



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:48 AM UTC

PDB ID : 1FBX / pdb_00001fbx
Title : CRYSTAL STRUCTURE OF ZINC-CONTAINING E.COLI GTP CYCLO-HYDROLASE I
Authors : Auerbach, G.; Herrmann, A.; Bracher, A.; Bader, A.; Gutlich, M.; Fischer, M.; Neukamm, M.; Nar, H.; Garrido-Franco, M.; Richardson, J.; Huber, R.; Bacher, A.
Deposited on : 2000-07-17
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

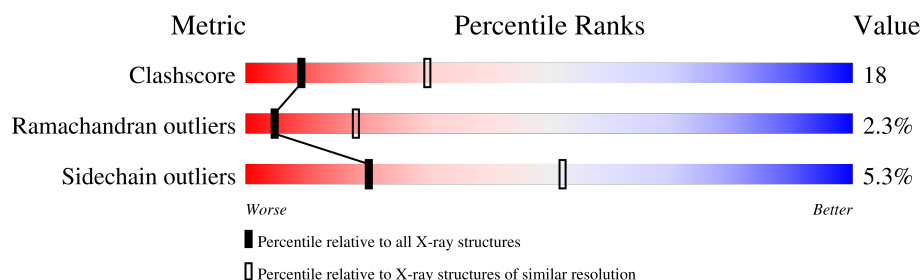
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	
1	F	221	
1	G	221	
1	H	221	

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Mol	Chain	Length	Quality of chain
1	I	221	
1	J	221	
1	K	221	
1	L	221	
1	M	221	
1	N	221	
1	O	221	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	3350	-	-	X	-
3	CL	F	3355	-	-	X	-
3	CL	J	3354	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26025 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 GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	B	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	C	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	D	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	E	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	F	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	G	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	H	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	I	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	J	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	K	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	L	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	M	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	N	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	O	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0
2	M	1	Total Zn 1 1	0	0
2	N	1	Total Zn 1 1	0	0
2	O	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0
3	M	1	Total Cl 1 1	0	0
3	N	1	Total Cl 1 1	0	0
3	O	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0
4	I	1	Total O 1 1	0	0

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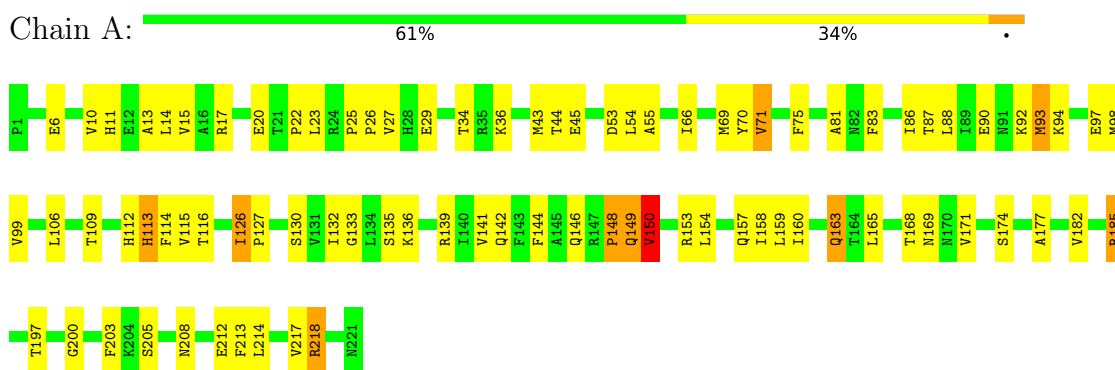
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total 1	O 1	0	0
4	K	1	Total 1	O 1	0	0
4	L	1	Total 1	O 1	0	0
4	M	1	Total 1	O 1	0	0
4	N	1	Total 1	O 1	0	0
4	O	1	Total 1	O 1	0	0

3 Residue-property plots

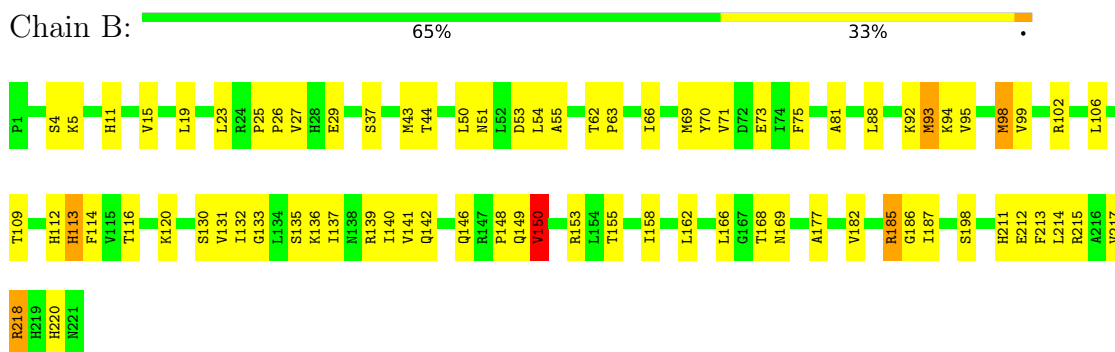
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

