22	1:C:181:ILE:HG23	1.88	0.55
1:A:69:VAL:HG21	1:A:158:VAL:HG21	1.87	0.55
1:C:12:PHE:HB3	1:C:27:PRO:HG3	1.87	0.55
1:C:126:ARG:HD3	1:C:143:TYR:O	2.07	0.55
1:B:62:GLU:HG3	1:B:66:ARG:NH2	2.22	0.55
1:G:126:ARG:HD2	1:G:145:MET:CA	2.37	0.55
1:E:11:ARG:CG	1:E:11:ARG:NH1	2.65	0.54
1:E:112:ARG:NE	2:E:267:HOH:O	2.41	0.54
1:H:53:GLU:OE1	1:H:126:ARG:NH2	2.40	0.54
1:I:55:VAL:O	1:I:59:ARG:HG3	2.08	0.54
1:C:200:MET:HE2	1:C:200:MET:HA	1.88	0.54
1:J:192:THR:OG1	1:J:195:GLN:HB2	2.07	0.54
1:E:228:ARG:HD3	2:E:259:HOH:O	2.06	0.54
1:J:129:PHE:HE2	1:J:140:MET:HE3	1.71	0.54
1:F:67:LEU:HD13	1:F:158:VAL:CG2	2.37	0.54
1:G:66:ARG:HD3	2:G:271:HOH:O	2.07	0.54
1:G:143:TYR:HD2	1:G:147:LEU:HD13	1.73	0.54
1:B:220:ARG:HB3	1:B:220:ARG:NH1	2.21	0.54
1:C:7:LEU:HB2	1:C:10:GLU:OE2	2.08	0.54
1:E:53:GLU:OE2	1:E:148:GLY:HA2	2.08	0.54
1:I:224:GLU:O	1:I:228:ARG:HB2	2.08	0.54
1:I:200:MET:HE3	1:I:210:TRP:HA	1.89	0.53
1:J:126:ARG:HD2	1:J:145:MET:HA	1.91	0.53
1:B:14:GLU:OE1	1:B:28:ASP:OD1	2.27	0.53
1:B:11:ARG:HG2	1:B:11:ARG:HH11	1.74	0.53
1:G:42:HIS:CE1	1:G:149:ARG:NH2	2.77	0.53
1:H:199:ARG:CD	2:H:259:HOH:O	2.45	0.53
1:I:53:GLU:OE1	1:I:126:ARG:NH2	2.40	0.53
1:A:123:HIS:HB3	1:A:145:MET:HE3	1.90	0.52
1:B:65:GLN:HG3	2:B:305:HOH:O	2.08	0.52
1:I:8:ILE:HD11	1:J:142:TYR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:75:SER:HB3	1:J:82:HIS:CE1	2.44	0.52
1:F:36:TRP:HB2	1:F:69:VAL:HG22	1.92	0.52
1:H:225:GLU:O	1:H:228:ARG:HG3	2.09	0.52
1:I:141:LEU:HD22	1:J:141:LEU:HD22	1.90	0.52
1:H:42:HIS:ND1	1:H:50:CYS:SG	2.78	0.52
1:A:200:MET:HA	1:A:200:MET:CE	2.40	0.52
1:B:140:MET:HE1	1:B:142:TYR:OH	2.09	0.52
1:B:241:LEU:HA	1:B:244:GLU:OE2	2.08	0.52
1:G:59:ARG:HH11	1:H:179:GLU:HG2	1.75	0.52
1:F:203:GLY:HA2	2:F:299:HOH:O	2.10	0.52
1:E:143:TYR:CD2	1:E:147:LEU:HD13	2.43	0.52
1:G:200:MET:HE3	1:G:210:TRP:HA	1.92	0.52
1:A:227:ARG:NH2	1:F:236:LYS:NZ	2.58	0.52
1:C:55:VAL:O	1:C:59:ARG:HG3	2.09	0.51
1:D:89:ILE:HG21	1:D:97:ILE:HD11	1.91	0.51
1:G:42:HIS:CG	1:G:50:CYS:HG	2.27	0.51
1:E:25:LYS:HD3	1:E:28:ASP:OD2	2.10	0.51
1:A:129:PHE:CE2	1:A:140:MET:HE2	2.44	0.51
1:B:192:THR:OG1	1:B:195:GLN:HB2	2.10	0.51
1:D:14:GLU:OE1	1:D:25:LYS:HE2	2.11	0.51
1:F:238:ALA:O	1:F:239:LYS:CB	2.58	0.51
1:G:129:PHE:CE2	1:G:140:MET:HE2	2.46	0.51
1:B:220:ARG:HH11	1:B:220:ARG:CB	2.21	0.51
