



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:47 AM UTC

PDB ID : 2NVL / pdb_00002nvl
Title : Crystal structure of archaeal peroxiredoxin, thioredoxin peroxidase from *Aeropyrum pernix* K1 (sulfonic acid form)
Authors : Nakamura, T.; Yamamoto, T.; Abe, M.; Matsumura, H.; Hagihara, Y.; Goto, T.; Yamaguchi, T.; Inoue, T.
Deposited on : 2006-11-13
Resolution : 2.36 Å(reported)

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

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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
Mogul	:	2022.3.0, CSD as543be (2022)
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

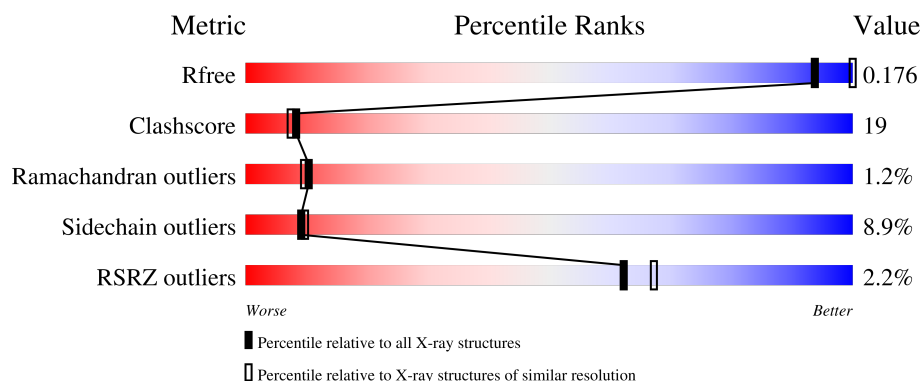
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	250	
1	B	250	
1	C	250	
1	D	250	
1	E	250	

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Mol	Chain	Length	Quality of chain
1	F	250	2% 61% 29% 5% • •
1	G	250	1% 62% 31% • •
1	H	250	2% 68% 23% 5% • •
1	I	250	4% 61% 28% 7% •
1	J	250	2% 66% 24% 7% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20328 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	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	B	240	Total	C	N	O	S	0	0	0
			1953	1254	343	350	6			
1	C	240	Total	C	N	O	S	0	0	0
			1950	1252	341	351	6			
1	D	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	E	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	F	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	G	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	H	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	I	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	J	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	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

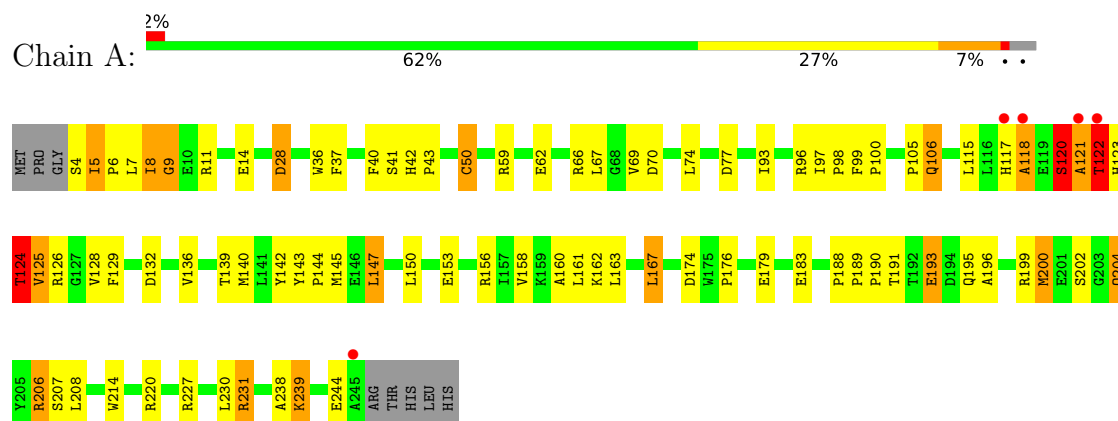
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	83	Total O 83 83	0	0
2	B	64	Total O 64 64	0	0
2	C	58	Total O 58 58	0	0
2	D	44	Total O 44 44	0	0
2	E	66	Total O 66 66	0	0
2	F	75	Total O 75 75	0	0
2	G	82	Total O 82 82	0	0
2	H	82	Total O 82 82	0	0
2	I	75	Total O 75 75	0	0
2	J	76	Total O 76 76	0	0

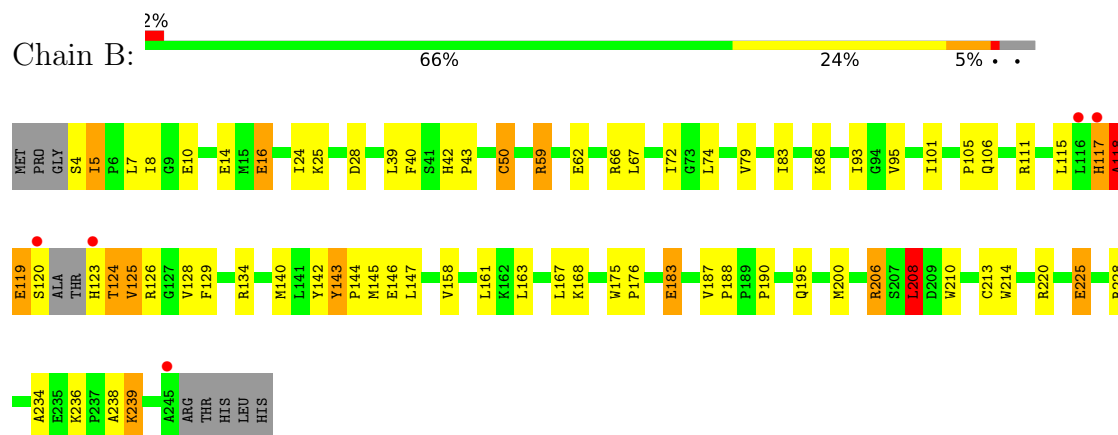
3 Residue-property plots

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

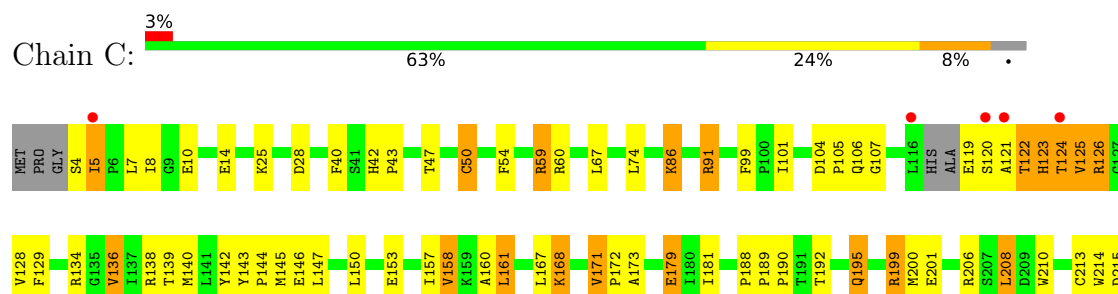
• Molecule 1: Probable peroxiredoxin

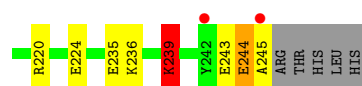


• Molecule 1: Probable peroxiredoxin

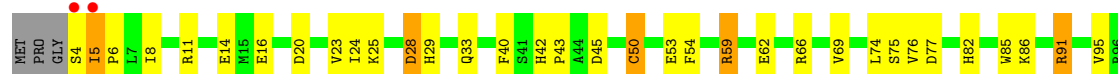


• Molecule 1: Probable peroxiredoxin

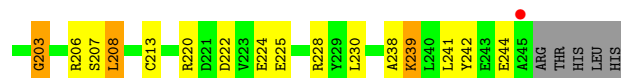




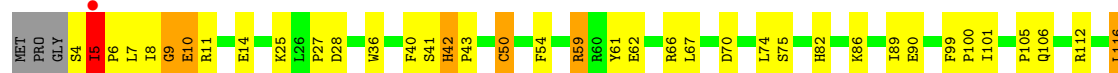
- Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin

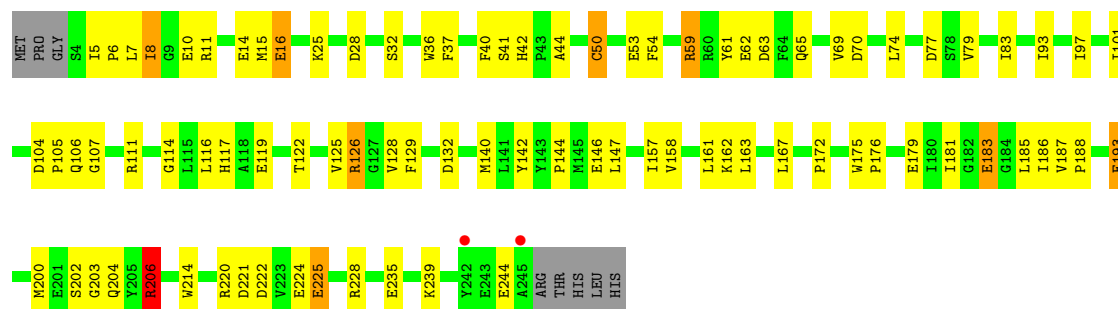


- Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin

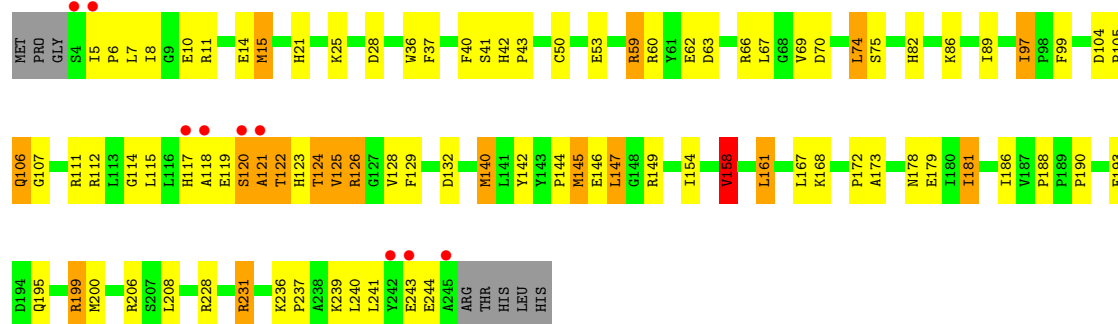




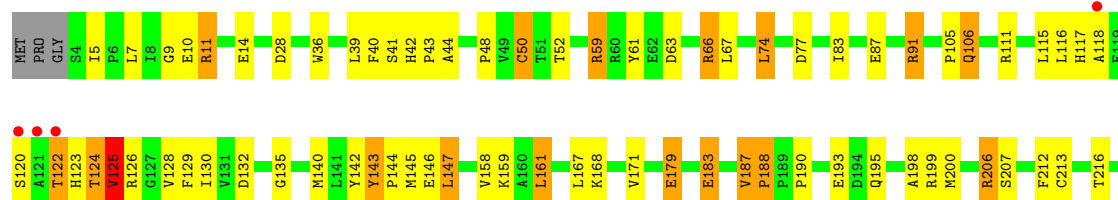
- Molecule 1: Probable peroxiredoxin

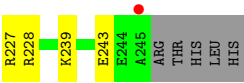


- Molecule 1: Probable peroxiredoxin



- 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	76.32Å 102.96Å 104.30Å 105.65° 105.26° 92.69°	Depositor
Resolution (Å)	50.00 – 2.36 50.00 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.36) 92.1 (50.00-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.219 0.167 , 0.176	Depositor DCC
R_{free} test set	11689 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20328	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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

Bond lengths and bond angles in the following residue types are not validated in this section: OCS