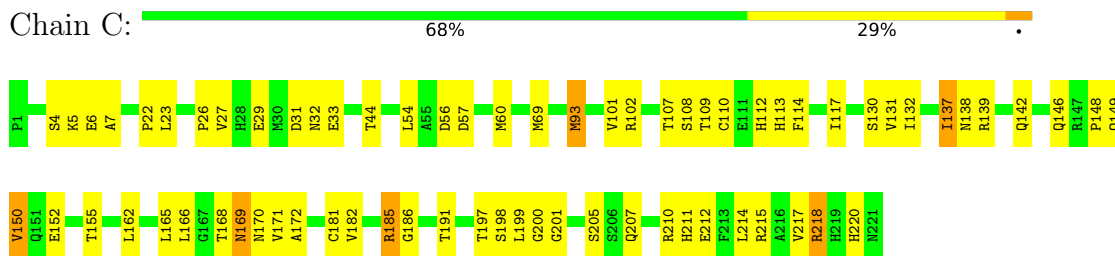
• Molecule 1: GTP CYCLOHYDROLASE I



• Molecule 1: GTP CYCLOHYDROLASE I

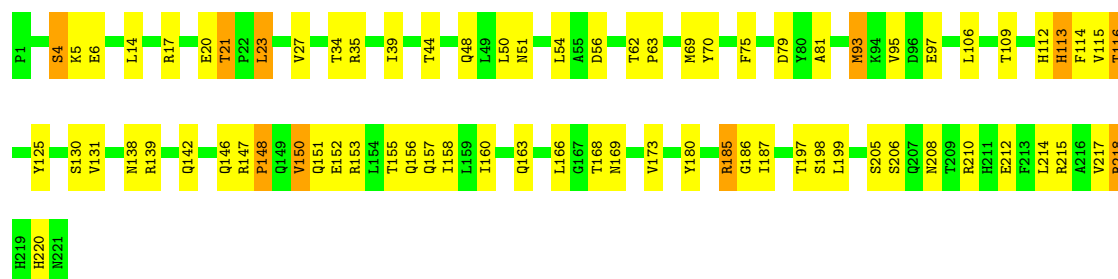


• Molecule 1: GTP CYCLOHYDROLASE I



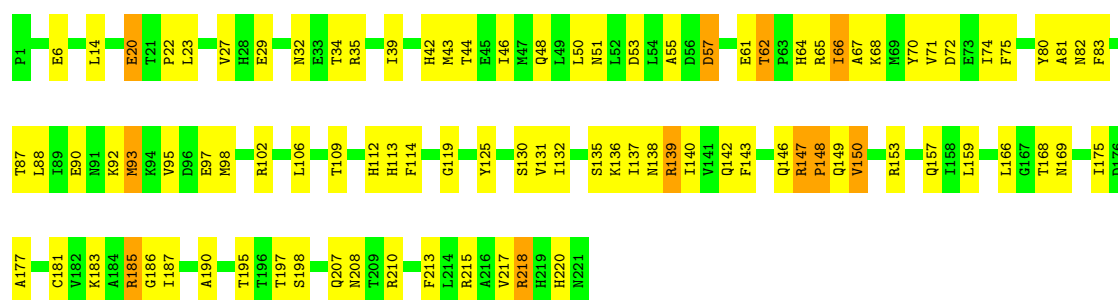
• Molecule 1: GTP CYCLOHYDROLASE I

Chain D:  66% 29% 5%



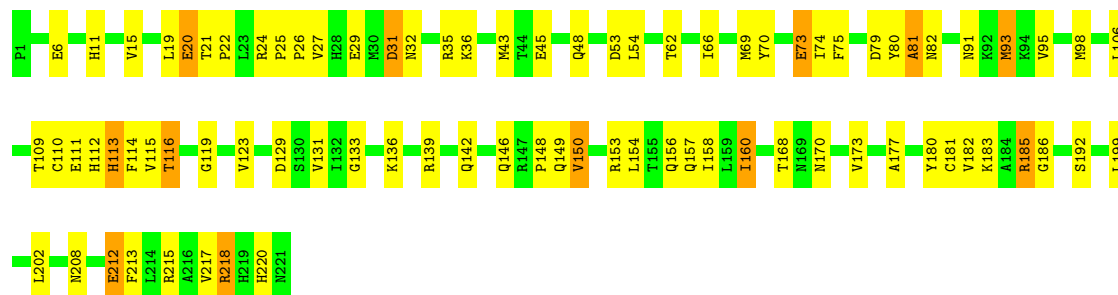
• Molecule 1: GTP CYCLOHYDROLASE I

Chain E:  57% 38% 5%



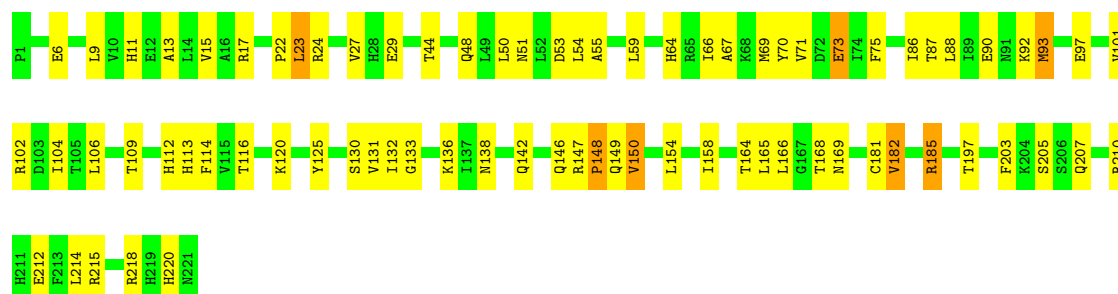
• Molecule 1: GTP CYCLOHYDROLASE I

Chain F:  62% 32% 5%



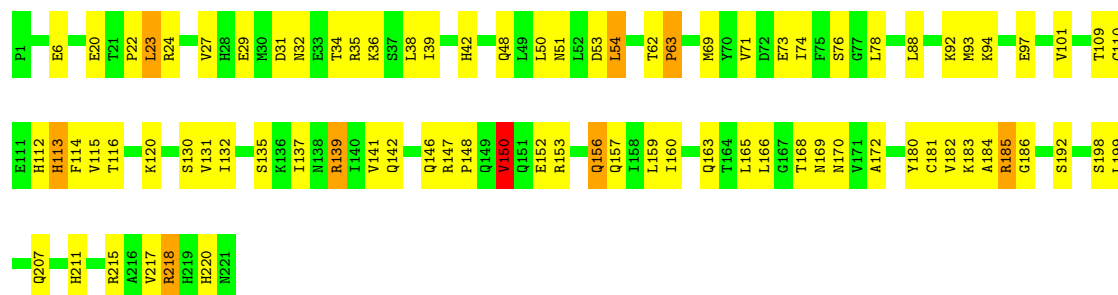
• Molecule 1: GTP CYCLOHYDROLASE I

Chain G:  65% 32% 3%



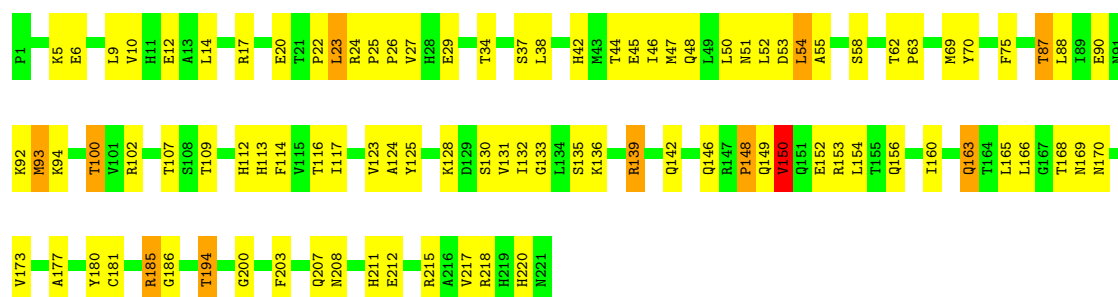
• Molecule 1: GTP CYCLOHYDROLASE I

Chain H:  62% 33%



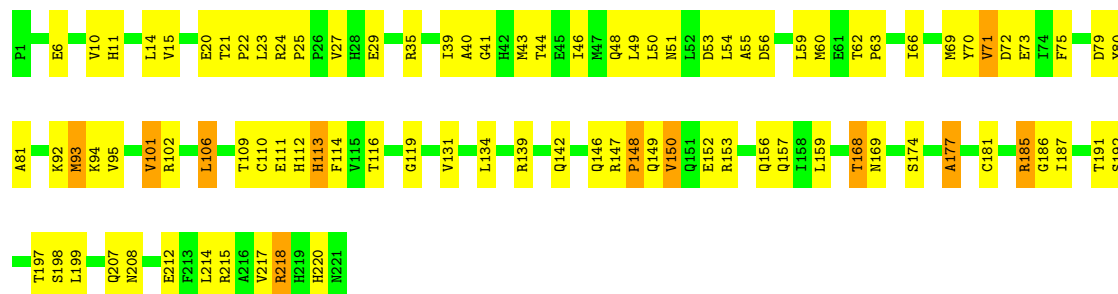
• Molecule 1: GTP CYCLOHYDROLASE I

Chain I:  57% 38% 5%



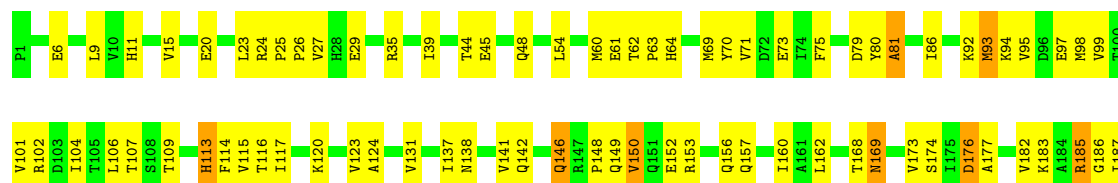
• Molecule 1: GTP CYCLOHYDROLASE I

Chain J:  58% 37% 5%



• Molecule 1: GTP CYCLOHYDROLASE I

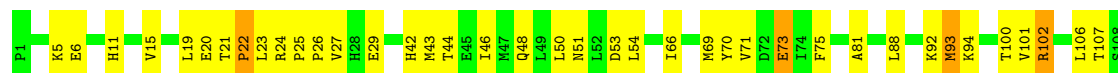
Chain K:  60% 36% 5%





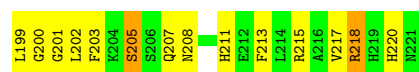
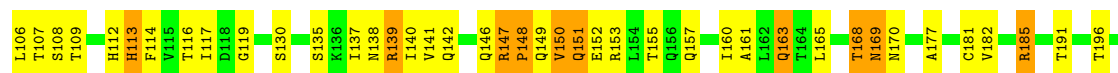
• Molecule 1: GTP CYCLOHYDROLASE I

Chain L: 58% 37% 5%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain M: 57% 36% 7%



• Molecule 1: GTP CYCLOHYDROLASE I

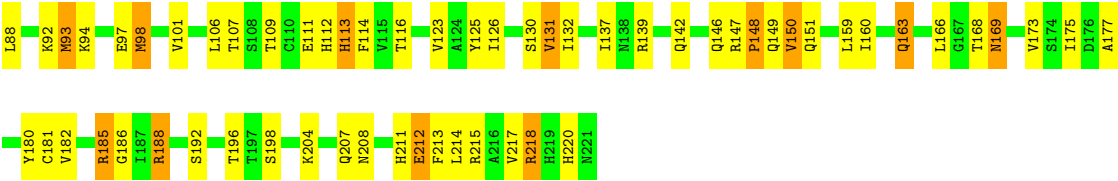
Chain N: 55% 40% 5%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain O: 55% 37% 8%





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	227.69Å 314.19Å 132.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.80	Depositor
% Data completeness (in resolution range)	91.2 (14.98-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26025	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.73	1/1760 (0.1%)	1.20	18/2384 (0.8%)
1	B	0.76	1/1760 (0.1%)	1.16	14/2384 (0.6%)
1	C	0.79	1/1760 (0.1%)	1.17	14/2384 (0.6%)
1	D	0.77	1/1760 (0.1%)	1.14	11/2384 (0.5%)
1	E	0.65	0/1760	1.18	13/2384 (0.5%)
1	F	0.69	0/1760	1.13	14/2384 (0.6%)
1	G	0.61	0/1760	1.08	13/2384 (0.5%)
1	H	0.69	0/1760	1.15	12/2384 (0.5%)
1	I	0.62	0/1760	1.05	7/2384 (0.3%)
1	J	0.65	0/1760	1.12	15/2384 (0.6%)
1	K	0.67	0/1760	1.13	12/2384 (0.5%)
1	L	0.59	0/1760	1.04	10/2384 (0.4%)
1	M	0.66	0/1760	1.18	20/2384 (0.8%)
1	N	0.60	0/1760	1.10	10/2384 (0.4%)
1	O	0.61	1/1760 (0.1%)	1.08	14/2384 (0.6%)
All	All	0.68	5/26400 (0.0%)	1.13	197/35760 (0.6%)

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	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	MET	SD-CE	-5.89	1.64	1.79
1	C	69	MET	SD-CE	-5.46	1.66	1.79
1	D	69	MET	SD-CE	-5.36	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	MET	SD-CE	-5.35	1.66	1.79
1	O	69	MET	SD-CE	-5.21	1.66	1.79