1:B:5:ILE:HG12	1:E:5:ILE:HG13	1.89	0.51
1:C:4:SER:N	2:C:288:HOH:O	2.43	0.51
1:H:208:LEU:CD2	1:H:214:TRP:CZ3	2.94	0.51
1:I:147:LEU:HG	1:J:161:LEU:HD13	1.92	0.51
1:J:55:VAL:O	1:J:59:ARG:HG3	2.11	0.51
1:B:143:TYR:HD2	1:B:147:LEU:HD13	1.74	0.50
1:B:123:HIS:HE1	2:B:293:HOH:O	1.94	0.50
1:B:132:ASP:OD2	1:B:138:ARG:HD3	2.11	0.50
1:G:92:HIS:CE1	2:G:259:HOH:O	2.64	0.50
1:I:53:GLU:OE2	1:I:148:GLY:HA2	2.11	0.50
1:G:25:LYS:HG2	1:G:28:ASP:OD2	2.11	0.50
1:C:42:HIS:ND1	1:C:50:CYS:SG	2.84	0.50
1:C:206:ARG:HG3	1:C:206:ARG:NH1	2.26	0.50
1:E:111:ARG:HH21	1:I:106:GLN:HE21	1.59	0.50
1:H:69:VAL:HG21	1:H:158:VAL:HG21	1.93	0.50
1:J:69:VAL:HG21	1:J:158:VAL:HG21	1.93	0.50
1:A:5:ILE:O	1:A:5:ILE:HG13	2.12	0.49
1:B:180:ILE:O	1:E:240:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:PRO:HG3	1:D:181:ILE:HD11	1.94	0.49
1:J:176:PRO:HG2	1:J:227:ARG:HG3	1.94	0.49
1:A:92:HIS:O	1:A:245:ALA:HB1	2.12	0.49
1:B:48:PRO:CD	1:E:189:PRO:HG3	2.43	0.49
1:D:169:ARG:HH11	1:D:169:ARG:CG	2.20	0.49
1:C:212:PHE:C	1:C:212:PHE:HD2	2.15	0.49
1:G:42:HIS:HE2	1:G:54:PHE:HE1	1.59	0.49
1:H:159:LYS:HD3	1:H:225:GLU:HG2	1.94	0.49
1:I:187:VAL:HG23	1:I:213:CYS:O	2.13	0.49
1:B:37:PHE:HA	1:B:70:ASP:O	2.12	0.49
1:C:225:GLU:HA	1:C:228:ARG:HD2	1.95	0.49
1:F:180:ILE:HG22	1:F:181:ILE:HG23	1.95	0.49
1:B:188:PRO:O	1:B:199:ARG:NH2	2.44	0.49
1:G:91:ARG:HG2	1:G:92:HIS:CD2	2.47	0.49
1:C:53:GLU:OE1	1:C:126:ARG:NH2	2.46	0.49
1:B:126:ARG:CD	1:B:143:TYR:O	2.61	0.49
1:C:185:LEU:O	1:C:214:TRP:HB2	2.12	0.49
1:H:143:TYR:HD2	1:H:147:LEU:HD13	1.78	0.49
1:F:122:THR:HA	1:F:125:VAL:HG23	1.94	0.48
1:G:210:TRP:NE1	1:J:87:GLU:OE1	2.45	0.48
1:H:42:HIS:CE1	1:H:149:ARG:NH2	2.81	0.48
1:C:212:PHE:C	1:C:212:PHE:CD2	2.86	0.48
1:D:238:ALA:O	1:D:239:LYS:HB2	2.13	0.48
1:C:161:LEU:HD13	1:D:147:LEU:HD12	1.95	0.48
1:A:123:HIS:CB	1:A:145:MET:HE1	2.40	0.48
1:A:200:MET:HA	1:A:200:MET:HE2	1.94	0.48
1:B:129:PHE:CE2	1:B:140:MET:HE2	2.49	0.48
1:D:25:LYS:CD	1:D:28:ASP:OD2	2.58	0.48
1:E:7:LEU:O	1:E:10:GLU:HB2	2.12	0.48
1:H:125:VAL:HG12	1:H:125:VAL:O	2.13	0.48
1:I:62:GLU:HB2	2:I:258:HOH:O	2.12	0.48
1:J:200:MET:HA	1:J:200:MET:HE2	1.95	0.48
1:A:40:PHE:HZ	1:A:99:PHE:CE1	2.32	0.48
1:G:128:VAL:HG21	1:G:149:ARG:HD2	1.96	0.48
1:C:142:TYR:O	1:D:8:ILE:HD11	2.13	0.48
1:F:6:PRO:O	1:F:140:MET:HE1	2.14	0.48