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	1.40	8/2009 (0.4%)	1.26	8/2730 (0.3%)
1	B	1.36	1/1996 (0.1%)	1.28	16/2710 (0.6%)
1	C	1.37	4/1992 (0.2%)	1.27	11/2705 (0.4%)
1	D	1.36	10/2009 (0.5%)	1.29	9/2730 (0.3%)
1	E	1.39	5/2009 (0.2%)	1.24	6/2730 (0.2%)
1	F	1.41	7/2009 (0.3%)	1.27	11/2730 (0.4%)
1	G	1.45	5/2009 (0.2%)	1.28	3/2730 (0.1%)
1	H	1.40	7/2009 (0.3%)	1.25	8/2730 (0.3%)
1	I	1.37	7/2009 (0.3%)	1.26	10/2730 (0.4%)
1	J	1.38	4/2009 (0.2%)	1.27	15/2730 (0.5%)
All	All	1.39	58/20060 (0.3%)	1.27	97/27255 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	VAL	CA-CB	8.33	1.64	1.54
1	J	171	VAL	CA-CB	7.73	1.60	1.54
1	E	189	PRO	CA-C	7.65	1.57	1.52
1	D	186	ILE	CA-CB	7.41	1.63	1.54
1	H	93	ILE	CA-CB	7.23	1.63	1.54
1	G	93	ILE	CA-CB	7.13	1.63	1.54
1	E	5	ILE	CA-CB	7.09	1.63	1.54
1	F	5	ILE	CA-CB	7.03	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	VAL	CA-CB	6.62	1.60	1.54
1	H	189	PRO	CA-C	6.50	1.55	1.51
1	G	188	PRO	CA-C	6.48	1.58	1.52
1	G	44	ALA	CA-CB	6.45	1.64	1.53
1	I	186	ILE	CA-CB	6.43	1.61	1.54
1	G	126	ARG	CA-C	6.40	1.60	1.52
1	H	131	VAL	CA-CB	6.36	1.62	1.54
1	D	189	PRO	CA-C	6.31	1.58	1.52
1	D	136	VAL	CA-CB	6.23	1.61	1.54
1	H	171	VAL	CA-CB	6.16	1.59	1.54
1	A	160	ALA	CA-CB	6.15	1.63	1.53
1	D	216	THR	CA-CB	-6.09	1.46	1.53
1	D	188	PRO	CA-C	6.03	1.57	1.52
1	F	216	THR	C-O	-5.88	1.17	1.24
1	A	179	GLU	CD-OE1	5.86	1.36	1.25
1	A	189	PRO	CA-C	5.81	1.56	1.52
1	F	136	VAL	CA-CB	5.80	1.61	1.54
1	D	95	VAL	CA-CB	5.76	1.61	1.54
1	E	183	GLU	CD-OE2	5.74	1.36	1.25
1	A	136	VAL	CA-CB	5.67	1.61	1.54
1	J	188	PRO	CA-C	5.66	1.57	1.52
1	I	173	ALA	C-O	5.61	1.30	1.23
1	C	5	ILE	CA-C	5.60	1.58	1.52
1	I	140	MET	C-O	-5.60	1.17	1.23
1	D	168	LYS	CA-C	5.56	1.60	1.53
1	A	122	THR	CA-CB	5.50	1.62	1.53
1	H	83	ILE	CA-CB	5.50	1.61	1.54
1	E	5	ILE	CA-C	5.49	1.58	1.52
1	F	90	GLU	N-CA	-5.49	1.39	1.46
1	A	5	ILE	CA-CB	5.46	1.61	1.54
1	I	99	PHE	CA-C	5.46	1.59	1.52
1	F	128	VAL	N-CA	5.45	1.52	1.46
1	A	69	VAL	CA-CB	5.44	1.61	1.54
1	I	126	ARG	CA-C	5.43	1.59	1.53
1	J	44	ALA	CA-CB	5.42	1.62	1.53
1	I	158	VAL	CA-CB	5.40	1.61	1.54
1	D	223	VAL	CA-CB	5.34	1.61	1.54
1	H	175	TRP	CA-C	5.33	1.58	1.53
1	G	97	ILE	N-CA	-5.32	1.42	1.46
1	F	89	ILE	C-O	-5.31	1.18	1.24
1	A	93	ILE	C-O	-5.31	1.18	1.24
1	F	70	ASP	N-CA	5.29	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	TRP	CA-C	5.29	1.58	1.53
1	C	91	ARG	C-O	-5.27	1.17	1.24
1	H	205	TYR	CA-C	-5.23	1.46	1.52
1	I	181	ILE	CA-CB	5.23	1.61	1.54
1	D	158	VAL	C-O	-5.21	1.18	1.24
1	B	163	LEU	C-O	-5.19	1.18	1.24
1	J	130	ILE	CA-CB	5.15	1.60	1.54
1	E	72	ILE	CA-CB	5.10	1.61	1.54

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	HIS	N-CA-C	11.79	127.51	109.23
1	D	216	THR	CA-C-N	8.84	129.85	120.83
1	D	216	THR	C-N-CA	8.84	129.85	120.83
1	I	97	ILE	CA-C-N	-7.87	111.54	120.04
1	I	97	ILE	C-N-CA	-7.87	111.54	120.04
1	J	143	TYR	CA-C-N	-7.19	113.40	120.52
1	J	143	TYR	C-N-CA	-7.19	113.40	120.52
1	I	53	GLU	N-CA-C	6.79	118.34	111.07
1	B	208	LEU	N-CA-C	-6.70	105.39	113.97
1	B	187	VAL	CA-C-N	-6.67	113.51	120.38
1	B	187	VAL	C-N-CA	-6.67	113.51	120.38
1	J	187	VAL	CA-C-N	-6.44	113.75	120.38
1	J	187	VAL	C-N-CA	-6.44	113.75	120.38
1	C	189	PRO	O-C-N	6.37	124.24	121.31
1	B	117	HIS	CA-C-N	6.31	133.59	121.54
1	B	117	HIS	C-N-CA	6.31	133.59	121.54
1	E	21	HIS	N-CA-C	-6.29	105.55	113.72
1	G	221	ASP	N-CA-C	6.13	117.63	111.07
1	J	216	THR	CA-C-N	6.13	125.83	119.64
1	J	216	THR	C-N-CA	6.13	125.83	119.64
1	B	143	TYR	CA-C-N	-6.07	114.51	120.52
1	B	143	TYR	C-N-CA	-6.07	114.51	120.52
1	I	179	GLU	N-CA-C	6.06	118.68	111.71
1	E	124	THR	N-CA-C	6.02	119.09	110.24
1	I	239	LYS	N-CA-C	6.01	118.20	108.34
1	G	187	VAL	N-CA-C	-5.99	103.48	108.63
1	F	9	GLY	N-CA-C	-5.95	107.47	115.21
1	C	179	GLU	N-CA-C	5.92	118.52	111.71
1	D	77	ASP	N-CA-C	5.90	118.32	110.53
1	F	227	ARG	NE-CZ-NH1	-5.90	115.60	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	PRO	N-CA-C	5.86	117.85	110.70
1	D	5	ILE	CA-C-N	-5.85	114.73	120.52
1	D	5	ILE	C-N-CA	-5.85	114.73	120.52
1	J	9	GLY	N-CA-C	-5.82	107.76	114.69
1	B	118	ALA	N-CA-C	5.80	123.16	110.80
1	C	171	VAL	CA-C-N	5.79	125.70	119.85
1	C	171	VAL	C-N-CA	5.79	125.70	119.85
1	E	123	HIS	CA-C-N	5.77	129.30	121.05
1	E	123	HIS	C-N-CA	5.77	129.30	121.05
1	H	32	SER	CA-CB-OG	-5.74	99.62	111.10
1	F	221	ASP	N-CA-C	5.70	117.50	111.28
1	A	124	THR	N-CA-C	5.68	118.72	110.42
1	F	126	ARG	CB-CA-C	5.67	120.88	112.03
1	J	125	VAL	CA-C-N	-5.64	113.03	122.17
1	J	125	VAL	C-N-CA	-5.64	113.03	122.17
1	A	238	ALA	N-CA-C	-5.64	101.94	110.28
1	A	93	ILE	N-CA-C	-5.63	108.01	113.53
1	B	183	GLU	N-CA-C	-5.61	106.10	113.17
1	H	105	PRO	N-CA-C	-5.57	102.52	111.38
1	J	61	TYR	N-CA-C	5.55	117.01	111.07
1	E	208	LEU	N-CA-C	-5.53	106.89	113.97
1	B	238	ALA	N-CA-C	-5.53	101.66	109.96
1	A	118	ALA	N-CA-C	5.48	119.14	112.23
1	C	143	TYR	CA-C-N	-5.43	114.98	120.31
1	C	143	TYR	C-N-CA	-5.43	114.98	120.31
1	F	186	ILE	N-CA-C	5.41	116.36	108.58
1	D	163	LEU	N-CA-C	5.40	117.61	111.02
1	I	126	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	A	9	GLY	N-CA-C	-5.33	107.99	114.92
1	I	241	LEU	N-CA-C	5.33	117.84	111.71
1	A	97	ILE	CA-C-N	-5.32	114.29	120.04
1	A	97	ILE	C-N-CA	-5.32	114.29	120.04
1	I	21	HIS	N-CA-C	-5.31	106.74	114.12
1	H	216	THR	CA-C-N	-5.28	114.50	120.89
1	H	216	THR	C-N-CA	-5.28	114.50	120.89
1	H	125	VAL	CA-C-N	-5.27	113.90	122.34
1	H	125	VAL	C-N-CA	-5.27	113.90	122.34
1	J	243	GLU	N-CA-C	-5.26	105.24	110.97
1	J	59	ARG	N-CA-C	5.23	116.98	111.28
1	C	123	HIS	CA-C-N	5.21	128.74	121.24
1	C	123	HIS	C-N-CA	5.21	128.74	121.24
1	G	206	ARG	N-CA-C	-5.21	102.57	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	LYS	N-CA-C	5.21	116.95	111.28
1	E	151	VAL	N-CA-C	5.20	115.93	110.62
1	F	42	HIS	CA-C-N	5.20	124.83	119.05
1	F	42	HIS	C-N-CA	5.20	124.83	119.05
1	B	236	LYS	CA-C-N	-5.20	114.40	119.76
1	B	236	LYS	C-N-CA	-5.20	114.40	119.76
1	A	207	SER	N-CA-C	5.16	117.09	108.99
1	D	168	LYS	CB-CA-C	5.15	119.20	111.89
1	F	234	ALA	N-CA-C	5.15	118.72	112.23
1	C	47	THR	CA-C-N	5.13	124.44	118.85
1	C	47	THR	C-N-CA	5.13	124.44	118.85
1	H	188	PRO	CA-C-N	5.08	123.37	119.66
1	H	188	PRO	C-N-CA	5.08	123.37	119.66
1	J	87	GLU	CB-CA-C	-5.08	102.88	110.90
1	J	118	ALA	N-CA-C	5.05	119.08	113.02
1	F	116	LEU	CA-CB-CG	-5.05	98.62	116.30
1	B	188	PRO	CA-C-N	5.05	125.58	120.38
1	B	188	PRO	C-N-CA	5.05	125.58	120.38
1	D	152	ASP	N-CA-C	5.04	116.77	111.28
1	I	15	MET	N-CA-C	5.03	116.17	108.52
1	B	117	HIS	CA-CB-CG	5.03	118.83	113.80
1	I	126	ARG	CB-CA-C	5.03	119.87	111.83
1	J	83	ILE	N-CA-C	5.03	115.75	110.62
1	F	27	PRO	CA-C-N	5.01	127.31	120.54
1	F	27	PRO	C-N-CA	5.01	127.31	120.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	SER	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	1965	0	1948	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1953	0	1935	75	0
1	C	1950	0	1935	76	0
1	D	1965	0	1948	103	0
1	E	1965	0	1948	99	0
1	F	1965	0	1948	98	0
1	G	1965	0	1948	72	0
1	H	1965	0	1948	64	0
1	I	1965	0	1948	88	0
1	J	1965	0	1947	86	0
2	A	83	0	0	5	0
2	B	64	0	0	6	0
2	C	58	0	0	5	0
2	D	44	0	0	3	0
2	E	66	0	0	5	0
2	F	75	0	0	5	0
2	G	82	0	0	4	0
2	H	82	0	0	6	0
2	I	75	0	0	3	0
2	J	76	0	0	3	0
All	All	20328	0	19453	751	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 19.