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	147	ARG	CA-C-N	-9.41	110.02	119.90
1	M	147	ARG	C-N-CA	-9.41	110.02	119.90
1	O	73	GLU	N-CA-C	9.25	123.75	108.48
1	H	150	VAL	N-CA-C	-9.25	94.80	108.12
1	K	150	VAL	N-CA-C	-9.21	94.86	108.12
1	B	182	VAL	N-CA-C	-9.09	104.53	111.90
1	M	182	VAL	N-CA-C	-8.96	104.00	112.96
1	A	182	VAL	CB-CA-C	-8.92	103.21	111.06
1	B	150	VAL	N-CA-C	-8.88	94.63	107.77
1	C	182	VAL	N-CA-C	-8.86	104.72	111.90
1	I	150	VAL	N-CA-C	-8.64	95.67	108.12
1	C	150	VAL	N-CA-C	-8.64	95.68	108.12
1	J	71	VAL	N-CA-C	8.55	119.11	110.82
1	M	116	THR	N-CA-C	8.52	122.28	110.35
1	N	182	VAL	N-CA-C	-8.52	104.97	112.12
1	J	150	VAL	N-CA-C	-8.43	95.29	107.77
1	H	148	PRO	N-CA-C	-8.32	98.23	110.80
1	H	71	VAL	N-CA-C	8.20	118.29	110.42
1	M	169	ASN	N-CA-C	-8.17	103.10	113.72
1	N	149	GLN	N-CA-C	8.14	121.41	109.69
1	G	149	GLN	N-CA-C	8.10	121.72	109.41
1	E	81	ALA	N-CA-C	-7.78	102.88	112.38
1	N	71	VAL	N-CA-C	7.77	117.83	110.53
1	H	169	ASN	N-CA-C	-7.76	103.39	113.17
1	F	150	VAL	N-CA-C	-7.75	96.29	107.77
1	D	205	SER	N-CA-C	7.71	119.47	111.14
1	G	182	VAL	N-CA-C	-7.65	105.09	113.43
1	L	73	GLU	N-CA-C	7.64	120.27	108.12
1	O	169	ASN	N-CA-C	-7.60	104.15	113.50
1	O	149	GLN	N-CA-C	7.59	119.96	109.18
1	A	205	SER	N-CA-C	7.56	119.31	111.14
1	H	182	VAL	N-CA-C	-7.54	105.79	111.90
1	D	148	PRO	N-CA-C	-7.53	99.44	111.03
1	A	81	ALA	N-CA-C	-7.45	104.07	113.01
1	N	81	ALA	N-CA-C	-7.37	103.24	111.71
1	M	150	VAL	N-CA-C	-7.17	97.10	107.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	148	PRO	N-CA-C	-7.17	100.00	111.03
1	E	97	GLU	N-CA-C	-7.13	99.66	110.14
1	A	169	ASN	N-CA-C	-7.13	104.61	113.38
1	K	60	MET	N-CA-C	7.08	118.68	110.97
1	O	177	ALA	N-CA-C	7.08	119.50	108.96
1	C	117	ILE	N-CA-C	-6.99	98.33	108.11
1	G	150	VAL	N-CA-C	-6.99	97.43	107.77
1	F	133	GLY	N-CA-C	-6.97	103.20	111.36
1	A	150	VAL	N-CA-C	-6.92	97.47	107.78
1	E	150	VAL	N-CA-C	-6.85	97.64	107.77
1	H	192	SER	N-CA-C	6.83	120.13	110.50
1	A	182	VAL	N-CA-C	-6.80	106.16	112.96
1	E	149	GLN	N-CA-C	6.77	119.70	109.41
1	A	177	ALA	N-CA-C	6.72	118.97	108.96
1	K	169	ASN	N-CA-C	-6.66	103.36	113.89
1	O	81	ALA	N-CA-C	-6.66	105.27	113.19
1	B	116	THR	N-CA-C	6.62	119.98	110.24
1	C	148	PRO	N-CA-C	-6.61	100.84	111.03
1	A	149	GLN	N-CA-C	6.57	119.14	109.69
1	J	116	THR	N-CA-C	6.52	119.69	110.23
1	M	191	THR	N-CA-C	6.52	121.64	113.43
1	B	177	ALA	N-CA-C	6.46	119.00	109.24
1	O	150	VAL	N-CA-C	-6.42	98.22	107.78
1	E	181	CYS	N-CA-C	-6.35	105.53	113.28
1	M	71	VAL	N-CA-C	6.34	116.97	110.82
1	L	181	CYS	N-CA-C	-6.34	105.51	113.18
1	J	191	THR	N-CA-C	6.31	121.26	113.50
1	M	181	CYS	N-CA-C	-6.29	105.36	113.16
1	O	181	CYS	N-CA-C	-6.28	105.67	113.15
1	K	212	GLU	N-CA-C	-6.28	104.49	111.71
1	B	73	GLU	N-CA-C	6.27	118.83	108.48
1	E	62	THR	N-CA-C	6.26	121.27	112.75
1	L	81	ALA	N-CA-C	-6.26	105.60	113.18
1	N	150	VAL	N-CA-C	-6.26	98.45	107.78
1	E	169	ASN	N-CA-C	-6.26	105.64	113.28
1	F	199	LEU	N-CA-C	6.25	118.71	108.52
1	O	126	ILE	N-CA-C	-6.24	100.92	107.60
1	K	192	SER	N-CA-C	6.20	118.55	110.43
1	F	116	THR	N-CA-C	6.17	119.29	110.10
1	J	169	ASN	N-CA-C	-6.17	105.58	113.23
1	B	81	ALA	N-CA-C	-6.13	105.65	113.01
1	B	71	VAL	N-CA-C	6.12	116.90	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	PRO	N-CA-C	-6.12	100.89	110.50
1	K	148	PRO	N-CA-C	-6.12	100.58	110.55
1	K	149	GLN	N-CA-C	6.11	118.70	109.41
1	J	177	ALA	N-CA-C	6.11	118.06	108.96
1	D	151	GLN	N-CA-C	6.08	118.69	111.33
1	G	66	ILE	N-CA-C	-6.08	104.42	110.62
1	G	116	THR	N-CA-C	6.07	118.80	110.24
1	H	181	CYS	N-CA-C	-6.06	105.87	113.20
1	C	101	VAL	N-CA-C	-6.02	99.07	107.80
1	B	137	ILE	N-CA-C	-6.02	104.64	110.42
1	F	81	ALA	N-CA-C	-6.01	105.80	113.01
1	D	150	VAL	N-CA-C	-5.97	99.52	108.12
1	M	78	LEU	N-CA-C	-5.97	106.00	113.28
1	F	181	CYS	N-CA-C	-5.96	106.35	113.21
1	C	32	ASN	N-CA-C	5.96	118.56	111.71
1	G	148	PRO	N-CA-C	-5.96	101.86	111.03
1	L	71	VAL	N-CA-C	5.94	117.88	111.58
1	I	181	CYS	N-CA-C	-5.92	105.82	113.16
1	M	149	GLN	N-CA-C	5.91	118.40	109.41
1	A	148	PRO	N-CA-C	-5.90	100.32	112.47
1	F	62	THR	CA-C-N	-5.89	112.80	119.28