1:G:136:VAL:O	1:G:138:ARG:HG2	2.14	0.48
1:D:129:PHE:CE2	1:D:140:MET:CE	2.97	0.48
1:H:129:PHE:CE2	1:H:140:MET:HE3	2.48	0.48
1:I:175:TRP:CG	1:I:176:PRO:HA	2.49	0.48
1:A:39:LEU:C	1:A:39:LEU:HD23	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:GLU:OE1	1:F:126:ARG:NH2	2.41	0.48
1:I:15:MET:HE2	1:I:112:ARG:HG2	1.95	0.48
1:J:136:VAL:O	1:J:138:ARG:HG2	2.14	0.48
1:B:142:TYR:O	1:E:139:THR:HG23	2.14	0.48
1:F:128:VAL:HG21	1:F:149:ARG:HD2	1.96	0.48
1:I:126:ARG:HD3	1:I:143:TYR:O	2.13	0.48
1:B:43:PRO:HG3	1:B:145:MET:CE	2.44	0.48
1:C:36:TRP:HB2	1:C:69:VAL:HG22	1.96	0.48
1:H:86:LYS:HE3	1:H:101:ILE:CD1	2.44	0.48
1:B:42:HIS:NE2	1:B:54:PHE:HE1	2.11	0.47
1:C:159:LYS:HD3	1:C:225:GLU:HG2	1.95	0.47
1:F:238:ALA:O	1:F:239:LYS:HB2	2.13	0.47
1:I:144:PRO:HD3	1:J:139:THR:OG1	2.14	0.47
1:J:13:PRO:HB2	1:J:15:MET:HE3	1.96	0.47
1:A:53:GLU:OE1	1:A:126:ARG:NH2	2.48	0.47
1:J:79:VAL:O	1:J:83:ILE:HG13	2.15	0.47
1:E:200:MET:HA	1:E:200:MET:CE	2.44	0.47
1:E:235:GLU:HG3	2:E:264:HOH:O	2.11	0.47
1:G:88:TRP:CZ2	1:H:209:ASP:HB2	2.50	0.47
1:G:60:ARG:HG3	1:G:60:ARG:HH11	1.80	0.47
1:G:67:LEU:HD13	1:G:158:VAL:HG23	1.95	0.47
1:A:53:GLU:CD	1:A:126:ARG:HH22	2.17	0.47
1:A:106:GLN:NE2	1:D:111:ARG:HH21	2.11	0.47
1:F:67:LEU:HD13	1:F:158:VAL:HG22	1.95	0.47
1:I:36:TRP:HB2	1:I:69:VAL:HG22	1.97	0.47
1:I:157:ILE:O	1:I:161:LEU:HB2	2.14	0.47
1:A:180:ILE:HG22	1:A:181:ILE:CG2	2.39	0.47
1:E:228:ARG:CD	2:E:259:HOH:O	2.62	0.47
1:G:190:PRO:HD3	2:G:311:HOH:O	2.14	0.47
1:C:6:PRO:HB2	1:C:137:ILE:HD12	1.97	0.47
1:H:159:LYS:CE	1:H:222:ASP:OD1	2.62	0.47
1:I:48:PRO:HG2	1:J:186:ILE:HG21	1.96	0.47
1:B:43:PRO:CG	1:B:145:MET:HE1	2.45	0.47
1:D:171:VAL:HG12	2:D:251:HOH:O	2.14	0.47
1:I:42:HIS:CE1	1:I:149:ARG:HH21	2.30	0.47
1:G:37:PHE:HA	1:G:70:ASP:O	2.15	0.46
1:I:15:MET:CE	1:I:112:ARG:HG2	2.45	0.46
1:I:180:ILE:HG22	1:I:181:ILE:HG23	1.96	0.46
1:C:86:LYS:NZ	1:H:193:GLU:OE1	2.41	0.46
1:F:126:ARG:CD	1:F:143:TYR:O	2.61	0.46
1:H:55:VAL:O	1:H:59:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:TYR:HD2	1:A:147:LEU:HD13	1.79	0.46
1:C:42:HIS:NE2	1:C:54:PHE:HE1	2.13	0.46
1:C:62:GLU:OE2	1:C:62:GLU:HA	2.15	0.46
1:E:75:SER:HB3	1:E:82:HIS:CE1	2.50	0.46
1:G:74:LEU:CD1	1:G:74:LEU:C	2.83	0.46
1:E:12:PHE:HA	1:E:13:PRO:HD2	1.73	0.46
1:E:19:THR:HA	1:E:101:ILE:O	2.16	0.46
1:F:128:VAL:CG2	1:F:149:ARG:HD2	2.46	0.46