All (751) 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:J:66:ARG:HH11	1:J:66:ARG:HG3	1.05	1.16
1:D:105:PRO:O	1:D:106:GLN:HB3	1.43	1.15
1:G:105:PRO:O	1:G:106:GLN:HB2	1.48	1.13
1:G:14:GLU:HG3	1:G:25:LYS:HZ1	1.05	1.13
1:B:126:ARG:HH11	1:B:145:MET:HA	1.11	1.08
1:D:206:ARG:HG3	1:D:206:ARG:HH11	1.18	1.07
1:H:206:ARG:HG3	1:H:206:ARG:HH11	1.08	1.06
1:J:206:ARG:HH11	1:J:206:ARG:HG3	0.91	1.06
1:G:14:GLU:HG3	1:G:25:LYS:NZ	1.71	1.05
1:F:206:ARG:HG3	1:F:206:ARG:HH11	1.18	1.04
1:A:200:MET:HE2	1:A:200:MET:HA	1.39	1.02
1:F:129:PHE:CE2	1:F:140:MET:HE3	1.95	1.02
1:E:11:ARG:HG2	1:E:11:ARG:HH11	1.25	1.01
1:E:129:PHE:CE2	1:E:140:MET:HE3	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:PRO:O	1:F:106:GLN:HB2	1.59	0.99
1:J:206:ARG:HG3	1:J:206:ARG:NH1	1.68	0.99
1:J:91:ARG:HG2	1:J:91:ARG:HH11	1.27	0.97
1:J:105:PRO:O	1:J:106:GLN:HB2	1.61	0.97
1:A:129:PHE:CE2	1:A:140:MET:HE3	2.00	0.96
1:C:125:VAL:HA	1:C:145:MET:HE2	1.44	0.96
1:I:5:ILE:HD12	1:I:6:PRO:O	1.64	0.96
1:J:11:ARG:HG2	1:J:11:ARG:HH11	1.28	0.96
1:E:11:ARG:HH11	1:E:11:ARG:CG	1.79	0.94
1:B:228:ARG:HD2	2:B:271:HOH:O	1.67	0.93
1:D:120:SER:CB	1:D:123:HIS:O	2.16	0.92
1:E:59:ARG:HG3	1:E:59:ARG:HH11	1.31	0.92
1:E:168:LYS:O	1:E:168:LYS:HD3	1.69	0.92
1:J:206:ARG:HH11	1:J:206:ARG:CG	1.83	0.91
1:H:106:GLN:O	1:H:111:ARG:NH2	2.04	0.91
1:B:126:ARG:NH1	1:B:145:MET:HA	1.84	0.91
1:E:242:TYR:CD1	1:F:214:TRP:HH2	1.89	0.90
1:C:214:TRP:HH2	1:D:242:TYR:CD1	1.90	0.90
1:H:111:ARG:HE	1:I:106:GLN:NE2	1.68	0.90
1:G:129:PHE:CE2	1:G:140:MET:HE3	2.07	0.89
1:E:129:PHE:HE2	1:E:140:MET:HE3	1.30	0.89
1:A:105:PRO:HG2	1:J:122:THR:HG22	1.53	0.89
1:G:206:ARG:HG3	1:G:206:ARG:HH11	1.38	0.88
1:A:7:LEU:HD13	1:B:117:HIS:HB3	1.54	0.88
1:C:14:GLU:OE1	1:C:28:ASP:OD1	1.92	0.88
1:D:188:PRO:O	1:D:199:ARG:NH2	2.07	0.88
1:I:140:MET:HE2	1:I:142:TYR:OH	1.74	0.87
1:F:40:PHE:HD1	1:F:42:HIS:HE2	1.19	0.87
1:I:8:ILE:H	1:J:117:HIS:HD2	1.18	0.87
1:J:140:MET:HE2	1:J:142:TYR:OH	1.74	0.86
1:I:117:HIS:HB2	1:I:125:VAL:CG1	2.05	0.86
1:A:126:ARG:NH1	1:A:145:MET:O	2.08	0.85
1:J:91:ARG:HG2	1:J:91:ARG:NH1	1.89	0.84
1:C:129:PHE:CE2	1:C:140:MET:HE3	2.12	0.84
1:B:200:MET:HE3	1:B:210:TRP:HA	1.59	0.84
1:D:105:PRO:O	1:D:106:GLN:CB	2.26	0.84
1:F:66:ARG:NH2	2:F:311:HOH:O	2.11	0.84
1:F:129:PHE:HE2	1:F:140:MET:HE3	1.40	0.84
1:F:206:ARG:HG3	1:F:206:ARG:NH1	1.89	0.84
1:D:69:VAL:HG21	1:D:158:VAL:HG11	1.60	0.83
1:G:7:LEU:HD12	1:G:10:GLU:OE2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:ILE:HD12	1:G:6:PRO:O	1.78	0.83
1:H:105:PRO:O	1:H:106:GLN:HB2	1.79	0.83
1:F:238:ALA:O	1:F:239:LYS:HB2	1.77	0.83
1:J:145:MET:HE3	2:J:295:HOH:O	1.77	0.83
1:J:129:PHE:CE2	1:J:140:MET:HE3	2.13	0.82
1:C:105:PRO:O	1:C:106:GLN:HB2	1.76	0.82
1:H:206:ARG:HG3	1:H:206:ARG:NH1	1.85	0.82
1:D:241:LEU:HA	1:D:244:GLU:HG3	1.61	0.82
1:B:183:GLU:OE2	2:B:301:HOH:O	1.97	0.82
1:I:8:ILE:N	1:J:117:HIS:HD2	1.77	0.82
1:E:200:MET:HE2	1:E:200:MET:HA	1.61	0.82
1:E:179:GLU:OE1	1:F:59:ARG:HG2	1.80	0.82
1:A:7:LEU:HB3	1:B:117:HIS:HB2	1.62	0.81
1:A:126:ARG:HH12	1:A:145:MET:C	1.88	0.81
1:J:66:ARG:HG3	1:J:66:ARG:NH1	1.81	0.81
1:J:11:ARG:HG2	1:J:11:ARG:NH1	1.93	0.81
1:D:206:ARG:HG3	1:D:206:ARG:NH1	1.89	0.81
1:E:40:PHE:HD1	1:E:42:HIS:HE2	1.28	0.81
1:F:62:GLU:HG3	1:F:66:ARG:NH2	1.94	0.81
1:B:129:PHE:CE2	1:B:140:MET:HE3	2.16	0.81
2:C:270:HOH:O	1:D:183:GLU:HG3	1.80	0.81
1:I:59:ARG:HH12	1:J:179:GLU:HG2	1.46	0.81
1:C:5:ILE:HD13	1:D:5:ILE:HD13	1.60	0.80
1:F:14:GLU:OE1	1:F:25:LYS:HE2	1.79	0.80
1:B:126:ARG:HB2	1:B:143:TYR:O	1.80	0.80
1:E:11:ARG:HG2	1:E:11:ARG:NH1	1.96	0.79
1:I:129:PHE:CE2	1:I:140:MET:HE3	2.17	0.79
1:F:11:ARG:HH11	1:F:11:ARG:HG2	1.45	0.79
1:E:126:ARG:NH1	1:E:145:MET:O	2.17	0.78
1:B:14:GLU:OE1	1:B:25:LYS:HE2	1.83	0.78
1:D:111:ARG:HD2	2:D:273:HOH:O	1.83	0.78
1:I:59:ARG:NH1	1:J:179:GLU:HG2	1.99	0.78
1:J:91:ARG:HH11	1:J:91:ARG:CG	1.97	0.77
1:G:200:MET:HA	1:G:200:MET:HE2	1.66	0.77
1:G:129:PHE:HE2	1:G:140:MET:HE3	1.48	0.77
1:J:115:LEU:O	1:J:125:VAL:HG23	1.85	0.77
1:D:120:SER:HB2	1:D:123:HIS:O	1.85	0.77
1:C:43:PRO:HD2	1:C:50:OCS:OD3	1.85	0.77
1:A:231:ARG:HH21	1:A:231:ARG:HB2	1.48	0.76
1:F:5:ILE:HG13	1:F:6:PRO:O	1.85	0.76
1:F:7:LEU:O	1:F:10:GLU:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:PRO:O	1:G:106:GLN:CB	2.27	0.76
1:B:105:PRO:O	1:B:106:GLN:HB2	1.84	0.76
1:D:117:HIS:HB2	1:D:125:VAL:CG1	2.15	0.76
1:I:8:ILE:H	1:J:117:HIS:CD2	2.03	0.75
1:J:7:LEU:HD12	1:J:10:GLU:OE2	1.84	0.75
2:A:262:HOH:O	1:B:146:GLU:HG3	1.87	0.75
1:J:50:OCS:OD1	1:J:126:ARG:NH2	2.20	0.75
1:E:43:PRO:HG2	1:E:145:MET:HG2	1.68	0.75
1:I:40:PHE:HD1	1:I:42:HIS:HE2	1.34	0.74
1:I:200:MET:HA	1:I:200:MET:HE2	1.68	0.74
1:H:59:ARG:HH11	1:H:59:ARG:CG	2.00	0.74
1:G:50:OCS:OD1	1:G:126:ARG:NH2	2.19	0.74
1:A:200:MET:HA	1:A:200:MET:CE	2.15	0.74
1:B:40:PHE:HD1	1:B:42:HIS:HE2	1.35	0.74
1:E:120:SER:HB2	1:E:123:HIS:O	1.88	0.74
1:C:168:LYS:O	1:C:168:LYS:HD3	1.88	0.74
1:E:50:OCS:OD1	1:E:126:ARG:NH2	2.20	0.74
1:C:8:ILE:H	1:D:117:HIS:HD2	1.34	0.73
1:B:206:ARG:HG3	1:B:206:ARG:HH11	1.52	0.73
1:G:5:ILE:HG22	1:G:114:GLY:HA3	1.69	0.73
1:D:200:MET:HE3	1:D:210:TRP:HA	1.69	0.73
1:A:231:ARG:HH21	1:A:231:ARG:CB	2.02	0.72
1:F:206:ARG:HH11	1:F:206:ARG:CG	1.98	0.72
1:H:59:ARG:HH11	1:H:59:ARG:HG3	1.53	0.72
1:G:69:VAL:HG21	1:G:158:VAL:HG11	1.69	0.72
1:E:140:MET:HE2	1:E:142:TYR:OH	1.89	0.72
1:H:11:ARG:NH1	1:H:14:GLU:OE2	2.22	0.72
1:D:120:SER:C	1:D:122:THR:H	1.98	0.72
1:E:117:HIS:CG	1:E:125:VAL:HG21	2.24	0.72
1:C:214:TRP:CH2	1:D:242:TYR:CD1	2.77	0.72
1:D:120:SER:HB3	1:D:123:HIS:O	1.88	0.72
1:I:117:HIS:HB2	1:I:125:VAL:HG11	1.72	0.72
1:G:206:ARG:HH11	1:G:206:ARG:CG	2.02	0.71
1:G:206:ARG:HG3	1:G:206:ARG:NH1	2.06	0.71
1:C:140:MET:HE2	1:C:142:TYR:OH	1.89	0.71
1:B:140:MET:CE	1:B:142:TYR:OH	2.39	0.71
1:G:140:MET:HE2	1:G:142:TYR:OH	1.90	0.71
2:I:295:HOH:O	1:J:146:GLU:HG3	1.90	0.71
1:I:106:GLN:O	1:I:111:ARG:NH2	2.24	0.71
1:F:124:THR:HG23	1:F:125:VAL:O	1.91	0.70
1:E:59:ARG:HG3	1:E:59:ARG:NH1	1.98	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:HE2	1:A:140:MET:HE3	1.57	0.70
1:G:8:ILE:H	1:H:117:HIS:HD2	1.38	0.70
1:I:125:VAL:HA	1:I:145:MET:HE2	1.71	0.70
1:D:86:LYS:HD3	1:D:97:ILE:HB	1.72	0.70
1:B:126:ARG:NH1	1:B:145:MET:CA	2.55	0.70
1:E:14:GLU:OE1	1:E:28:ASP:OD1	2.10	0.69
1:F:185:LEU:O	1:F:214:TRP:HB2	1.92	0.69
1:G:11:ARG:NH1	1:G:14:GLU:OE2	2.22	0.69
1:I:5:ILE:HG22	1:I:114:GLY:HA3	1.72	0.69
1:I:60:ARG:HH11	1:I:60:ARG:HG3	1.58	0.69
1:A:7:LEU:HD22	1:B:117:HIS:CG	2.28	0.69
1:G:63:ASP:CG	1:G:228:ARG:HH12	2.00	0.69
1:E:168:LYS:HD2	2:E:284:HOH:O	1.94	0.68
1:G:117:HIS:HD2	1:H:8:ILE:H	1.40	0.68
1:E:242:TYR:CD1	1:F:214:TRP:CH2	2.77	0.68
1:F:140:MET:HE2	1:F:142:TYR:OH	1.92	0.68
1:G:14:GLU:OE1	1:G:28:ASP:OD1	2.12	0.68
1:A:118:ALA:HB2	1:B:10:GLU:HG3	1.75	0.68
1:J:117:HIS:ND1	1:J:125:VAL:HG21	2.09	0.68
1:D:228:ARG:NH1	2:D:268:HOH:O	2.25	0.68
1:F:106:GLN:HE22	1:G:107:GLY:HA3	1.56	0.68
1:I:117:HIS:HB2	1:I:125:VAL:HG13	1.74	0.68
1:B:106:GLN:O	1:B:111:ARG:NH2	2.26	0.68
1:C:214:TRP:HH2	1:D:242:TYR:CE1	2.12	0.68
1:A:239:LYS:HD2	1:A:244:GLU:HG2	1.75	0.67
1:G:40:PHE:HD1	1:G:42:HIS:HE2	1.40	0.67
1:A:231:ARG:HB2	1:A:231:ARG:NH2	2.10	0.67
1:C:120:SER:O	1:C:122:THR:N	2.27	0.67
1:H:111:ARG:HE	1:I:106:GLN:HE22	1.40	0.67
1:A:126:ARG:NH1	1:A:145:MET:C	2.50	0.67
1:E:8:ILE:H	1:F:117:HIS:HD2	1.40	0.67
1:F:188:PRO:O	1:F:199:ARG:NH2	2.27	0.67
1:D:50:OCS:OD1	1:D:126:ARG:NH2	2.27	0.67
1:C:125:VAL:CA	1:C:145:MET:HE2	2.21	0.67
1:E:115:LEU:HB3	1:E:124:THR:HG23	1.76	0.67
1:B:43:PRO:HB3	1:B:123:HIS:HB3	1.77	0.67
1:B:67:LEU:HD13	1:B:158:VAL:HG23	1.76	0.67
1:E:40:PHE:HD1	1:E:42:HIS:NE2	1.92	0.67
1:E:190:PRO:HB3	1:E:195:GLN:HB3	1.77	0.66
1:J:67:LEU:HD13	1:J:158:VAL:HG23	1.76	0.66
1:A:208:LEU:CD1	1:A:214:TRP:CZ3	2.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:PHE:HD1	1:G:42:HIS:NE2	1.92	0.66
1:H:69:VAL:HG21	1:H:158:VAL:HG21	1.78	0.66
1:I:14:GLU:OE1	1:I:25:LYS:HE2	1.96	0.66
1:J:105:PRO:O	1:J:106:GLN:CB	2.37	0.66
1:D:167:LEU:HD23	1:D:217:PRO:HG2	1.78	0.66
1:D:241:LEU:HA	1:D:244:GLU:CG	2.27	0.65
1:I:240:LEU:O	1:I:243:GLU:HG2	1.96	0.65
1:H:122:THR:HG22	1:H:123:HIS:CD2	2.32	0.65
1:E:117:HIS:CD2	1:E:125:VAL:HG21	2.31	0.65
1:A:7:LEU:HB3	1:B:117:HIS:CB	2.26	0.65
1:B:59:ARG:HH11	1:B:59:ARG:HG2	1.62	0.65
1:A:120:SER:C	1:A:121:ALA:O	2.39	0.65