1	F	62	THR	C-N-CA	-5.89	112.80	119.28
1	D	81	ALA	N-CA-C	-5.86	105.39	112.54
1	J	147	ARG	CA-C-N	-5.85	113.03	120.23
1	J	147	ARG	C-N-CA	-5.85	113.03	120.23
1	M	73	GLU	N-CA-C	5.84	123.24	110.80
1	C	205	SER	N-CA-C	5.83	117.31	111.07
1	N	116	THR	N-CA-C	5.83	118.69	110.23
1	I	148	PRO	N-CA-C	-5.81	100.50	112.47
1	K	81	ALA	N-CA-C	-5.80	106.18	113.20
1	L	116	THR	N-CA-C	5.79	118.76	110.24
1	A	133	GLY	N-CA-C	-5.79	105.27	111.93
1	K	182	VAL	N-CA-C	-5.79	107.17	112.96
1	O	148	PRO	N-CA-C	-5.79	102.06	110.80
1	H	116	THR	N-CA-C	5.79	118.75	110.24
1	M	81	ALA	N-CA-C	-5.78	105.49	112.54
1	C	182	VAL	CB-CA-C	-5.76	105.77	111.30
1	M	148	PRO	N-CA-C	-5.76	102.11	110.80
1	G	169	ASN	N-CA-C	-5.75	106.42	113.50
1	A	116	THR	N-CA-C	5.74	118.33	110.24
1	I	117	ILE	N-CA-C	-5.74	100.07	108.11
1	F	73	GLU	N-CA-C	5.72	117.23	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	149	GLN	N-CA-C	5.72	118.56	109.81
1	N	169	ASN	N-CA-C	-5.72	106.31	113.28
1	E	147	ARG	CA-C-N	-5.71	113.66	119.83
1	E	147	ARG	C-N-CA	-5.71	113.66	119.83
1	C	149	GLN	N-CA-C	5.69	118.06	109.41
1	F	74	ILE	N-CA-C	5.69	119.02	111.17
1	L	149	GLN	N-CA-C	5.69	118.95	109.96
1	G	71	VAL	N-CA-C	5.67	116.73	111.45
1	O	188	ARG	N-CA-C	5.66	119.24	111.54
1	N	39	ILE	N-CA-C	-5.66	105.58	111.58
1	E	71	VAL	N-CA-C	5.66	116.31	110.82
1	M	205	SER	N-CA-C	5.66	118.30	111.40
1	C	169	ASN	N-CA-C	-5.64	106.40	113.28
1	H	147	ARG	CA-C-N	-5.63	113.99	119.90
1	H	147	ARG	C-N-CA	-5.63	113.99	119.90
1	J	192	SER	N-CA-C	5.62	118.14	110.55
1	C	181	CYS	N-CA-C	-5.59	106.44	113.20
1	F	149	GLN	N-CA-C	5.59	118.36	109.81
1	D	17	ARG	N-CA-C	-5.57	106.25	113.16
1	G	181	CYS	N-CA-C	-5.57	106.25	113.16
1	J	148	PRO	N-CA-C	-5.56	101.77	110.50
1	D	116	THR	N-CA-C	5.51	118.21	110.23
1	C	33	GLU	N-CA-C	-5.49	105.45	111.82
1	B	99	VAL	N-CA-C	-5.48	100.55	108.71
1	M	151	GLN	N-CA-C	5.46	117.94	111.33
1	L	148	PRO	N-CA-C	-5.45	101.24	112.47
1	A	99	VAL	N-CA-C	-5.42	100.59	108.17
1	M	74	ILE	N-CA-C	5.40	119.67	111.89
1	E	74	ILE	N-CA-C	5.39	119.66	111.89
1	J	168	THR	CB-CA-C	-5.38	100.31	110.16
1	L	177	ALA	N-CA-C	5.38	116.98	108.96
1	E	66	ILE	N-CA-C	-5.38	104.36	111.09
1	I	177	ALA	N-CA-C	5.38	116.98	108.96
1	B	169	ASN	N-CA-C	-5.38	106.09	113.30
1	G	203	PHE	N-CA-C	-5.37	106.23	112.89
1	D	212	GLU	N-CA-C	-5.35	105.45	111.28
1	N	151	GLN	N-CA-C	5.35	117.81	111.33
1	B	182	VAL	CB-CA-C	-5.34	106.17	111.30
1	B	149	GLN	N-CA-C	5.33	117.97	109.81
1	G	133	GLY	N-CA-C	-5.33	105.80	111.93
1	D	206	SER	N-CA-C	5.32	117.38	108.23
1	O	147	ARG	CA-C-N	-5.31	114.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	147	ARG	C-N-CA	-5.31	114.33	119.90
1	K	101	VAL	N-CA-C	-5.30	100.01	107.75
1	L	102	ARG	N-CA-C	5.30	118.36	110.14
1	B	98	MET	N-CA-C	5.30	117.71	110.24
1	A	126	ILE	CA-C-N	5.30	125.60	119.93
1	A	126	ILE	C-N-CA	5.30	125.60	119.93
1	N	78	LEU	N-CA-C	-5.28	106.79	113.18
1	O	212	GLU	N-CA-C	-5.28	105.61	111.36
1	F	160	ILE	CB-CA-C	-5.27	105.14	111.88
1	K	177	ALA	N-CA-C	5.25	117.16	109.24
1	J	181	CYS	N-CA-C	-5.23	106.68	113.16
1	I	149	GLN	N-CA-C	5.22	117.47	109.95
1	C	191	THR	N-CA-C	5.21	121.03	114.31
1	I	116	THR	N-CA-C	5.18	117.54	110.24
1	G	205	SER	N-CA-C	5.16	119.67	112.90
1	J	199	LEU	N-CA-C	5.16	117.21	108.02
1	A	163	GLN	N-CA-C	-5.15	105.56	111.07
1	M	199	LEU	N-CA-C	5.14	117.10	108.73
1	A	71	VAL	N-CA-C	5.13	115.36	110.53
1	G	73	GLU	N-CA-C	5.13	121.73	110.80
1	C	137	ILE	N-CA-C	-5.12	105.60	110.42
1	M	140	ILE	N-CA-C	-5.11	105.61	110.42
1	A	34	THR	N-CA-C	-5.11	105.60	111.07
1	F	212	GLU	N-CA-C	-5.10	105.72	111.28
1	K	71	VAL	N-CA-C	5.10	116.56	111.00
1	D	34	THR	N-CA-C	-5.09	105.64	111.14
1	D	56	ASP	N-CA-C	5.09	117.61	110.23
1	O	98	MET	N-CA-C	5.08	117.23	110.53
1	H	101	VAL	N-CA-C	-5.07	100.58	107.99
1	A	45	GLU	N-CA-C	-5.05	105.47	110.97
1	L	130	SER	N-CA-C	5.05	117.63	109.40
1	J	101	VAL	N-CA-C	-5.03	100.40	107.75
1	H	156	GLN	N-CA-C	5.02	118.18	111.75
1	M	165	LEU	N-CA-C	5.01	117.40	111.33
1	F	148	PRO	N-CA-C	-5.01	102.16	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	180	TYR	Sidechain