1:E:156:ARG:HD3	1:E:230:LEU:HD21	1.97	0.46
1:I:43:PRO:HG2	1:I:145:MET:HG3	1.98	0.46
1:I:139:THR:OG1	1:J:144:PRO:HD3	2.15	0.46
1:I:67:LEU:CD1	1:I:158:VAL:HG23	2.44	0.46
1:D:127:GLY:HA2	1:D:141:LEU:O	2.16	0.46
1:G:42:HIS:CD2	1:G:54:PHE:HE1	2.32	0.46
1:I:28:ASP:O	1:I:29:HIS:C	2.53	0.46
1:C:74:LEU:C	1:C:74:LEU:HD13	2.37	0.46
1:A:188:PRO:O	1:A:199:ARG:NH2	2.40	0.46
1:G:11:ARG:HD2	2:G:302:HOH:O	2.14	0.46
1:G:74:LEU:HD13	1:G:74:LEU:C	2.36	0.46
1:G:236:LYS:HD2	1:G:237:PRO:HD2	1.98	0.46
1:A:67:LEU:HD13	1:A:158:VAL:CG2	2.42	0.46
1:B:147:LEU:HG	1:E:161:LEU:HD13	1.98	0.46
1:F:214:TRP:NE1	2:F:295:HOH:O	2.33	0.46
1:H:128:VAL:HG21	1:H:149:ARG:HD2	1.97	0.46
1:H:159:LYS:HE2	1:H:222:ASP:OD1	2.15	0.46
1:B:41:SER:O	1:B:149:ARG:NH2	2.50	0.45
1:C:74:LEU:CD2	1:C:104:ASP:HB2	2.46	0.45
1:C:157:ILE:O	1:C:161:LEU:HB2	2.16	0.45
1:F:84:LYS:HE3	1:F:84:LYS:HB3	1.77	0.45
1:C:231:ARG:NH1	2:C:273:HOH:O	2.40	0.45
1:F:156:ARG:HD3	1:F:230:LEU:HD21	1.98	0.45
1:J:45:ASP:OD2	1:J:82:HIS:ND1	2.38	0.45
1:A:6:PRO:HB2	1:A:137:ILE:HD13	1.98	0.45
1:B:154:ILE:O	1:B:158:VAL:HG22	2.17	0.45
1:F:43:PRO:O	1:F:44:ALA:HB2	2.16	0.45
1:G:67:LEU:O	1:G:162:LYS:HE3	2.16	0.45
1:G:129:PHE:CE2	1:G:140:MET:CE	3.00	0.45
1:C:157:ILE:HG23	1:D:147:LEU:HD11	1.99	0.45
1:A:75:SER:HB3	1:A:82:HIS:CE1	2.52	0.45
1:C:53:GLU:CD	1:C:126:ARG:HH22	2.21	0.45
1:F:228:ARG:HD3	2:F:284:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.52	0.45
1:E:11:ARG:HG3	1:E:11:ARG:NH1	2.23	0.45
1:H:156:ARG:HD3	1:H:230:LEU:HD21	1.99	0.45
1:J:53:GLU:OE2	1:J:148:GLY:HA2	2.16	0.45
1:J:106:GLN:O	1:J:111:ARG:NH2	2.47	0.45
1:C:106:GLN:HA	1:G:106:GLN:C	2.38	0.44
1:B:147:LEU:HD11	1:E:157:ILE:HG23	1.98	0.44
1:C:188:PRO:O	1:C:199:ARG:NH2	2.50	0.44
1:D:42:HIS:HE1	1:D:149:ARG:HH21	1.62	0.44
1:B:93:ILE:HG22	1:B:95:VAL:CG2	2.41	0.44
1:I:171:VAL:HG22	1:I:185:LEU:HD22	1.99	0.44
1:B:129:PHE:CE2	1:B:140:MET:CE	3.01	0.44
1:F:116:LEU:CD2	1:F:121:ALA:HB3	2.47	0.44
1:G:231:ARG:HG3	2:G:268:HOH:O	2.16	0.44
1:A:105:PRO:O	1:A:106:GLN:CB	2.39	0.44
1:A:126:ARG:HD2	1:A:144:PRO:C	2.38	0.44
1:B:35:LYS:HE2	1:B:68:GLY:HA2	1.98	0.44
1:H:37:PHE:HA	1:H:70:ASP:O	2.18	0.44
1:A:129:PHE:CE2	1:A:140:MET:HE3	2.53	0.44
1:C:67:LEU:HD13	1:C:158:VAL:HG23	1.99	0.44
1:E:111:ARG:NH2	1:I:106:GLN:HE21	2.16	0.44