1:A:67:LEU:HD13	1:A:158:VAL:HG23	1.80	0.64
1:A:140:MET:HE2	1:A:142:TYR:OH	1.97	0.64
1:B:126:ARG:HH12	1:B:145:MET:CG	2.09	0.64
1:F:106:GLN:NE2	1:G:107:GLY:HA3	2.12	0.64
1:F:129:PHE:CE2	1:F:140:MET:CE	2.77	0.64
1:G:40:PHE:CD1	1:G:42:HIS:NE2	2.63	0.64
1:H:67:LEU:HD13	1:H:158:VAL:HG22	1.78	0.64
1:D:117:HIS:HB2	1:D:125:VAL:HG13	1.80	0.63
1:I:126:ARG:HH12	1:I:145:MET:C	2.05	0.63
1:I:43:PRO:HG3	1:I:145:MET:HG2	1.78	0.63
1:B:126:ARG:HH11	1:B:145:MET:CA	1.99	0.63
1:F:11:ARG:HG2	1:F:11:ARG:NH1	2.11	0.63
1:B:106:GLN:HE22	1:C:107:GLY:HA3	1.63	0.63
1:H:40:PHE:HD1	1:H:42:HIS:HE2	1.47	0.63
1:I:7:LEU:HD12	1:I:10:GLU:OE2	1.98	0.63
1:E:168:LYS:O	1:E:168:LYS:CD	2.43	0.63
1:C:172:PRO:HG3	1:C:181:ILE:HD11	1.80	0.63
1:E:168:LYS:HE3	1:E:188:PRO:HD2	1.79	0.63
1:F:42:HIS:NE2	1:F:54:PHE:HE1	1.97	0.63
1:D:42:HIS:NE2	1:D:54:PHE:HE1	1.97	0.62
1:F:120:SER:HA	1:F:145:MET:HE1	1.81	0.62
1:I:161:LEU:HD11	1:J:144:PRO:HG3	1.81	0.62
1:G:220:ARG:O	1:G:224:GLU:HG3	1.99	0.62
1:H:105:PRO:O	1:H:106:GLN:CB	2.45	0.62
1:F:194:ASP:OD1	1:F:197:ARG:NH2	2.31	0.62
1:G:42:HIS:NE2	1:G:54:PHE:HE1	1.97	0.62
1:C:200:MET:HE3	1:C:210:TRP:HA	1.81	0.62
1:I:105:PRO:O	1:I:106:GLN:HB2	1.97	0.62
1:I:115:LEU:HD21	1:I:129:PHE:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:125:VAL:HA	1:I:145:MET:CE	2.29	0.62
1:G:193:GLU:OE2	1:I:86:LYS:HD2	1.99	0.61
1:A:14:GLU:OE1	1:A:28:ASP:OD1	2.18	0.61
1:B:145:MET:O	1:B:145:MET:HG2	1.99	0.61
1:D:206:ARG:HH11	1:D:206:ARG:CG	2.04	0.61
1:F:86:LYS:HE3	1:F:101:ILE:CD1	2.30	0.61
1:A:7:LEU:HD22	1:B:117:HIS:CD2	2.35	0.61
1:J:129:PHE:HE2	1:J:140:MET:HE3	1.63	0.61
1:H:125:VAL:HA	1:H:145:MET:CE	2.31	0.61
1:G:59:ARG:HH11	1:G:59:ARG:HG2	1.65	0.61
1:J:111:ARG:HG3	1:J:116:LEU:HD12	1.83	0.61
1:B:115:LEU:HB3	1:B:124:THR:HG23	1.82	0.61
1:C:129:PHE:HE2	1:C:140:MET:HE3	1.65	0.61
1:D:14:GLU:OE1	1:D:28:ASP:OD1	2.19	0.61
1:A:208:LEU:CD1	1:A:214:TRP:HZ3	2.13	0.60
1:E:146:GLU:HG3	2:F:287:HOH:O	2.01	0.60
1:F:40:PHE:HD1	1:F:42:HIS:NE2	1.94	0.60
1:B:126:ARG:HH12	1:B:145:MET:HG2	1.66	0.60
1:C:125:VAL:HA	1:C:145:MET:CE	2.25	0.60
1:A:117:HIS:O	1:A:120:SER:HB2	2.00	0.60
1:G:202:SER:OG	1:G:204:GLN:HG2	2.02	0.60
1:D:154:ILE:O	1:D:158:VAL:HG23	2.01	0.60
1:D:228:ARG:HH11	1:D:228:ARG:CG	2.15	0.60
1:A:4:SER:HA	1:B:4:SER:HB2	1.84	0.60
1:E:134:ARG:NH1	2:E:306:HOH:O	2.31	0.60
1:F:62:GLU:CG	1:F:66:ARG:NH2	2.64	0.60
1:B:206:ARG:HG3	1:B:206:ARG:NH1	2.14	0.60
1:E:5:ILE:HD13	1:F:5:ILE:HD13	1.83	0.60
1:H:106:GLN:HG3	1:I:121:ALA:O	2.02	0.60
1:I:40:PHE:HD1	1:I:42:HIS:NE2	2.00	0.60
1:D:140:MET:HE2	1:D:142:TYR:OH	2.02	0.59
1:E:242:TYR:CE1	1:F:214:TRP:HH2	2.19	0.59
1:H:59:ARG:HG3	1:H:59:ARG:NH1	2.14	0.59
1:C:50:OCS:OD1	1:C:126:ARG:NH2	2.36	0.59
1:A:122:THR:HG22	1:A:123:HIS:CD2	2.38	0.59
1:E:42:HIS:NE2	1:E:54:PHE:HE1	2.01	0.59
1:I:5:ILE:HG12	1:J:5:ILE:HG12	1.83	0.59
1:J:206:ARG:NH1	1:J:206:ARG:CG	2.53	0.59
1:F:62:GLU:HG3	1:F:66:ARG:CZ	2.32	0.59
1:F:167:LEU:HD12	1:F:167:LEU:N	2.18	0.59
1:D:126:ARG:HD2	1:D:144:PRO:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:ARG:HH12	1:J:179:GLU:CG	2.13	0.59
1:J:200:MET:HE2	1:J:200:MET:HA	1.84	0.59
1:B:40:PHE:HD1	1:B:42:HIS:NE2	2.00	0.59
1:C:43:PRO:HB3	1:C:123:HIS:HB3	1.84	0.59
1:I:11:ARG:NH2	2:I:302:HOH:O	2.35	0.59
1:B:43:PRO:HG2	1:B:145:MET:HG3	1.84	0.59
1:E:129:PHE:CE2	1:E:140:MET:CE	2.80	0.58
1:B:140:MET:HE2	1:B:142:TYR:OH	2.02	0.58
1:B:190:PRO:HB3	1:B:195:GLN:HB3	1.86	0.58
1:J:67:LEU:HD21	1:J:159:LYS:HD3	1.85	0.58
1:A:105:PRO:O	1:A:106:GLN:HB2	2.03	0.58
1:G:104:ASP:OD2	1:G:107:GLY:HA2	2.04	0.58
1:D:69:VAL:CG2	1:D:158:VAL:HG11	2.32	0.58
1:J:14:GLU:OE1	1:J:28:ASP:OD1	2.21	0.58
1:A:163:LEU:O	1:A:167:LEU:HB2	2.04	0.57
1:G:172:PRO:HG3	1:G:181:ILE:HD11	1.85	0.57
1:H:159:LYS:NZ	1:H:225:GLU:OE2	2.33	0.57
1:I:120:SER:HB3	1:I:123:HIS:O	2.04	0.57
1:I:144:PRO:HB3	2:J:326:HOH:O	2.03	0.57
1:G:144:PRO:HG3	1:H:161:LEU:HD11	1.86	0.57
1:A:62:GLU:HG3	1:A:66:ARG:NH1	2.18	0.57
1:E:4:SER:HA	1:F:4:SER:HA	1.85	0.57
1:F:167:LEU:N	1:F:167:LEU:CD1	2.67	0.57
1:C:244:GLU:HG3	1:C:245:ALA:N	2.19	0.57
1:D:117:HIS:HB2	1:D:125:VAL:HG11	1.87	0.57
1:G:183:GLU:OE1	1:H:236:LYS:NZ	2.27	0.57
1:E:238:ALA:O	1:E:239:LYS:CB	2.52	0.57
1:D:75:SER:HB3	1:D:82:HIS:CE1	2.39	0.57
1:A:188:PRO:O	1:A:199:ARG:NH2	2.38	0.56
1:B:86:LYS:HE3	1:B:101:ILE:HD12	1.87	0.56
1:C:214:TRP:HH2	1:D:242:TYR:CG	2.23	0.56
1:C:105:PRO:O	1:C:106:GLN:CB	2.48	0.56
1:A:118:ALA:CB	1:B:10:GLU:HG3	2.35	0.56
1:B:206:ARG:HH11	1:B:206:ARG:CG	2.17	0.56
1:E:105:PRO:O	1:E:106:GLN:CB	2.54	0.56
1:I:89:ILE:HG21	1:I:97:ILE:HD11	1.86	0.56
1:E:118:ALA:HB2	1:F:10:GLU:HG3	1.87	0.56
1:F:163:LEU:O	1:F:167:LEU:HD13	2.06	0.56
1:D:28:ASP:OD1	1:D:28:ASP:N	2.39	0.56
1:D:110:ALA:HB1	1:D:124:THR:HG22	1.86	0.56
1:D:146:GLU:OE2	1:D:146:GLU:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:CD1	1:D:5:ILE:HD13	2.35	0.56
1:E:118:ALA:CB	1:F:10:GLU:HG3	2.35	0.56
1:E:206:ARG:HG3	1:E:206:ARG:HH11	1.71	0.56
1:F:126:ARG:HH12	1:F:145:MET:C	2.14	0.56
1:E:50:OCS:SG	1:E:126:ARG:NH2	2.79	0.56
1:E:117:HIS:HB2	1:E:125:VAL:CG2	2.36	0.56
1:E:144:PRO:HD3	1:F:139:THR:OG1	2.06	0.56
1:J:40:PHE:CD1	1:J:42:HIS:NE2	2.72	0.56
1:F:124:THR:CG2	1:F:125:VAL:O	2.54	0.55
1:D:200:MET:CE	1:D:210:TRP:HA	2.36	0.55
1:A:193:GLU:OE2	1:C:86:LYS:HD2	2.06	0.55
1:C:126:ARG:HD2	1:C:144:PRO:O	2.07	0.55
1:F:190:PRO:HB3	1:F:195:GLN:HB3	1.88	0.55
1:F:67:LEU:HD21	1:F:159:LYS:HD2	1.89	0.55
1:D:228:ARG:HH11	1:D:228:ARG:HG2	1.71	0.55
1:F:67:LEU:HD13	1:F:158:VAL:HG23	1.89	0.55
1:A:139:THR:HG1	1:B:144:PRO:HD3	1.72	0.55
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.06	0.55
1:H:40:PHE:HD1	1:H:42:HIS:NE2	2.04	0.55
1:I:126:ARG:HG3	1:I:149:ARG:CZ	2.36	0.55
1:F:220:ARG:NH1	1:F:224:GLU:OE2	2.40	0.55
1:H:190:PRO:HB3	1:H:195:GLN:HB3	1.89	0.55
1:D:144:PRO:HG2	1:D:147:LEU:HB2	1.89	0.54
1:H:228:ARG:HD3	2:H:266:HOH:O	2.07	0.54
1:C:134:ARG:NH1	2:C:308:HOH:O	2.26	0.54
1:C:146:GLU:HG3	2:D:258:HOH:O	2.06	0.54
1:H:11:ARG:NH2	2:H:271:HOH:O	2.40	0.54
1:H:238:ALA:O	1:H:239:LYS:HB3	2.08	0.54
1:H:67:LEU:HD21	1:H:159:LYS:HD3	1.90	0.54
1:B:225:GLU:HB2	1:B:228:ARG:HH22	1.73	0.54
1:H:14:GLU:OE1	1:H:28:ASP:OD1	2.24	0.54
1:I:120:SER:C	1:I:122:THR:H	2.16	0.54
1:F:215:ASP:OD1	1:F:217:PRO:HD3	2.08	0.53
1:I:59:ARG:HH12	1:J:179:GLU:HB3	1.72	0.53
1:A:117:HIS:HB2	1:A:125:VAL:HG13	1.90	0.53
1:D:16:GLU:OE1	1:D:23:VAL:CG1	2.56	0.53
1:H:35:LYS:NZ	2:H:308:HOH:O	2.40	0.53
1:F:239:LYS:HE2	1:F:244:GLU:OE1	2.08	0.53
1:C:220:ARG:NH1	1:C:224:GLU:OE2	2.41	0.53
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.43	0.53
1:E:115:LEU:HB3	1:E:124:THR:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:OCS:OD1	1:B:126:ARG:NH2	2.42	0.53
2:C:259:HOH:O	1:D:146:GLU:HG3	2.07	0.53
1:H:106:GLN:NE2	1:I:111:ARG:HE	2.07	0.53
1:J:126:ARG:HD2	1:J:144:PRO:O	2.08	0.53
1:I:11:ARG:NH1	1:I:14:GLU:OE2	2.40	0.53
1:A:62:GLU:HG3	1:A:66:ARG:HH11	1.74	0.53
1:E:122:THR:HG23	1:E:123:HIS:CD2	2.44	0.53
1:B:200:MET:HE1	1:B:213:CYS:SG	2.49	0.53
1:E:11:ARG:HH11	1:E:11:ARG:HG3	1.71	0.53
1:G:146:GLU:HG3	2:H:267:HOH:O	2.08	0.53
1:B:126:ARG:NH1	1:B:145:MET:O	2.42	0.52
1:D:66:ARG:HG3	1:D:66:ARG:NH1	2.24	0.52
1:D:122:THR:HG23	1:D:123:HIS:CD2	2.45	0.52
1:H:124:THR:HG23	1:H:125:VAL:O	2.08	0.52
1:I:236:LYS:HD2	1:I:237:PRO:HD2	1.91	0.52
1:D:228:ARG:NH1	1:D:228:ARG:HG2	2.25	0.52
1:I:5:ILE:CD1	1:I:6:PRO:O	2.48	0.52
1:I:63:ASP:HA	1:I:66:ARG:NH1	2.24	0.52
1:D:16:GLU:OE1	1:D:23:VAL:HG12	2.10	0.52
2:G:268:HOH:O	1:H:146:GLU:HG3	2.10	0.52
1:I:144:PRO:HG3	1:J:161:LEU:HD11	1.90	0.52
1:A:202:SER:C	1:A:204:GLN:N	2.65	0.52
1:C:104:ASP:OD2	1:C:107:GLY:HA2	2.10	0.52
1:I:7:LEU:HB2	1:I:10:GLU:CD	2.34	0.52
1:A:128:VAL:O	1:A:140:MET:HA	2.10	0.52
1:I:36:TRP:HB2	1:I:69:VAL:HG22	1.91	0.52
1:D:122:THR:CG2	1:D:123:HIS:CD2	2.93	0.51
1:E:117:HIS:HB2	1:E:125:VAL:HG22	1.92	0.51
1:F:36:TRP:CD2	1:F:132:ASP:HA	2.44	0.51
1:I:117:HIS:CB	1:I:125:VAL:HG11	2.40	0.51
1:A:239:LYS:HG2	1:A:244:GLU:OE1	2.10	0.51
1:I:147:LEU:HG	1:J:161:LEU:HD13	1.93	0.51
1:D:117:HIS:CG	1:D:125:VAL:HG11	2.46	0.51
1:J:63:ASP:CG	1:J:228:ARG:NH2	2.68	0.51
1:A:139:THR:OG1	1:B:144:PRO:HD3	2.11	0.51
1:E:5:ILE:CD1	1:F:5:ILE:HD13	2.41	0.51
1:E:188:PRO:O	1:E:199:ARG:NH2	2.43	0.51
1:E:242:TYR:HD1	1:F:208:LEU:HD11	1.76	0.51