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	1732	0	1766	56	0
1	B	1732	0	1766	49	0
1	C	1732	0	1766	42	0
1	D	1732	0	1766	43	0
1	E	1732	0	1766	60	0
1	F	1732	0	1766	76	0
1	G	1732	0	1766	69	0
1	H	1732	0	1766	68	0
1	I	1732	0	1766	88	0
1	J	1732	0	1766	98	0
1	K	1732	0	1766	75	0
1	L	1732	0	1766	79	0
1	M	1732	0	1766	84	0
1	N	1732	0	1766	94	0
1	O	1732	0	1766	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
3	A	1	0	0	2	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
3	E	1	0	0	1	0
3	F	1	0	0	2	0
3	G	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	1	0
3	I	1	0	0	1	0
3	J	1	0	0	2	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	N	1	0	0	1	0
3	O	1	0	0	1	0
4	A	1	0	0	1	0
4	B	1	0	0	2	0
4	C	1	0	0	1	0
4	D	1	0	0	1	0
4	E	1	0	0	1	0
4	F	1	0	0	2	0
4	G	1	0	0	1	0
4	H	1	0	0	2	0
4	I	1	0	0	1	0
4	J	1	0	0	3	0
4	K	1	0	0	0	0
4	L	1	0	0	1	0
4	M	1	0	0	1	0
4	N	1	0	0	1	0
4	O	1	0	0	2	0
All	All	26025	0	26490	919	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 18.