1:E:124:THR:O	1:E:126:ARG:N	2.51	0.44
1:B:11:ARG:HG2	1:B:11:ARG:NH1	2.33	0.43
1:C:206:ARG:HH11	1:C:206:ARG:CG	2.31	0.43
1:D:200:MET:HA	1:D:200:MET:CE	2.49	0.43
1:B:105:PRO:O	1:B:106:GLN:CB	2.61	0.43
1:I:129:PHE:N	1:I:129:PHE:CD1	2.87	0.43
1:H:11:ARG:NH1	1:H:14:GLU:OE2	2.51	0.43
1:I:128:VAL:HB	1:I:141:LEU:HB2	2.00	0.43
1:D:126:ARG:HD3	1:D:143:TYR:O	2.19	0.43
1:F:157:ILE:O	1:F:161:LEU:HB2	2.18	0.43
1:G:143:TYR:CD2	1:G:147:LEU:HD13	2.53	0.43
1:J:129:PHE:CE2	1:J:140:MET:HE3	2.50	0.43
1:B:16:GLU:HG2	1:B:25:LYS:HG3	2.01	0.43
1:B:173:ALA:HB2	1:E:53:GLU:HG3	2.01	0.43
1:F:61:TYR:HE1	2:F:273:HOH:O	2.01	0.43
1:J:67:LEU:HD13	1:J:158:VAL:CG2	2.48	0.43
1:A:206:ARG:O	1:A:213:CYS:HA	2.18	0.43
1:G:161:LEU:HD13	1:H:147:LEU:HG	2.00	0.43
1:I:42:HIS:CE1	1:I:149:ARG:HH22	2.36	0.42
1:J:150:LEU:HD23	1:J:153:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HB2	1:C:102:ILE:HD12	2.02	0.42
1:E:42:HIS:CE1	1:E:149:ARG:NH2	2.87	0.42
1:E:149:ARG:HD3	2:E:251:HOH:O	2.19	0.42
1:A:7:LEU:HB2	1:A:10:GLU:OE2	2.20	0.42
1:A:227:ARG:HH21	1:F:236:LYS:HZ2	1.65	0.42
1:G:53:GLU:CD	1:G:126:ARG:HH22	2.22	0.42
1:H:84:LYS:HD2	1:I:210:TRP:HE1	1.83	0.42
1:G:60:ARG:HD3	1:G:151:VAL:HG12	2.00	0.42
1:H:14:GLU:OE1	1:H:25:LYS:HE2	2.20	0.42
1:H:28:ASP:OD1	1:H:28:ASP:N	2.53	0.42
1:I:169:ARG:HB3	1:I:185:LEU:HB3	2.02	0.42
1:A:238:ALA:O	1:A:239:LYS:CB	2.61	0.42
1:C:202:SER:OG	1:C:204:GLN:HG2	2.20	0.42
1:D:42:HIS:ND1	1:D:50:CYS:SG	2.89	0.42
1:F:115:LEU:HD22	1:F:126:ARG:O	2.20	0.42
1:J:38:VAL:HG23	1:J:69:VAL:HG11	2.00	0.42
1:A:123:HIS:CB	1:A:145:MET:HE3	2.47	0.42
1:G:140:MET:CE	1:G:142:TYR:OH	2.68	0.42
1:A:105:PRO:C	1:A:107:GLY:H	2.23	0.42
1:G:185:LEU:O	1:G:214:TRP:HB2	2.20	0.42
1:J:67:LEU:HD13	1:J:158:VAL:HG22	2.00	0.42
1:B:43:PRO:HB3	1:B:122:THR:O	2.20	0.41
1:C:7:LEU:O	1:C:10:GLU:HB2	2.20	0.41
1:C:184:GLY:HA2	1:C:216:THR:HG22	2.01	0.41
1:H:79:VAL:O	1:H:83:ILE:HG13	2.20	0.41
1:A:231:ARG:HH11	1:A:231:ARG:HD2	1.71	0.41
1:B:175:TRP:CG	1:B:176:PRO:HA	2.54	0.41
1:D:156:ARG:HD3	1:D:230:LEU:HD21	2.01	0.41
1:E:127:GLY:HA2	1:E:141:LEU:O	2.20	0.41
1:E:185:LEU:O	1:E:214:TRP:HB2	2.20	0.41
1:H:99:PHE:HB2	1:H:100:PRO:HD2	2.02	0.41
1:I:20:ASP:OD2	1:I:86:LYS:NZ	2.50	0.41
1:J:53:GLU:OE1	1:J:126:ARG:NH2	2.53	0.41
1:C:178:ASN:HD21	1:D:52:THR:HB	1.84	0.41
1:I:128:VAL:O	1:I:140:MET:HA	2.21	0.41