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.46	0.51
1:E:43:PRO:HB2	1:E:145:MET:HE2	1.92	0.51
1:E:144:PRO:HB3	2:E:286:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:115:LEU:HD21	1:I:129:PHE:CE1	2.44	0.51
1:I:178:ASN:HD21	1:J:52:THR:HB	1.76	0.51
1:B:126:ARG:NH1	1:B:145:MET:CG	2.73	0.51
1:B:134:ARG:NH1	2:B:297:HOH:O	2.44	0.51
1:I:190:PRO:HB3	1:I:195:GLN:HB3	1.91	0.51
1:E:39:LEU:HD23	1:E:39:LEU:C	2.36	0.51
1:E:122:THR:HG23	1:E:123:HIS:CG	2.46	0.51
1:E:220:ARG:HG3	2:E:264:HOH:O	2.11	0.51
1:F:42:HIS:CD2	1:F:54:PHE:HE1	2.29	0.51
1:E:238:ALA:O	1:E:239:LYS:HB2	2.11	0.51
1:E:200:MET:HA	1:E:200:MET:CE	2.37	0.51
1:F:126:ARG:HG2	1:F:143:TYR:O	2.10	0.51
1:I:37:PHE:HA	1:I:70:ASP:O	2.11	0.51
1:J:63:ASP:OD1	1:J:228:ARG:NH2	2.43	0.51
1:A:122:THR:HG22	1:A:123:HIS:CG	2.46	0.50
1:F:75:SER:HB3	1:F:82:HIS:CE1	2.46	0.50
1:J:120:SER:CB	1:J:123:HIS:O	2.60	0.50
1:D:66:ARG:HG3	1:D:66:ARG:HH11	1.75	0.50
1:D:76:VAL:O	1:D:105:PRO:HA	2.11	0.50
1:F:220:ARG:HG3	1:F:220:ARG:HH11	1.76	0.50
1:C:206:ARG:HH12	1:C:215:ASP:HA	1.75	0.50
1:G:163:LEU:HD11	1:G:222:ASP:HB3	1.93	0.50
1:H:104:ASP:OD2	1:H:107:GLY:HA2	2.12	0.50
1:C:86:LYS:HE2	1:C:101:ILE:HD11	1.93	0.50
1:E:7:LEU:HD12	1:E:10:GLU:OE2	2.11	0.50
1:G:7:LEU:HB2	1:G:10:GLU:OE2	2.12	0.50
1:G:63:ASP:OD1	1:G:228:ARG:NH1	2.45	0.50
1:A:43:PRO:HD2	1:A:50:OCS:OD3	2.11	0.50
1:E:43:PRO:CG	1:E:145:MET:HG2	2.39	0.50
1:J:190:PRO:HB3	1:J:195:GLN:HB3	1.94	0.50
1:J:120:SER:HB2	1:J:123:HIS:O	2.11	0.50
1:H:122:THR:CG2	1:H:123:HIS:CD2	2.95	0.50
1:I:59:ARG:HH12	1:J:179:GLU:CB	2.24	0.50
1:A:191:THR:H	1:A:195:GLN:NE2	2.10	0.50
1:C:40:PHE:CD1	1:C:42:HIS:NE2	2.79	0.50
1:D:14:GLU:OE1	1:D:25:LYS:HE3	2.12	0.50
1:I:60:ARG:HG3	1:I:60:ARG:NH1	2.27	0.50
1:A:9:GLY:HA3	1:B:119:GLU:HG2	1.94	0.49
1:J:63:ASP:OD2	1:J:228:ARG:NH2	2.45	0.49
1:J:207:SER:HB3	1:J:213:CYS:SG	2.52	0.49
1:C:214:TRP:CH2	1:D:242:TYR:CG	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:NH1	1:A:145:MET:HA	2.27	0.49
1:B:67:LEU:HD13	1:B:158:VAL:CG2	2.42	0.49
1:C:8:ILE:HD11	1:D:142:TYR:HB3	1.94	0.49
1:F:200:MET:HE2	1:F:200:MET:HA	1.94	0.49
1:I:43:PRO:CB	1:I:123:HIS:HB3	2.42	0.49
1:E:7:LEU:O	1:E:10:GLU:HB2	2.12	0.49
1:I:236:LYS:HD3	1:J:227:ARG:NH2	2.27	0.49
1:D:106:GLN:CD	1:E:111:ARG:HH21	2.19	0.49
1:E:105:PRO:O	1:E:106:GLN:HB2	2.12	0.49
1:E:129:PHE:HE2	1:E:140:MET:CE	2.15	0.49
1:F:14:GLU:OE1	1:F:28:ASP:OD1	2.30	0.49
1:I:146:GLU:HG3	2:J:263:HOH:O	2.13	0.49
1:A:144:PRO:HB3	2:A:333:HOH:O	2.12	0.49
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.77	0.49
1:D:16:GLU:OE2	1:D:25:LYS:HB2	2.13	0.49
1:B:208:LEU:HD22	1:B:214:TRP:HZ3	1.77	0.49
1:H:126:ARG:HG3	1:H:143:TYR:O	2.13	0.49
1:B:117:HIS:NE2	1:B:125:VAL:HG21	2.27	0.49
1:A:105:PRO:HG2	1:J:122:THR:CG2	2.34	0.49
1:B:124:THR:HG22	1:B:125:VAL:O	2.12	0.49
1:F:238:ALA:O	1:F:239:LYS:CB	2.52	0.49
1:G:14:GLU:O	1:G:15:MET:HB3	2.13	0.49
1:A:142:TYR:HB3	1:B:8:ILE:HD11	1.95	0.49
1:E:4:SER:HA	1:F:4:SER:N	2.27	0.49
1:G:14:GLU:CG	1:G:25:LYS:NZ	2.61	0.49
1:G:54:PHE:CE2	1:G:101:ILE:HD11	2.48	0.49
1:J:41:SER:HB2	1:J:124:THR:HG21	1.94	0.49
1:C:206:ARG:NH1	1:C:215:ASP:HA	2.28	0.48
1:C:42:HIS:NE2	1:C:54:PHE:HE1	2.12	0.48
1:C:157:ILE:O	1:C:161:LEU:HB2	2.13	0.48
1:C:200:MET:HE1	1:C:213:CYS:SG	2.53	0.48
1:F:41:SER:HB2	1:F:124:THR:HG21	1.95	0.48
1:G:117:HIS:CD2	1:H:8:ILE:H	2.25	0.48
1:C:4:SER:HA	1:D:4:SER:HA	1.96	0.48
1:I:43:PRO:HB2	1:I:123:HIS:HB3	1.94	0.48
1:J:117:HIS:HB2	1:J:125:VAL:HG22	1.95	0.48
1:D:200:MET:HE1	1:D:213:CYS:SG	2.54	0.48
1:E:11:ARG:CG	1:E:11:ARG:NH1	2.50	0.48
1:H:120:SER:HA	2:H:279:HOH:O	2.14	0.48
1:J:115:LEU:HD11	1:J:129:PHE:CE1	2.48	0.48
1:A:40:PHE:HZ	1:A:99:PHE:CE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:HB2	2:A:324:HOH:O	2.12	0.48
1:B:228:ARG:CD	2:B:271:HOH:O	2.44	0.48
1:F:129:PHE:HE2	1:F:140:MET:CE	2.20	0.48
1:G:79:VAL:O	1:G:83:ILE:HG13	2.13	0.48
1:C:214:TRP:CH2	1:D:242:TYR:CE1	2.96	0.47
1:I:154:ILE:O	1:I:158:VAL:HG13	2.14	0.47
1:A:156:ARG:HD3	1:A:230:LEU:HD21	1.96	0.47
1:C:40:PHE:HD1	1:C:42:HIS:NE2	2.12	0.47
1:I:41:SER:HB2	1:I:124:THR:HG21	1.95	0.47
1:I:59:ARG:NH1	1:J:179:GLU:CG	2.73	0.47
1:A:117:HIS:C	1:A:120:SER:HB2	2.39	0.47
1:D:6:PRO:O	1:D:140:MET:HE1	2.13	0.47
1:F:140:MET:HE2	1:F:142:TYR:HH	1.79	0.47
1:F:228:ARG:HD3	2:F:268:HOH:O	2.15	0.47
1:J:198:ALA:O	1:J:199:ARG:C	2.56	0.47
1:H:146:GLU:OE2	1:H:146:GLU:N	2.42	0.47
1:I:126:ARG:NH1	1:I:145:MET:O	2.31	0.47
1:C:153:GLU:O	1:C:157:ILE:HG13	2.14	0.47
1:D:172:PRO:HG3	1:D:181:ILE:HD11	1.95	0.47
1:E:4:SER:HA	1:F:4:SER:CA	2.44	0.47
1:E:144:PRO:HG2	1:E:147:LEU:HB2	1.97	0.47
1:E:140:MET:HE2	1:E:142:TYR:HH	1.79	0.47
1:F:86:LYS:HE3	1:F:101:ILE:HD11	1.95	0.47
1:H:122:THR:HG23	1:I:105:PRO:HG2	1.97	0.47
1:B:115:LEU:HB3	1:B:124:THR:CG2	2.45	0.47
1:G:200:MET:HE2	1:G:200:MET:CA	2.40	0.47
1:H:44:ALA:O	1:H:47:THR:OG1	2.30	0.47
1:H:111:ARG:HH21	1:I:106:GLN:HE21	1.61	0.47
1:I:104:ASP:OD2	1:I:107:GLY:HA2	2.14	0.47
1:C:7:LEU:O	1:C:10:GLU:HB2	2.15	0.47
1:F:167:LEU:HD23	1:F:217:PRO:HG2	1.97	0.47
1:G:63:ASP:CG	1:G:228:ARG:NH1	2.71	0.47
1:G:128:VAL:O	1:G:140:MET:HA	2.15	0.47
1:D:110:ALA:HB2	1:D:124:THR:HG21	1.97	0.46
1:J:128:VAL:O	1:J:140:MET:HA	2.15	0.46
1:B:208:LEU:HD22	1:B:214:TRP:CZ3	2.50	0.46
1:D:120:SER:C	1:D:122:THR:N	2.64	0.46
1:E:220:ARG:O	1:E:224:GLU:HG3	2.15	0.46
1:B:106:GLN:NE2	1:C:107:GLY:HA3	2.29	0.46
1:J:124:THR:HG23	1:J:125:VAL:O	2.16	0.46
1:B:105:PRO:O	1:B:106:GLN:CB	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:GLU:OE2	1:F:146:GLU:N	2.36	0.46
1:G:146:GLU:OE2	1:G:146:GLU:N	2.45	0.46
1:A:174:ASP:HB3	2:B:279:HOH:O	2.15	0.46
1:D:110:ALA:CB	1:D:124:THR:CG2	2.93	0.46
1:I:118:ALA:HB2	1:J:10:GLU:CG	2.46	0.46
1:J:39:LEU:HD23	1:J:39:LEU:C	2.41	0.46
1:J:40:PHE:HD1	1:J:42:HIS:NE2	2.13	0.46
1:A:115:LEU:O	1:A:125:VAL:HG22	2.16	0.46
1:E:242:TYR:CE1	1:F:214:TRP:CH2	3.02	0.46
1:G:157:ILE:O	1:G:161:LEU:HB2	2.16	0.46
1:D:45:ASP:HA	1:D:85:TRP:CE3	2.51	0.46
1:D:228:ARG:NH1	1:D:228:ARG:CG	2.79	0.46
1:E:203:GLY:HA2	2:E:269:HOH:O	2.16	0.46
1:G:106:GLN:O	1:G:111:ARG:NH2	2.49	0.46
1:I:128:VAL:HG23	1:I:149:ARG:HH11	1.80	0.46
1:A:124:THR:HG23	1:A:125:VAL:O	2.15	0.46
1:D:45:ASP:HA	1:D:85:TRP:CZ3	2.51	0.46
1:J:11:ARG:HH11	1:J:11:ARG:CG	2.12	0.46
1:A:126:ARG:HB3	1:A:143:TYR:O	2.16	0.46
1:D:110:ALA:HB1	1:D:124:THR:CG2	2.44	0.46
1:G:16:GLU:HG2	1:G:25:LYS:CD	2.45	0.46
1:I:117:HIS:CG	1:I:125:VAL:HG11	2.51	0.46
1:E:128:VAL:O	1:E:140:MET:HA	2.16	0.46
1:H:125:VAL:HA	1:H:145:MET:HE3	1.98	0.46
1:A:43:PRO:HB3	1:A:123:HIS:HB3	1.98	0.45
1:C:200:MET:HG2	1:C:210:TRP:HB3	1.97	0.45
1:H:126:ARG:NH1	1:H:145:MET:O	2.49	0.45
1:A:5:ILE:HD13	1:B:5:ILE:HG12	1.97	0.45
1:A:77:ASP:OD2	1:J:77:ASP:OD2	2.33	0.45
1:F:67:LEU:O	1:F:162:LYS:HE2	2.16	0.45
1:F:99:PHE:HB2	1:F:100:PRO:HD2	1.98	0.45
1:H:74:LEU:HD13	1:H:75:SER:N	2.32	0.45
1:I:69:VAL:HG21	1:I:158:VAL:HG21	1.97	0.45
1:B:43:PRO:CB	1:B:123:HIS:HB3	2.44	0.45
1:F:239:LYS:CE	1:F:244:GLU:OE1	2.65	0.45
1:I:75:SER:HB3	1:I:82:HIS:CE1	2.52	0.45
1:A:67:LEU:CD1	1:A:158:VAL:HG23	2.46	0.45
1:A:117:HIS:O	1:A:120:SER:CB	2.63	0.45
1:C:86:LYS:HE3	1:C:101:ILE:HD12	1.97	0.45
1:C:160:ALA:HB1	1:C:171:VAL:HG11	1.97	0.45
1:E:84:LYS:HD2	1:E:87:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:HD13	1:C:158:VAL:CG2	2.46	0.45
1:F:126:ARG:HG3	1:F:126:ARG:O	2.16	0.45
1:A:11:ARG:NH1	1:A:14:GLU:OE2	2.50	0.45
1:C:40:PHE:HZ	1:C:99:PHE:CE1	2.35	0.45
1:D:220:ARG:O	1:D:224:GLU:HG3	2.16	0.45
1:F:124:THR:O	1:F:124:THR:HG22	2.17	0.45
1:H:39:LEU:C	1:H:39:LEU:HD23	2.41	0.45
1:J:66:ARG:NH1	1:J:66:ARG:CG	2.65	0.45
1:A:5:ILE:HG13	1:A:6:PRO:O	2.17	0.45
1:C:144:PRO:HG3	1:D:161:LEU:HD11	1.99	0.45
1:H:111:ARG:HG3	1:H:116:LEU:HD12	1.99	0.45
1:H:244:GLU:HG2	2:H:296:HOH:O	2.16	0.45
1:C:43:PRO:CB	1:C:123:HIS:HB3	2.45	0.45
1:C:54:PHE:CE2	1:C:101:ILE:HD13	2.52	0.45
1:D:43:PRO:HB3	1:D:123:HIS:HB3	1.99	0.45
1:A:117:HIS:CD2	1:A:125:VAL:HG21	2.52	0.45
1:A:231:ARG:NH2	1:B:234:ALA:HB1	2.32	0.45
1:D:122:THR:HA	1:E:106:GLN:CG	2.47	0.45
1:F:105:PRO:O	1:F:106:GLN:CB	2.38	0.45
2:I:251:HOH:O	1:J:183:GLU:HG2	2.16	0.45
1:B:59:ARG:HG2	1:B:59:ARG:NH1	2.28	0.44
1:H:124:THR:O	1:H:145:MET:HE2	2.17	0.44
1:E:171:VAL:HB	1:F:147:LEU:HD23	1.98	0.44
1:E:207:SER:HB2	1:E:213:CYS:SG	2.57	0.44
1:G:36:TRP:HB2	1:G:69:VAL:HG22	1.98	0.44
1:G:37:PHE:HA	1:G:70:ASP:O	2.17	0.44