All (919) 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:69:MET:HE2	1:N:185:ARG:HD2	1.27	1.14
1:C:168:THR:HG22	1:C:170:ASN:H	1.14	1.11
1:I:168:THR:HG22	1:I:170:ASN:H	1.22	1.04
1:F:185:ARG:HD2	1:M:69:MET:HE2	1.39	1.02
1:K:61:GLU:OE1	1:K:64:HIS:HD2	1.41	1.00
1:J:24:ARG:NH2	1:N:54:LEU:HB2	1.80	0.97
1:H:48:GLN:HG2	1:K:24:ARG:HH12	1.31	0.95
1:I:185:ARG:HG2	1:I:186:GLY:N	1.81	0.94
1:L:142:GLN:O	1:L:146:GLN:HG2	1.68	0.94
1:I:54:LEU:HB2	1:O:24:ARG:HH22	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:93:MET:HE1	1:L:131:VAL:HG21	1.51	0.92
1:G:54:LEU:HB2	1:L:24:ARG:NH2	1.85	0.91
1:F:168:THR:HG22	1:F:170:ASN:H	1.37	0.90
1:C:142:GLN:O	1:C:146:GLN:HG2	1.71	0.89
1:H:48:GLN:HG2	1:K:24:ARG:NH1	1.87	0.89
1:G:48:GLN:HE21	1:L:24:ARG:HH12	1.17	0.89
1:G:54:LEU:HB2	1:L:24:ARG:HH22	1.39	0.87
1:K:61:GLU:OE1	1:K:64:HIS:CD2	2.27	0.86
1:E:142:GLN:O	1:E:146:GLN:HG2	1.78	0.83
1:B:185:ARG:HH11	1:B:185:ARG:CG	1.90	0.82
1:C:93:MET:HE1	1:C:131:VAL:HG21	1.59	0.82
1:J:69:MET:CE	1:N:185:ARG:HD2	2.09	0.81
1:J:24:ARG:HH22	1:N:54:LEU:HB2	1.47	0.80
1:I:54:LEU:HB2	1:O:24:ARG:NH2	1.96	0.80
1:G:70:TYR:O	1:G:75:PHE:HB2	1.82	0.80
1:F:69:MET:HE2	1:M:185:ARG:HD2	1.62	0.80
1:O:11:HIS:O	1:O:15:VAL:HG23	1.82	0.80
1:F:48:GLN:HE21	1:M:24:ARG:HH12	1.29	0.79
1:K:92:LYS:O	1:K:94:LYS:HG3	1.83	0.79
1:N:11:HIS:O	1:N:15:VAL:HG23	1.83	0.78
1:B:141:VAL:HG22	1:B:158:ILE:HD13	1.64	0.78
1:N:6:GLU:CD	1:N:6:GLU:H	1.91	0.78
1:J:185:ARG:HD2	1:N:69:MET:HE2	1.65	0.78
1:J:142:GLN:O	1:J:146:GLN:HG2	1.83	0.78
1:C:214:LEU:HD13	1:D:215:ARG:HH22	1.47	0.77
1:E:159:LEU:HD22	1:E:198:SER:HB3	1.65	0.77
1:M:200:GLY:O	1:M:203:PHE:HB2	1.86	0.76
1:G:212:GLU:HG2	1:G:215:ARG:HH22	1.50	0.76
1:O:139:ARG:NH1	3:O:3359:CL:CL	2.55	0.76
1:L:187:ILE:HD12	1:M:139:ARG:HG2	1.68	0.75
1:F:98:MET:HE1	1:F:213:PHE:HA	1.69	0.75
1:B:185:ARG:NH1	1:B:185:ARG:HG2	2.01	0.75
1:D:35:ARG:O	1:D:39:ILE:HG13	1.86	0.74
1:I:93:MET:HE1	1:I:131:VAL:HG21	1.70	0.74
1:L:212:GLU:HA	1:L:215:ARG:NH1	2.02	0.74
1:H:69:MET:HE2	1:K:185:ARG:HD2	1.68	0.74
1:A:90:GLU:OE2	1:A:92:LYS:HG2	1.88	0.73
1:E:90:GLU:OE2	1:E:92:LYS:HG2	1.88	0.73
1:O:6:GLU:CD	1:O:6:GLU:H	1.96	0.73
1:I:70:TYR:O	1:I:75:PHE:HB2	1.88	0.73
1:N:142:GLN:O	1:N:146:GLN:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:21:THR:O	1:N:23:LEU:HD13	1.88	0.73
1:E:112:HIS:ND1	4:E:3335:HOH:O	2.21	0.73
1:M:153:ARG:O	1:M:157:GLN:HG3	1.89	0.73
1:G:185:ARG:HD2	1:L:69:MET:HE2	1.70	0.72
1:L:149:GLN:HE21	1:L:154:LEU:HD13	1.53	0.72
1:F:142:GLN:O	1:F:146:GLN:HG2	1.89	0.72
1:I:142:GLN:O	1:I:146:GLN:HG2	1.90	0.72
1:A:185:ARG:HH11	1:A:185:ARG:CG	2.03	0.72
1:A:92:LYS:O	1:A:94:LYS:HG3	1.89	0.71
1:D:163:GLN:HG2	1:D:169:ASN:HA	1.73	0.71
1:F:24:ARG:HH12	1:M:48:GLN:HG2	1.56	0.71
1:O:92:LYS:O	1:O:94:LYS:HG3	1.91	0.71
1:D:185:ARG:HG2	1:D:186:GLY:N	2.05	0.70
1:O:88:LEU:HD23	1:O:132:ILE:HA	1.73	0.70
1:L:106:LEU:HD23	1:L:106:LEU:C	2.17	0.70
1:H:185:ARG:HD2	1:K:69:MET:HE2	1.74	0.70
1:L:214:LEU:HD13	1:M:215:ARG:HH22	1.57	0.70
1:A:11:HIS:O	1:A:15:VAL:HG23	1.92	0.69
1:I:24:ARG:NH2	1:O:54:LEU:HB2	2.06	0.69
1:O:185:ARG:HG2	1:O:186:GLY:N	2.07	0.69
1:N:75:PHE:CE1	1:N:148:PRO:HG3	2.27	0.69
1:D:44:THR:HG23	1:D:54:LEU:CD1	2.23	0.69
1:M:185:ARG:HH11	1:M:185:ARG:CG	2.06	0.69
1:A:142:GLN:O	1:A:146:GLN:HG2	1.93	0.69
1:L:70:TYR:O	1:L:75:PHE:HB2	1.93	0.69
1:B:185:ARG:CG	1:B:185:ARG:NH1	2.50	0.68
1:N:207:GLN:NE2	1:O:208:ASN:ND2	2.42	0.68
1:E:50:LEU:O	1:E:51:ASN:HB2	1.93	0.68
1:I:139:ARG:NH1	3:I:3353:CL:CL	2.64	0.68
1:H:112:HIS:HB2	4:H:3338:HOH:O	1.94	0.67
1:H:168:THR:HG22	1:H:170:ASN:H	1.60	0.67
1:J:24:ARG:NH2	1:N:54:LEU:H	1.92	0.67
1:O:53:ASP:OD1	1:O:55:ALA:HB3	1.95	0.67
1:N:207:GLN:NE2	1:O:208:ASN:HD21	1.93	0.66
1:F:32:ASN:O	1:F:36:LYS:HG3	1.94	0.66
1:G:87:THR:HG23	1:G:136:LYS:HE3	1.76	0.66
1:H:156:GLN:O	1:H:160:ILE:HG12	1.95	0.66
1:H:159:LEU:HD22	1:H:198:SER:HB3	1.76	0.66
1:J:112:HIS:ND1	4:J:3340:HOH:O	2.28	0.66
1:K:11:HIS:O	1:K:15:VAL:HG23	1.96	0.66
1:N:185:ARG:HG2	1:N:186:GLY:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLU:HA	1:B:215:ARG:NH1	2.11	0.66
1:F:24:ARG:HH12	1:M:48:GLN:HE21	1.44	0.66
1:A:97:GLU:HA	1:A:97:GLU:OE1	1.95	0.66
1:J:56:ASP:O	1:J:60:MET:HB2	1.96	0.66
1:L:44:THR:O	1:L:48:GLN:HG3	1.96	0.65