1:J:127:GLY:HA2	1:J:141:LEU:O	2.20	0.41
1:C:7:LEU:HD23	1:C:7:LEU:HA	1.86	0.41
1:C:96:ARG:NH2	1:C:98:PRO:HB3	2.35	0.41
1:F:63:ASP:OD1	1:F:66:ARG:NH1	2.38	0.41
1:D:7:LEU:H	1:D:10:GLU:CD	2.23	0.41
1:G:128:VAL:O	1:G:140:MET:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:THR:O	2:D:306:HOH:O	2.22	0.41
1:I:200:MET:CE	1:I:200:MET:HA	2.49	0.41
1:C:15:MET:HE2	1:C:112:ARG:HG2	2.03	0.41
1:E:163:LEU:HD22	1:E:167:LEU:HD22	2.02	0.41
1:A:129:PHE:CD2	1:A:140:MET:CE	3.03	0.41
1:F:40:PHE:HD1	1:F:42:HIS:HE2	1.69	0.41
1:D:31:VAL:C	1:D:33:GLN:H	2.24	0.41
1:D:190:PRO:HB3	1:D:195:GLN:HB3	2.03	0.41
1:G:60:ARG:HG3	1:G:60:ARG:NH1	2.35	0.41
1:G:89:ILE:HG23	1:G:93:ILE:HD12	2.03	0.41
1:H:188:PRO:O	1:H:199:ARG:NH2	2.49	0.41
1:B:153:GLU:O	1:B:157:ILE:HG13	2.21	0.41
1:H:39:LEU:O	1:H:128:VAL:HA	2.21	0.41
1:I:126:ARG:HD2	1:I:144:PRO:C	2.42	0.41
1:C:63:ASP:OD1	1:C:66:ARG:NH1	2.53	0.40
1:A:180:ILE:HA	1:F:241:LEU:HB2	2.03	0.40
1:E:28:ASP:OD1	1:E:28:ASP:N	2.55	0.40
1:E:128:VAL:O	1:E:140:MET:HA	2.21	0.40
1:H:53:GLU:CD	1:H:126:ARG:HH22	2.23	0.40
1:H:231:ARG:O	1:H:235:GLU:HG2	2.20	0.40
1:A:42:HIS:HA	1:A:43:PRO:HD3	1.87	0.40
1:F:242:TYR:CE2	1:F:243:GLU:HG3	2.56	0.40
1:H:105:PRO:O	1:H:105:PRO:HG2	2.22	0.40
1:I:112:ARG:O	1:I:112:ARG:HG3	2.20	0.40
1:E:197:ARG:HH11	1:E:197:ARG:HG3	1.86	0.40
1:I:177:ASN:HB3	1:J:237:PRO:HD3	2.03	0.40
1:C:153:GLU:OE1	1:D:150:LEU:HD22	2.19	0.40
1:C:219:SER:O	1:C:222:ASP:HB2	2.21	0.40
1:E:53:GLU:OE1	1:E:126:ARG:NH2	2.55	0.40
1:E:152:ASP:HB2	1:E:233:ALA:HB2	2.03	0.40
1:J:28:ASP:OD1	1:J:28:ASP:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:ARG:NH1	1:H:228:ARG:CB[1_544]	2.19	0.01

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	234/250 (94%)	224 (96%)	7 (3%)	3 (1%)	12	17
1	B	235/250 (94%)	228 (97%)	6 (3%)	1 (0%)	34	48
1	C	235/250 (94%)	219 (93%)	15 (6%)	1 (0%)	34	48
1	D	234/250 (94%)	219 (94%)	13 (6%)	2 (1%)	17	25
1	E	234/250 (94%)	223 (95%)	11 (5%)	0	100	100
1	F	234/250 (94%)	224 (96%)	8 (3%)	2 (1%)	17	25
1	G	234/250 (94%)	217 (93%)	15 (6%)	2 (1%)	17	25
1	H	234/250 (94%)	221 (94%)	10 (4%)	3 (1%)	12	17
1	I	234/250 (94%)	221 (94%)	10 (4%)	3 (1%)	12	17
1	J	234/250 (94%)	211 (90%)	21 (9%)	2 (1%)	17	25
All	All	2342/2500 (94%)	2207 (94%)	116 (5%)	19 (1%)	19	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	C	121	ALA