1:A:67:LEU:HD13	1:A:158:VAL:CG2	2.45	0.44
1:C:60:ARG:HA	2:C:273:HOH:O	2.18	0.44
1:C:188:PRO:O	1:C:199:ARG:NH2	2.50	0.44
1:H:238:ALA:O	1:H:239:LYS:CB	2.62	0.44
1:A:96:ARG:NH2	1:A:98:PRO:HB3	2.33	0.44
1:A:183:GLU:HG2	2:A:286:HOH:O	2.17	0.44
1:A:190:PRO:HG2	1:A:196:ALA:HA	2.00	0.44
1:B:93:ILE:HG22	1:B:95:VAL:HG23	1.99	0.44
1:D:167:LEU:HD12	1:D:167:LEU:N	2.32	0.44
1:E:126:ARG:NH1	1:E:145:MET:HA	2.33	0.44
1:E:156:ARG:HD3	1:E:230:LEU:HD21	1.99	0.44
1:G:16:GLU:HG2	1:G:25:LYS:HD2	1.98	0.44
1:I:172:PRO:HG3	1:I:181:ILE:HD11	2.00	0.44
1:J:43:PRO:CB	1:J:123:HIS:HB3	2.48	0.44
1:C:150:LEU:HD22	1:D:153:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:GLY:HA2	2:G:289:HOH:O	2.18	0.44
1:A:40:PHE:HD1	1:A:42:HIS:HE2	1.65	0.44
1:G:175:TRP:CG	1:G:176:PRO:HA	2.53	0.44
1:C:124:THR:O	1:C:124:THR:CG2	2.66	0.44
1:D:228:ARG:HH11	1:D:228:ARG:CB	2.31	0.44
1:E:42:HIS:CD2	1:E:54:PHE:HE1	2.36	0.44
1:E:163:LEU:HD11	1:E:222:ASP:HB3	2.00	0.44
1:H:111:ARG:HE	1:I:106:GLN:HE21	1.57	0.44
1:I:118:ALA:HB2	1:J:10:GLU:HG3	2.00	0.44
1:I:140:MET:CE	1:I:142:TYR:OH	2.56	0.44
1:D:224:GLU:O	1:D:228:ARG:HD3	2.17	0.43
1:E:206:ARG:HG3	1:E:206:ARG:NH1	2.31	0.43
1:F:116:LEU:HD13	1:G:106:GLN:NE2	2.33	0.43
1:F:159:LYS:HD3	1:F:225:GLU:OE2	2.17	0.43
1:B:175:TRP:CG	1:B:176:PRO:HA	2.54	0.43
1:E:45:ASP:HA	1:E:85:TRP:CZ3	2.53	0.43
1:E:59:ARG:HH11	1:E:59:ARG:CG	2.13	0.43
1:F:112:ARG:HG2	2:F:264:HOH:O	2.17	0.43
1:E:157:ILE:O	1:E:161:LEU:HB2	2.18	0.43
1:F:106:GLN:NE2	1:G:116:LEU:HD11	2.33	0.43
1:G:225:GLU:HG2	2:G:266:HOH:O	2.18	0.43
1:H:45:ASP:HA	1:H:85:TRP:CZ3	2.52	0.43
1:A:117:HIS:HB2	1:A:125:VAL:CG1	2.49	0.43
1:A:208:LEU:HD12	1:A:214:TRP:CZ3	2.52	0.43
1:C:239:LYS:HB3	1:C:239:LYS:HE2	1.56	0.43
1:D:122:THR:HA	1:E:106:GLN:HG3	1.99	0.43
1:E:228:ARG:HD3	1:E:228:ARG:C	2.44	0.43
1:I:74:LEU:HD13	1:I:75:SER:N	2.34	0.43
1:A:208:LEU:HD12	1:A:214:TRP:HZ3	1.80	0.43
1:E:4:SER:CA	1:F:4:SER:HA	2.49	0.43
1:H:50:OCS:OD1	1:H:126:ARG:NH2	2.50	0.43
1:J:106:GLN:O	1:J:111:ARG:NH2	2.52	0.43
1:H:157:ILE:O	1:H:161:LEU:HB2	2.19	0.43
1:H:59:ARG:CG	1:H:59:ARG:NH1	2.66	0.43
1:A:206:ARG:NH1	2:A:309:HOH:O	2.51	0.43
1:I:124:THR:O	1:I:124:THR:HG22	2.18	0.43
1:C:14:GLU:HG3	1:C:25:LYS:HE2	2.00	0.43
1:C:120:SER:OG	1:C:125:VAL:CG1	2.67	0.43
1:C:208:LEU:HD13	1:D:242:TYR:HD1	1.83	0.43
1:D:120:SER:O	1:D:122:THR:N	2.52	0.43
1:A:99:PHE:HB2	1:A:100:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:ARG:HH11	1:I:126:ARG:HD2	1.51	0.43
1:B:225:GLU:CG	1:B:228:ARG:HH12	2.32	0.42
1:D:189:PRO:HA	1:D:190:PRO:HD3	1.96	0.42
1:A:121:ALA:O	1:A:123:HIS:N	2.50	0.42
1:C:236:LYS:HD2	1:D:227:ARG:NH2	2.33	0.42
1:D:20:ASP:OD2	1:D:86:LYS:NZ	2.51	0.42
1:D:106:GLN:HE21	1:D:106:GLN:HB2	1.50	0.42
1:J:11:ARG:HG3	1:J:135:GLY:O	2.19	0.42
1:A:11:ARG:NH2	1:A:14:GLU:OE2	2.52	0.42
1:B:50:OCS:SG	1:B:126:ARG:NH2	2.93	0.42
1:C:214:TRP:NE1	2:C:302:HOH:O	2.07	0.42
1:D:117:HIS:CB	1:D:125:VAL:HG11	2.49	0.42
1:F:50:OCS:OD1	1:F:126:ARG:NH2	2.50	0.42
1:J:140:MET:HE2	1:J:142:TYR:HH	1.81	0.42
1:A:202:SER:C	1:A:204:GLN:H	2.26	0.42
1:B:39:LEU:HA	1:B:72:ILE:O	2.20	0.42
1:C:59:ARG:HH11	1:D:179:GLU:HG2	1.85	0.42
1:D:106:GLN:O	1:D:106:GLN:HG3	2.18	0.42
1:G:228:ARG:NH2	2:G:292:HOH:O	2.47	0.42
1:B:79:VAL:O	1:B:83:ILE:HG13	2.19	0.42
1:F:220:ARG:NH1	1:F:220:ARG:HG3	2.34	0.42
1:G:54:PHE:CE2	1:G:101:ILE:CD1	3.02	0.42
1:I:120:SER:C	1:I:122:THR:N	2.77	0.42
1:J:168:LYS:HE3	1:J:168:LYS:HB3	1.83	0.42
1:A:41:SER:HB2	1:A:124:THR:HG21	2.00	0.42
1:E:107:GLY:O	1:E:111:ARG:HB2	2.20	0.42
1:G:172:PRO:HB3	1:G:186:ILE:HD11	2.00	0.42
1:A:143:TYR:CD2	1:A:147:LEU:HD13	2.54	0.42
1:D:40:PHE:HZ	1:D:99:PHE:CE1	2.38	0.42
1:I:188:PRO:O	1:I:199:ARG:NH2	2.53	0.42
1:A:150:LEU:HD23	1:A:153:GLU:HB2	2.01	0.42
1:D:185:LEU:O	1:D:214:TRP:HB2	2.19	0.42
1:E:119:GLU:HB3	1:F:9:GLY:HA3	2.01	0.42
1:F:122:THR:HA	1:G:106:GLN:OE1	2.19	0.42
1:A:176:PRO:HG2	1:A:227:ARG:HG2	2.02	0.42
1:C:192:THR:OG1	1:C:195:GLN:HB2	2.20	0.42
1:F:153:GLU:HA	1:F:153:GLU:OE1	2.20	0.42
1:H:74:LEU:HD13	1:H:74:LEU:C	2.45	0.42
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.55	0.42
1:B:128:VAL:O	1:B:140:MET:HA	2.19	0.42
1:B:220:ARG:HG3	2:B:288:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:VAL:O	1:C:140:MET:HA	2.20	0.42
1:C:136:VAL:O	1:C:138:ARG:HG2	2.20	0.42
1:E:69:VAL:HG21	1:E:158:VAL:HG11	2.02	0.42
1:I:128:VAL:O	1:I:140:MET:HA	2.19	0.42
1:J:48:PRO:O	1:J:52:THR:HG23	2.19	0.42
1:B:7:LEU:HD12	1:B:10:GLU:OE2	2.20	0.41
1:C:140:MET:HE2	1:C:142:TYR:HH	1.82	0.41
1:D:91:ARG:O	1:D:91:ARG:HG3	2.17	0.41
1:H:40:PHE:HZ	1:H:99:PHE:CE1	2.37	0.41
1:G:129:PHE:CE2	1:G:140:MET:CE	2.92	0.41
1:A:120:SER:O	1:A:121:ALA:O	2.39	0.41
1:B:126:ARG:NH1	1:B:145:MET:HG3	2.34	0.41
1:C:139:THR:OG1	1:D:144:PRO:HD3	2.20	0.41
1:E:168:LYS:O	1:E:168:LYS:CG	2.68	0.41
1:F:11:ARG:NH2	1:F:14:GLU:OE2	2.44	0.41
1:H:120:SER:O	1:H:121:ALA:HB3	2.19	0.41
1:I:231:ARG:HG2	1:I:231:ARG:HH11	1.85	0.41
1:A:208:LEU:HD13	1:A:214:TRP:CZ3	2.54	0.41
1:D:43:PRO:CB	1:D:123:HIS:HB3	2.50	0.41
1:G:8:ILE:H	1:H:117:HIS:CD2	2.27	0.41
1:H:120:SER:O	1:H:121:ALA:CB	2.68	0.41
1:I:36:TRP:CD2	1:I:132:ASP:HA	2.55	0.41
1:J:144:PRO:HB2	1:J:146:GLU:OE1	2.20	0.41
1:F:61:TYR:HB3	2:F:325:HOH:O	2.21	0.41
1:H:119:GLU:OE2	1:H:145:MET:HE3	2.21	0.41
1:J:74:LEU:C	1:J:74:LEU:HD13	2.45	0.41
1:J:207:SER:CB	1:J:213:CYS:SG	3.09	0.41
1:C:179:GLU:CB	1:D:59:ARG:HH12	2.33	0.41
1:F:122:THR:HB	1:G:105:PRO:HG2	2.03	0.41
1:H:54:PHE:CZ	1:H:101:ILE:HD13	2.55	0.41
1:A:126:ARG:NH1	1:A:145:MET:CA	2.84	0.41
1:C:173:ALA:HB2	1:D:53:GLU:HG2	2.02	0.41
1:E:24:ILE:HD11	1:E:72:ILE:CD1	2.51	0.41
1:F:116:LEU:HA	1:F:116:LEU:HD23	1.78	0.41
1:F:208:LEU:HD13	1:F:214:TRP:HZ3	1.86	0.41
1:J:146:GLU:H	1:J:146:GLU:CD	2.29	0.41
1:A:231:ARG:HA	1:A:231:ARG:HD3	1.89	0.41
1:B:129:PHE:HE2	1:B:140:MET:HE3	1.78	0.41
1:D:29:HIS:O	1:D:33:GLN:NE2	2.46	0.41
1:F:122:THR:HA	1:G:106:GLN:CD	2.46	0.41
1:H:43:PRO:HB3	1:H:123:HIS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:67:LEU:HA	1:I:67:LEU:HD23	1.89	0.41
1:J:43:PRO:HG3	1:J:145:MET:HE2	2.03	0.41
1:J:200:MET:HE1	1:J:213:CYS:SG	2.61	0.41
1:B:16:GLU:HG2	1:B:25:LYS:HD3	2.01	0.41
1:C:43:PRO:CG	1:C:145:MET:HG2	2.51	0.41
1:D:146:GLU:H	1:D:146:GLU:CD	2.26	0.41
1:A:8:ILE:HG21	1:A:8:ILE:HD13	1.72	0.40
1:A:8:ILE:HD11	1:A:139:THR:HA	2.02	0.40
1:C:190:PRO:HB3	1:C:195:GLN:HB3	2.03	0.40
1:D:159:LYS:HE2	1:D:225:GLU:OE2	2.21	0.40
1:E:126:ARG:HG3	1:E:143:TYR:O	2.21	0.40
1:F:126:ARG:NH1	1:F:145:MET:HA	2.36	0.40
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.56	0.40
1:H:103:ALA:C	1:H:105:PRO:HD3	2.46	0.40
1:I:15:MET:HE2	1:I:112:ARG:HG2	2.03	0.40
1:I:59:ARG:NH1	1:J:179:GLU:HB3	2.36	0.40
1:A:8:ILE:O	1:B:118:ALA:HB3	2.21	0.40
1:C:179:GLU:CG	1:D:59:ARG:HH12	2.34	0.40
1:D:183:GLU:HG2	1:D:227:ARG:HH22	1.85	0.40
1:G:61:TYR:O	1:G:65:GLN:HG2	2.21	0.40
1:J:143:TYR:CD2	1:J:147:LEU:HD13	2.56	0.40
1:D:167:LEU:HD12	1:D:167:LEU:H	1.86	0.40
1:E:84:LYS:HD2	1:E:84:LYS:HA	1.78	0.40
1:E:125:VAL:HG11	1:F:8:ILE:HD12	2.01	0.40
1:F:129:PHE:CD2	1:F:140:MET:HE3	2.51	0.40
1:G:185:LEU:O	1:G:214:TRP:HB2	2.21	0.40
1:J:115:LEU:HD11	1:J:129:PHE:HE1	1.85	0.40
1:A:37:PHE:HA	1:A:70:ASP:O	2.21	0.40
1:C:200:MET:HA	1:C:200:MET:HE2	2.02	0.40
1:D:86:LYS:HE3	1:D:101:ILE:HD12	2.03	0.40
1:E:122:THR:CG2	1:E:123:HIS:CD2	3.04	0.40
1:E:150:LEU:HD22	1:F:153:GLU:OE1	2.20	0.40
1:G:41:SER:HB2	1:G:74:LEU:HD12	2.03	0.40
1:I:118:ALA:C	1:I:120:SER:H	2.29	0.40
1:J:187:VAL:O	1:J:188:PRO:C	2.64	0.40
1:J:212:PHE:HD2	1:J:212:PHE:C	2.30	0.40
1:E:241:LEU:HD23	1:E:241:LEU:HA	1.88	0.40
1:F:42:HIS:HA	1:F:43:PRO:HD3	1.92	0.40
1:G:53:GLU:OE1	1:G:126:ARG:NH2	2.53	0.40
1:J:126:ARG:NH1	1:J:145:MET:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	239/250 (96%)	221 (92%)	16 (7%)	2 (1%)	16	17
1	B	235/250 (94%)	223 (95%)	9 (4%)	3 (1%)	9	8
1	C	235/250 (94%)	224 (95%)	8 (3%)	3 (1%)	9	8
1	D	239/250 (96%)	226 (95%)	10 (4%)	3 (1%)	9	8
1	E	239/250 (96%)	220 (92%)	15 (6%)	4 (2%)	7	6
1	F	239/250 (96%)	228 (95%)	10 (4%)	1 (0%)	30	34
1	G	239/250 (96%)	227 (95%)	10 (4%)	2 (1%)	16	17
1	H	239/250 (96%)	226 (95%)	8 (3%)	5 (2%)	5	4
1	I	239/250 (96%)	226 (95%)	10 (4%)	3 (1%)	9	8
1	J	239/250 (96%)	223 (93%)	14 (6%)	2 (1%)	16	17
All	All	2382/2500 (95%)	2244 (94%)	110 (5%)	28 (1%)	10	9