1:A:106:LEU:C	1:A:106:LEU:HD23	2.21	0.65
1:I:102:ARG:HG3	1:I:102:ARG:HH11	1.61	0.65
1:O:112:HIS:HD2	4:O:3345:HOH:O	1.78	0.65
1:H:185:ARG:HH11	1:H:185:ARG:CG	2.10	0.64
1:L:212:GLU:HA	1:L:215:ARG:HH12	1.61	0.64
1:B:43:MET:HE2	1:B:66:ILE:CD1	2.27	0.64
1:I:185:ARG:HG2	1:I:186:GLY:H	1.60	0.64
1:J:185:ARG:HH11	1:J:185:ARG:CG	2.10	0.64
1:C:168:THR:HG22	1:C:170:ASN:N	2.00	0.64
1:A:141:VAL:HG22	1:A:158:ILE:HD13	1.79	0.64
1:I:194:THR:HG23	1:J:101:VAL:HG22	1.78	0.64
1:I:212:GLU:HA	1:I:215:ARG:HH12	1.62	0.64
1:L:119:GLY:O	1:L:120:LYS:HD2	1.98	0.64
1:D:142:GLN:O	1:D:146:GLN:HG2	1.98	0.63
1:F:208:ASN:CG	1:J:207:GLN:HE22	2.06	0.63
1:I:23:LEU:HD12	1:O:51:ASN:O	1.97	0.63
1:M:19:LEU:CD2	1:N:93:MET:HA	2.28	0.63
1:F:185:ARG:HG2	1:F:186:GLY:N	2.14	0.63
1:N:56:ASP:C	1:N:58:SER:H	2.05	0.63
1:D:93:MET:HE1	1:D:131:VAL:HG21	1.79	0.63
1:C:185:ARG:HH11	1:C:185:ARG:CG	2.12	0.63
1:G:24:ARG:NH2	1:L:54:LEU:HB2	2.14	0.63
1:C:185:ARG:HG2	1:C:186:GLY:N	2.12	0.63
1:J:24:ARG:NE	1:N:53:ASP:HA	2.14	0.63
1:B:44:THR:HG23	1:B:54:LEU:CD1	2.29	0.62
1:G:73:GLU:OE1	1:L:185:ARG:NH1	2.32	0.62
1:J:106:LEU:C	1:J:106:LEU:HD23	2.24	0.62
1:J:70:TYR:O	1:J:75:PHE:HB2	1.98	0.62
1:M:70:TYR:O	1:M:75:PHE:HB2	1.99	0.62
1:N:44:THR:O	1:N:48:GLN:HG3	1.99	0.62
1:L:101:VAL:HG21	1:L:137:ILE:HD12	1.82	0.62
1:A:174:SER:OG	1:A:197:THR:HG22	1.98	0.62
1:B:43:MET:HE2	1:B:66:ILE:HD13	1.80	0.62
1:N:86:ILE:HG13	1:N:165:LEU:HD13	1.81	0.62
1:A:185:ARG:NH1	1:A:185:ARG:HG2	2.15	0.62
1:I:212:GLU:HA	1:I:215:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:LEU:O	1:G:158:ILE:HG13	2.00	0.62
1:H:69:MET:HE1	1:K:113:HIS:HB3	1.81	0.62
1:A:75:PHE:CE1	1:A:148:PRO:HG3	2.35	0.62
1:F:24:ARG:NH2	1:M:54:LEU:HB2	2.15	0.62
1:A:139:ARG:NH1	3:A:3350:CL:CL	2.70	0.61
1:B:185:ARG:HH11	1:B:185:ARG:HG3	1.63	0.61
1:D:155:THR:HG22	1:D:198:SER:OG	2.00	0.61
1:G:93:MET:HE1	1:G:131:VAL:HG21	1.82	0.61
1:N:19:LEU:HD12	1:N:160:ILE:HG13	1.81	0.61
1:N:123:VAL:HG22	1:N:173:VAL:HG22	1.81	0.61
1:B:212:GLU:HA	1:B:215:ARG:HH12	1.65	0.61
1:F:69:MET:CE	1:M:185:ARG:HD2	2.29	0.61
1:F:91:ASN:HB2	1:F:129:ASP:O	2.00	0.61
1:J:24:ARG:HH12	1:N:48:GLN:HE21	1.49	0.61
1:O:30:MET:HE3	1:O:35:ARG:HG2	1.81	0.61
1:H:69:MET:HE1	1:K:113:HIS:CB	2.29	0.61
1:H:137:ILE:O	1:H:141:VAL:HG23	2.01	0.61
1:I:69:MET:HE2	1:O:185:ARG:HD2	1.81	0.61
1:O:163:GLN:HG2	1:O:169:ASN:HA	1.81	0.61
1:B:88:LEU:HD23	1:B:132:ILE:HA	1.83	0.61
1:H:185:ARG:HG2	1:H:186:GLY:N	2.15	0.61
1:I:217:VAL:HG12	1:I:218:ARG:N	2.15	0.61
1:J:185:ARG:HD2	1:N:69:MET:CE	2.31	0.61
1:E:185:ARG:HH11	1:E:185:ARG:CG	2.14	0.61
1:M:163:GLN:HG2	1:M:169:ASN:HA	1.82	0.61
1:G:106:LEU:HD23	1:G:106:LEU:C	2.26	0.60
1:F:106:LEU:C	1:F:106:LEU:HD23	2.25	0.60
1:G:101:VAL:HG12	1:G:104:ILE:HD11	1.82	0.60
1:J:110:CYS:HB2	4:J:3340:HOH:O	2.00	0.60
1:K:106:LEU:C	1:K:106:LEU:HD23	2.27	0.60
1:H:54:LEU:HB2	1:K:24:ARG:NH2	2.17	0.60
1:I:152:GLU:HB3	1:J:95:VAL:HG21	1.83	0.60
1:M:106:LEU:O	1:M:106:LEU:HD23	2.01	0.60
1:D:109:THR:CG2	1:D:114:PHE:HA	2.31	0.60
1:E:64:HIS:O	1:E:67:ALA:HB3	2.01	0.60
1:N:185:ARG:CG	1:N:185:ARG:HH11	2.15	0.60
1:I:75:PHE:CE1	1:I:148:PRO:HG3	2.36	0.60
1:H:88:LEU:HD23	1:H:132:ILE:HA	1.84	0.60
1:I:211:HIS:NE2	1:J:212:GLU:HG3	2.17	0.60
1:J:24:ARG:HH12	1:N:48:GLN:HG2	1.66	0.60
1:G:142:GLN:O	1:G:146:GLN:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:LEU:HB2	1:K:24:ARG:HH22	1.67	0.60
1:E:106:LEU:C	1:E:106:LEU:HD23	2.26	0.59
1:E:139:ARG:NH1	3:E:3349:CL:CL	2.72	0.59
1:F:43:MET:HE2	1:F:66:ILE:HD13	1.83	0.59
1:O:112:HIS:CD2	4:O:3345:HOH:O	2.53	0.59
1:A:106:LEU:HD23	1:A:106:LEU:O	2.01	0.59
1:B:142:GLN:O	1:B:146:GLN:HG2	2.02	0.59
1:K:152:GLU:OE1	1:K:152:GLU:N	2.26	0.59
1:E:102:ARG:HG3	1:E:102:ARG:HH11	1.68	0.59
1:I:87:THR:HG23	1:I:136:LYS:HE3	1.83	0.59
1:K:115:VAL:HG12	1:K:116:THR:N	2.16	0.59
1:G:106:LEU:HD11	1:G:154:LEU:HD21	1.83	0.59
1:N:168:THR:HG22	1:N:170:ASN:H	1.67	0.59
1:A:159:LEU:HD12	1:A:171:VAL:HG12	1.83	0.59
1:F:24:ARG:NH1	1:M:48:GLN:HE21	1.99	0.59
1:B:211:HIS:HD2	1:B:214:LEU:HD12	1.67	0.59
1:F:73:GLU:OE1	1:M:185:ARG:NH1	2.36	0.59
1:G:69:MET:HE2	1:L:185:ARG:HD2	1.85	0.59
1:J:22:PRO:O	1:J:23:LEU:HD12	2.03	0.59
1:J:43:MET:HE2	1:J:66:ILE:HD12	1.85	0.59
1:J:54:LEU:HB2	1:N:24:ARG:NH2	2.17	0.59