1	F	32	SER
1	F	122	THR
1	I	122	THR
1	J	32	SER
1	J	106	GLN
1	H	106	GLN
1	H	122	THR
1	I	32	SER
1	I	239	LYS
1	A	20	ASP
1	B	122	THR
1	D	122	THR

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Mol	Chain	Res	Type
1	D	239	LYS
1	G	243	GLU
1	A	239	LYS
1	G	122	THR
1	H	239	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	206/216 (95%)	189 (92%)	17 (8%)	11 17
1	B	207/216 (96%)	182 (88%)	25 (12%)	5 6
1	C	207/216 (96%)	191 (92%)	16 (8%)	13 20
1	D	206/216 (95%)	188 (91%)	18 (9%)	10 15
1	E	206/216 (95%)	185 (90%)	21 (10%)	7 10
1	F	206/216 (95%)	188 (91%)	18 (9%)	10 15
1	G	206/216 (95%)	191 (93%)	15 (7%)	14 22
1	H	206/216 (95%)	185 (90%)	21 (10%)	7 10
1	I	206/216 (95%)	188 (91%)	18 (9%)	10 15
1	J	206/216 (95%)	190 (92%)	16 (8%)	12 19
All	All	2062/2160 (96%)	1877 (91%)	185 (9%)	9 14

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	5	ILE
1	A	28	ASP
1	A	62	GLU
1	A	74	LEU
1	A	77	ASP
1	A	106	GLN
1	A	122	THR

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Mol	Chain	Res	Type
1	A	147	LEU
1	A	161	LEU
1	A	167	LEU
1	A	199	ARG
1	A	206	ARG
1	A	208	LEU
1	A	212	PHE
1	A	220	ARG
1	A	242	TYR
1	B	24	ILE
1	B	28	ASP
1	B	32	SER
1	B	35	LYS
1	B	59	ARG
1	B	66	ARG
1	B	74	LEU
1	B	77	ASP
1	B	116	LEU
1	B	122	THR
1	B	126	ARG
1	B	145	MET
1	B	147	LEU
1	B	159	LYS
1	B	161	LEU
1	B	167	LEU
1	B	193	GLU
1	B	197	ARG
1	B	199	ARG
1	B	204	GLN
1	B	206	ARG
1	B	208	LEU
1	B	212	PHE
1	B	220	ARG
1	B	242	TYR
1	C	11	ARG
1	C	25	LYS
1	C	28	ASP
1	C	74	LEU
1	C	116	LEU
1	C	122	THR
1	C	147	LEU
1	C	167	LEU

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Mol	Chain	Res	Type
1	C	183	GLU
1	C	195	GLN
1	C	199	ARG
1	C	206	ARG
1	C	212	PHE
1	C	228	ARG
1	C	239	LYS
1	C	242	TYR
1	D	11	ARG
1	D	28	ASP
1	D	62	GLU
1	D	74	LEU
1	D	91	ARG
1	D	126	ARG
1	D	147	LEU
1	D	158	VAL
1	D	161	LEU
1	D	166	SER
1	D	167	LEU
1	D	169	ARG
1	D	179	GLU
1	D	199	ARG
1	D	204	GLN
1	D	206	ARG
1	D	208	LEU
1	D	212	PHE
1	E	11	ARG
1	E	28	ASP
1	E	41	SER
1	E	66	ARG
1	E	74	LEU
1	E	122	THR
1	E	126	ARG
1	E	145	MET
1	E	147	LEU
1	E	158	VAL
1	E	161	LEU
1	E	166	SER
1	E	167	LEU
1	E	179	GLU
1	E	197	ARG
1	E	199	ARG

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Mol	Chain	Res	Type
1	E	204	GLN
1	E	208	LEU
1	E	212	PHE
1	E	220	ARG
1	E	242	TYR
1	F	14	GLU