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	B	118	ALA
1	C	121	ALA
1	E	239	LYS
1	G	239	LYS
1	H	120	SER
1	H	125	VAL
1	E	203	GLY
1	E	244	GLU
1	H	121	ALA
1	I	119	GLU
1	C	239	LYS
1	I	121	ALA
1	B	239	LYS

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Mol	Chain	Res	Type
1	D	121	ALA
1	G	32	SER
1	A	239	LYS
1	B	124	THR
1	D	239	LYS
1	H	124	THR
1	H	243	GLU
1	J	106	GLN
1	I	125	VAL
1	D	184	GLY
1	E	125	VAL
1	C	125	VAL
1	J	125	VAL
1	F	125	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%)	189 (91%)	19 (9%)	9	9
1	B	207/215 (96%)	188 (91%)	19 (9%)	8	9
1	C	207/215 (96%)	187 (90%)	20 (10%)	8	7
1	D	208/215 (97%)	187 (90%)	21 (10%)	7	6
1	E	208/215 (97%)	191 (92%)	17 (8%)	10	11
1	F	208/215 (97%)	192 (92%)	16 (8%)	12	13
1	G	208/215 (97%)	190 (91%)	18 (9%)	9	10
1	H	208/215 (97%)	190 (91%)	18 (9%)	9	10
1	I	208/215 (97%)	187 (90%)	21 (10%)	7	6
1	J	208/215 (97%)	192 (92%)	16 (8%)	12	13
All	All	2078/2150 (97%)	1893 (91%)	185 (9%)	9	10