1	F	32	SER
1	F	62	GLU
1	F	74	LEU
1	F	116	LEU
1	F	126	ARG
1	F	145	MET
1	F	147	LEU
1	F	158	VAL
1	F	161	LEU
1	F	167	LEU
1	F	199	ARG
1	F	204	GLN
1	F	206	ARG
1	F	208	LEU
1	F	212	PHE
1	F	236	LYS
1	F	242	TYR
1	G	24	ILE
1	G	32	SER
1	G	74	LEU
1	G	79	VAL
1	G	88	TRP
1	G	108	THR
1	G	122	THR
1	G	147	LEU
1	G	161	LEU
1	G	167	LEU
1	G	199	ARG
1	G	206	ARG
1	G	212	PHE
1	G	231	ARG
1	G	242	TYR
1	H	11	ARG
1	H	28	ASP
1	H	62	GLU
1	H	65	GLN

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Mol	Chain	Res	Type
1	H	91	ARG
1	H	116	LEU
1	H	147	LEU
1	H	158	VAL
1	H	159	LYS
1	H	161	LEU
1	H	167	LEU
1	H	179	GLU
1	H	183	GLU
1	H	197	ARG
1	H	199	ARG
1	H	201	GLU
1	H	207	SER
1	H	212	PHE
1	H	214	TRP
1	H	228	ARG
1	H	242	TYR
1	I	16	GLU
1	I	24	ILE
1	I	41	SER
1	I	61	TYR
1	I	82	HIS
1	I	116	LEU
1	I	126	ARG
1	I	147	LEU
1	I	161	LEU
1	I	167	LEU
1	I	195	GLN
1	I	199	ARG
1	I	208	LEU
1	I	212	PHE
1	I	220	ARG
1	I	236	LYS
1	I	242	TYR
1	I	243	GLU
1	J	7	LEU
1	J	41	SER
1	J	62	GLU
1	J	74	LEU
1	J	116	LEU
1	J	147	LEU
1	J	149	ARG

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Mol	Chain	Res	Type
1	J	158	VAL
1	J	161	LEU
1	J	167	LEU
1	J	174	ASP
1	J	193	GLU
1	J	195	GLN
1	J	199	ARG
1	J	212	PHE
1	J	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	B	106	GLN
1	C	106	GLN
1	D	106	GLN
1	E	21	HIS
1	E	106	GLN
1	F	106	GLN
1	F	204	GLN
1	G	92	HIS
1	G	106	GLN
1	I	92	HIS
1	I	106	GLN
1	I	195	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	238/250 (95%)	-0.75	2 (0%) 86 84	12, 22, 45, 72	0
1	B	239/250 (95%)	-0.63	0 100 100	14, 24, 44, 62	0
1	C	239/250 (95%)	-0.59	0 100 100	15, 25, 44, 71	0
1	D	238/250 (95%)	-0.66	0 100 100	13, 25, 46, 76	0
1	E	238/250 (95%)	-0.59	2 (0%) 86 84	13, 25, 44, 65	0
1	F	238/250 (95%)	-0.70	0 100 100	11, 22, 41, 65	0
1	G	238/250 (95%)	-0.63	0 100 100	14, 24, 44, 59	0
1	H	238/250 (95%)	-0.69	0 100 100	13, 24, 45, 63	0
1	I	238/250 (95%)	-0.56	1 (0%) 92 91	18, 30, 49, 68	0
1	J	238/250 (95%)	-0.69	1 (0%) 92 91	15, 27, 48, 63	0
All	All	2382/2500 (95%)	-0.65	6 (0%) 94 93	11, 25, 46, 76	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	238	ALA	4.3
1	A	245	ALA	2.8
1	A	244	GLU	2.7
1	E	242	TYR	2.4
1	E	244	GLU	2.4
1	I	220	ARG	2.1

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

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.