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

Mol	Chain	Res	Type
1	A	8	ILE
1	A	28	ASP
1	A	59	ARG
1	A	74	LEU
1	A	106	GLN
1	A	120	SER
1	A	122	THR
1	A	124	THR
1	A	125	VAL
1	A	147	LEU
1	A	161	LEU
1	A	162	LYS
1	A	167	LEU
1	A	193	GLU
1	A	200	MET
1	A	204	GLN
1	A	206	ARG
1	A	220	ARG
1	A	231	ARG
1	B	5	ILE
1	B	16	GLU
1	B	24	ILE
1	B	28	ASP
1	B	59	ARG
1	B	62	GLU
1	B	66	ARG
1	B	74	LEU
1	B	119	GLU
1	B	120	SER
1	B	125	VAL
1	B	147	LEU
1	B	161	LEU
1	B	167	LEU
1	B	168	LYS
1	B	206	ARG
1	B	208	LEU
1	B	225	GLU
1	B	239	LYS
1	C	59	ARG
1	C	74	LEU
1	C	91	ARG
1	C	119	GLU
1	C	122	THR

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Mol	Chain	Res	Type
1	C	124	THR
1	C	126	ARG
1	C	147	LEU
1	C	158	VAL
1	C	161	LEU
1	C	167	LEU
1	C	168	LYS
1	C	195	GLN
1	C	199	ARG
1	C	201	GLU
1	C	208	LEU
1	C	235	GLU
1	C	239	LYS
1	C	243	GLU
1	C	244	GLU
1	D	8	ILE
1	D	11	ARG
1	D	24	ILE
1	D	28	ASP
1	D	59	ARG
1	D	62	GLU
1	D	74	LEU
1	D	91	ARG
1	D	106	GLN
1	D	111	ARG
1	D	120	SER
1	D	122	THR
1	D	140	MET
1	D	147	LEU
1	D	168	LYS
1	D	193	GLU
1	D	199	ARG
1	D	206	ARG
1	D	208	LEU
1	D	228	ARG
1	D	244	GLU
1	E	11	ARG
1	E	16	GLU
1	E	59	ARG
1	E	62	GLU
1	E	74	LEU
1	E	79	VAL

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Mol	Chain	Res	Type
1	E	91	ARG
1	E	122	THR
1	E	125	VAL
1	E	145	MET
1	E	147	LEU
1	E	161	LEU
1	E	167	LEU
1	E	168	LYS
1	E	193	GLU
1	E	208	LEU
1	E	225	GLU
1	F	5	ILE
1	F	10	GLU
1	F	59	ARG
1	F	74	LEU
1	F	119	GLU
1	F	124	THR
1	F	125	VAL
1	F	126	ARG
1	F	145	MET
1	F	147	LEU
1	F	161	LEU
1	F	167	LEU
1	F	188	PRO
1	F	193	GLU
1	F	206	ARG
1	F	208	LEU
1	G	8	ILE
1	G	16	GLU
1	G	59	ARG
1	G	62	GLU
1	G	77	ASP
1	G	119	GLU
1	G	122	THR
1	G	125	VAL
1	G	147	LEU
1	G	162	LYS
1	G	167	LEU
1	G	179	GLU
1	G	183	GLU
1	G	193	GLU
1	G	206	ARG

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Mol	Chain	Res	Type
1	G	225	GLU
1	G	235	GLU
1	G	244	GLU
1	H	59	ARG
1	H	62	GLU
1	H	74	LEU
1	H	96	ARG
1	H	106	GLN
1	H	119	GLU
1	H	122	THR
1	H	124	THR
1	H	145	MET
1	H	147	LEU
1	H	158	VAL
1	H	161	LEU
1	H	167	LEU
1	H	193	GLU
1	H	199	ARG
1	H	206	ARG
1	H	208	LEU
1	H	227	ARG
1	I	28	ASP
1	I	59	ARG
1	I	62	GLU
1	I	74	LEU
1	I	106	GLN
1	I	120	SER
1	I	122	THR
1	I	124	THR
1	I	145	MET
1	I	147	LEU
1	I	158	VAL
1	I	161	LEU
1	I	167	LEU
1	I	168	LYS
1	I	193	GLU
1	I	199	ARG
1	I	206	ARG
1	I	208	LEU
1	I	228	ARG
1	I	231	ARG
1	I	244	GLU

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Mol	Chain	Res	Type
1	J	11	ARG
1	J	59	ARG
1	J	66	ARG
1	J	74	LEU
1	J	91	ARG
1	J	122	THR
1	J	124	THR
1	J	125	VAL
1	J	147	LEU
1	J	161	LEU
1	J	167	LEU
1	J	179	GLU
1	J	183	GLU
1	J	193	GLU
1	J	206	ARG
1	J	239	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	J	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	OCS	B	50	1	6,8,9	2.57	2 (33%)	7,11,13	2.32	2 (28%)
1	OCS	J	50	1	6,8,9	2.37	1 (16%)	7,11,13	1.96	2 (28%)
1	OCS	G	50	1	6,8,9	2.42	3 (50%)	7,11,13	1.48	2 (28%)
1	OCS	H	50	1	6,8,9	1.47	1 (16%)	7,11,13	1.66	3 (42%)
1	OCS	I	50	1	6,8,9	2.19	1 (16%)	7,11,13	1.48	2 (28%)
1	OCS	C	50	1	6,8,9	2.36	2 (33%)	7,11,13	2.31	3 (42%)
1	OCS	E	50	1	6,8,9	2.42	2 (33%)	7,11,13	1.93	3 (42%)
1	OCS	A	50	1	6,8,9	2.30	2 (33%)	7,11,13	0.83	0
1	OCS	F	50	1	6,8,9	2.61	2 (33%)	7,11,13	1.78	1 (14%)
1	OCS	D	50	1	6,8,9	2.33	2 (33%)	7,11,13	1.65	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	B	50	1	-	0/4/7/9	-
1	OCS	J	50	1	-	0/4/7/9	-
1	OCS	G	50	1	-	0/4/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	H	50	1	-	0/4/7/9	-
1	OCS	I	50	1	-	0/4/7/9	-
1	OCS	C	50	1	-	0/4/7/9	-
1	OCS	E	50	1	-	0/4/7/9	-
1	OCS	A	50	1	-	0/4/7/9	-
1	OCS	F	50	1	-	0/4/7/9	-
1	OCS	D	50	1	-	0/4/7/9	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	50	OCS	O-C	5.50	1.40	1.20
1	D	50	OCS	O-C	4.96	1.38	1.20
1	A	50	OCS	O-C	4.92	1.38	1.20
1	I	50	OCS	O-C	4.92	1.38	1.20
1	C	50	OCS	O-C	4.75	1.38	1.20
1	F	50	OCS	O-C	4.75	1.38	1.20
1	G	50	OCS	O-C	4.75	1.38	1.20
1	E	50	OCS	O-C	4.74	1.38	1.20
1	B	50	OCS	O-C	4.36	1.36	1.20
1	B	50	OCS	CB-CA	3.75	1.56	1.53
1	F	50	OCS	CB-CA	3.69	1.56	1.53
1	H	50	OCS	O-C	3.23	1.32	1.20
1	G	50	OCS	CB-CA	2.72	1.55	1.53
1	E	50	OCS	CB-CA	2.59	1.55	1.53
1	A	50	OCS	OD3-SG	2.45	1.52	1.45
1	D	50	OCS	OD3-SG	2.34	1.51	1.45
1	C	50	OCS	OD3-SG	2.24	1.51	1.45
1	G	50	OCS	OD3-SG	2.07	1.51	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	OCS	OD1-SG-CB	4.83	113.97	106.76
1	C	50	OCS	OD3-SG-CB	4.76	113.87	106.76
1	F	50	OCS	OD2-SG-CB	4.12	113.92	105.97
1	J	50	OCS	OD2-SG-CB	3.17	112.09	105.97
1	D	50	OCS	OD2-SG-CB	3.04	111.84	105.97
1	E	50	OCS	OD2-SG-CB	2.74	111.27	105.97
1	B	50	OCS	OD3-SG-OD1	-2.71	104.99	113.82
1	J	50	OCS	OD1-SG-CB	-2.59	102.89	106.76
1	G	50	OCS	OD2-SG-CB	2.58	110.95	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	50	OCS	OD3-SG-OD1	-2.38	106.08	113.82
1	H	50	OCS	OD1-SG-CB	2.31	110.21	106.76
1	E	50	OCS	OD3-SG-OD1	-2.27	106.44	113.82
1	I	50	OCS	OD2-SG-OD1	2.24	117.00	111.40
1	H	50	OCS	OD3-SG-OD1	-2.22	106.61	113.82
1	H	50	OCS	OD2-SG-CB	2.21	110.24	105.97
1	E	50	OCS	OD3-SG-CB	2.21	110.05	106.76
1	D	50	OCS	OD3-SG-OD1	-2.20	106.67	113.82
1	C	50	OCS	OD2-SG-CB	2.17	110.17	105.97
1	G	50	OCS	OD1-SG-CB	-2.01	103.76	106.76
1	C	50	OCS	OD2-SG-OD3	-2.00	106.39	111.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	50	OCS	2	0
1	J	50	OCS	1	0
1	G	50	OCS	1	0
1	H	50	OCS	1	0
1	C	50	OCS	2	0
1	E	50	OCS	2	0
1	A	50	OCS	1	0
1	F	50	OCS	1	0
1	D	50	OCS	1	0

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 ⓘ

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	241/250 (96%)	-0.25	5 (2%) 63 68	19, 30, 60, 79	0
1	B	239/250 (95%)	-0.28	5 (2%) 63 68	21, 31, 59, 79	0
1	C	239/250 (95%)	-0.21	7 (2%) 53 60	22, 33, 61, 74	0
1	D	241/250 (96%)	-0.04	5 (2%) 63 68	25, 38, 63, 79	0
1	E	241/250 (96%)	-0.27	4 (1%) 69 74	19, 33, 62, 78	0
1	F	241/250 (96%)	-0.36	6 (2%) 58 64	20, 29, 57, 72	0
1	G	241/250 (96%)	-0.37	2 (0%) 82 86	18, 28, 54, 73	0
1	H	241/250 (96%)	-0.40	6 (2%) 58 64	19, 28, 59, 78	0
1	I	241/250 (96%)	-0.28	9 (3%) 45 51	20, 31, 63, 83	0
1	J	241/250 (96%)	-0.27	5 (2%) 63 68	22, 32, 59, 76	0
All	All	2406/2500 (96%)	-0.27	54 (2%) 62 67	18, 32, 61, 83	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	245	ALA	5.2
1	A	121	ALA	5.0
1	I	121	ALA	4.9
1	D	245	ALA	4.6
1	B	245	ALA	4.4
1	G	245	ALA	4.1
1	J	122	THR	4.1
1	I	118	ALA	3.8
1	J	245	ALA	3.6
1	E	245	ALA	3.6
1	C	245	ALA	3.5
1	H	121	ALA	3.5
1	D	118	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	121	ALA	3.1
1	E	4	SER	3.0
1	I	120	SER	3.0
1	C	121	ALA	2.9
1	H	118	ALA	2.9
1	A	245	ALA	2.8
1	I	117	HIS	2.8
1	D	121	ALA	2.8
1	F	118	ALA	2.8
1	H	245	ALA	2.8
1	A	118	ALA	2.7
1	F	245	ALA	2.7
1	I	4	SER	2.7
1	B	116	LEU	2.7
1	B	117	HIS	2.6
1	F	121	ALA	2.6
1	J	120	SER	2.6
1	C	124	THR	2.6
1	H	120	SER	2.5
1	C	116	LEU	2.5
1	B	120	SER	2.5
1	A	122	THR	2.4
1	C	242	TYR	2.4
1	B	123	HIS	2.4
1	F	5	ILE	2.4
1	H	122	THR	2.4
1	E	117	HIS	2.3
1	I	242	TYR	2.3
1	J	118	ALA	2.3
1	H	242	TYR	2.3
1	A	117	HIS	2.2
1	E	122	THR	2.2
1	F	120	SER	2.2
1	C	5	ILE	2.1
1	D	4	SER	2.1
1	D	5	ILE	2.1
1	C	120	SER	2.1
1	F	238	ALA	2.1
1	G	242	TYR	2.0
1	I	243	GLU	2.0
1	I	5	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OCS	F	50	9/10	0.96	0.07	25,27,33,34	0
1	OCS	C	50	9/10	0.97	0.07	26,27,33,33	0
1	OCS	D	50	9/10	0.97	0.07	28,30,36,41	0
1	OCS	E	50	9/10	0.97	0.07	27,28,38,38	0
1	OCS	B	50	9/10	0.97	0.07	23,24,33,33	0
1	OCS	G	50	9/10	0.97	0.06	23,25,29,31	0
1	OCS	H	50	9/10	0.97	0.06	20,21,31,31	0
1	OCS	J	50	9/10	0.97	0.07	27,29,35,35	0
1	OCS	I	50	9/10	0.98	0.06	25,26,33,34	0
1	OCS	A	50	9/10	0.98	0.06	26,28,35,35	0

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.