1:C:185:ARG:CG	1:C:185:ARG:NH1	2.66	0.58
1:B:217:VAL:CG1	1:B:218:ARG:N	2.67	0.58
1:K:137:ILE:O	1:K:141:VAL:HG23	2.02	0.58
1:M:106:LEU:HD23	1:M:106:LEU:C	2.28	0.58
1:O:159:LEU:HD22	1:O:198:SER:HB3	1.84	0.58
1:G:44:THR:HG23	1:G:54:LEU:CD1	2.33	0.58
1:I:34:THR:HG22	1:I:38:LEU:HD12	1.84	0.58
1:J:159:LEU:HD22	1:J:198:SER:HB3	1.85	0.58
1:A:154:LEU:O	1:A:158:ILE:HG13	2.04	0.58
1:D:139:ARG:NH1	3:D:3348:CL:CL	2.73	0.58
1:E:42:HIS:O	1:E:46:ILE:HG13	2.04	0.58
1:N:217:VAL:HG12	1:N:218:ARG:N	2.18	0.58
1:F:185:ARG:NH1	1:M:73:GLU:OE1	2.37	0.58
1:A:185:ARG:CG	1:A:185:ARG:NH1	2.61	0.58
1:K:70:TYR:O	1:K:75:PHE:HB2	2.03	0.58
1:B:112:HIS:HB2	4:B:3332:HOH:O	2.03	0.58
1:C:211:HIS:CD2	1:D:215:ARG:HH12	2.22	0.58
1:H:142:GLN:O	1:H:146:GLN:HG2	2.04	0.58
1:M:139:ARG:NH1	3:M:3357:CL:CL	2.74	0.58
1:O:70:TYR:O	1:O:75:PHE:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:GLN:HE21	1:L:24:ARG:NH1	1.96	0.58
1:E:43:MET:HE2	1:E:66:ILE:HD12	1.85	0.57
1:H:92:LYS:O	1:H:94:LYS:HG3	2.04	0.57
1:I:185:ARG:CG	1:I:185:ARG:HH11	2.17	0.57
1:H:48:GLN:CG	1:K:24:ARG:HH12	2.11	0.57
1:I:135:SER:O	1:I:139:ARG:HG3	2.03	0.57
1:J:185:ARG:HG2	1:J:186:GLY:N	2.20	0.57
1:G:6:GLU:CD	1:G:6:GLU:H	2.13	0.57
1:J:6:GLU:O	1:J:10:VAL:HG23	2.04	0.57
1:N:50:LEU:O	1:N:51:ASN:HB2	2.04	0.57
1:G:48:GLN:NE2	1:L:24:ARG:HH12	1.96	0.57
1:D:153:ARG:O	1:D:157:GLN:HG3	2.05	0.56
1:A:153:ARG:O	1:A:157:GLN:HG3	2.04	0.56
1:E:125:TYR:CD2	1:E:166:LEU:HD13	2.39	0.56
1:F:11:HIS:O	1:F:15:VAL:HG23	2.04	0.56
1:I:24:ARG:HH12	1:O:48:GLN:HG2	1.69	0.56
1:A:10:VAL:HG21	1:A:83:PHE:CZ	2.41	0.56
1:J:109:THR:CG2	1:J:114:PHE:HA	2.36	0.56
1:M:35:ARG:O	1:M:39:ILE:HG13	2.05	0.56
1:K:185:ARG:HG2	1:K:186:GLY:N	2.20	0.56
1:M:169:ASN:O	1:M:201:GLY:N	2.39	0.56
1:O:207:GLN:OE1	1:O:211:HIS:CE1	2.59	0.56
1:G:185:ARG:HH11	1:G:185:ARG:CG	2.17	0.56
1:J:49:LEU:O	1:N:35:ARG:HD2	2.06	0.56
1:B:185:ARG:HH11	1:B:185:ARG:HG2	1.64	0.56
1:F:110:CYS:HB2	4:F:3336:HOH:O	2.04	0.56
1:H:110:CYS:HB2	4:H:3338:HOH:O	2.06	0.56
1:J:119:GLY:HA3	1:J:177:ALA:HB2	1.87	0.56
1:J:75:PHE:CE1	1:J:148:PRO:HG3	2.41	0.56
1:I:112:HIS:HB2	4:I:3339:HOH:O	2.06	0.56
1:G:17:ARG:O	1:H:94:LYS:NZ	2.29	0.56
1:O:43:MET:HE2	1:O:66:ILE:HD12	1.88	0.56
1:H:185:ARG:HH11	1:H:185:ARG:HG3	1.71	0.55
1:H:185:ARG:CG	1:H:185:ARG:NH1	2.66	0.55
1:I:90:GLU:HB3	1:I:92:LYS:HG3	1.87	0.55
1:L:135:SER:O	1:L:139:ARG:HG3	2.06	0.55
1:L:217:VAL:HG12	1:L:218:ARG:N	2.21	0.55
1:B:132:ILE:HG12	1:B:133:GLY:N	2.21	0.55
1:C:214:LEU:HD13	1:D:215:ARG:NH2	2.21	0.55
1:J:112:HIS:HB2	4:J:3340:HOH:O	2.06	0.55
1:J:174:SER:OG	1:J:197:THR:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:THR:O	1:L:23:LEU:HD13	2.06	0.55
1:H:73:GLU:OE1	1:K:185:ARG:NH1	2.39	0.55
1:H:93:MET:HE1	1:H:131:VAL:HG21	1.88	0.55
1:K:142:GLN:O	1:K:146:GLN:HG2	2.06	0.55
1:N:20:GLU:OE2	1:N:80:TYR:OH	2.10	0.55
1:B:93:MET:HE1	1:B:131:VAL:HG21	1.89	0.55
1:K:185:ARG:CG	1:K:185:ARG:HH11	2.19	0.55
1:A:36:LYS:HG2	1:A:71:VAL:HG21	1.89	0.55
1:E:102:ARG:HG3	1:E:102:ARG:NH1	2.22	0.55
1:O:217:VAL:HG12	1:O:218:ARG:N	2.21	0.55
1:C:185:ARG:HH11	1:C:185:ARG:HG3	1.72	0.55
1:I:163:GLN:HG2	1:I:169:ASN:HA	1.89	0.55
1:O:185:ARG:HH11	1:O:185:ARG:CG	2.19	0.55
1:E:70:TYR:O	1:E:75:PHE:HB2	2.07	0.55
1:F:119:GLY:HA3	1:F:177:ALA:HB2	1.87	0.55
1:H:135:SER:O	1:H:139:ARG:HG3	2.08	0.55
1:M:168:THR:HG22	1:M:169:ASN:H	1.70	0.55
1:G:102:ARG:HG3	1:G:102:ARG:HH11	1.72	0.54
1:E:153:ARG:O	1:E:157:GLN:HG3	2.07	0.54
1:J:212:GLU:HG2	1:J:215:ARG:HH12	1.72	0.54
1:M:168:THR:HG22	1:M:170:ASN:H	1.72	0.54
1:M:185:ARG:CG	1:M:185:ARG:NH1	2.67	0.54
1:E:87:THR:HG23	1:E:136:LYS:HE3	1.90	0.54
1:H:132:ILE:HB	1:H:166:LEU:HD21	1.89	0.54
1:L:6:GLU:CD	1:L:6:GLU:H	2.15	0.54
1:O:35:ARG:O	1:O:39:ILE:HG13	2.07	0.54
1:G:44:THR:O	1:G:48:GLN:HG3	2.07	0.54
1:O:125:TYR:CD2	1:O:166:LEU:HD13	2.42	0.54
1:F:31:ASP:O	1:F:35:ARG:HG3	2.08	0.54
1:F:154:LEU:O	1:F:158:ILE:HG13	2.07	0.54
1:G:185:ARG:NH1	1:G:185:ARG:HG2	2.21	0.54
1:H:185:ARG:HD2	1:K:69:MET:CE	2.36	0.54
1:J:44:THR:O	1:J:48:GLN:HG3	2.08	0.54
1:O:32:ASN:OD1	1:O:35:ARG:NH2	2.36	0.54
1:E:44:THR:O	1:E:48:GLN:HG3	2.07	0.54
1:G:75:PHE:CE1	1:G:148:PRO:HG3	2.43	0.54
1:G:112:HIS:HB2	4:G:3337:HOH:O	2.06	0.54
1:I:123:VAL:HG22	1:I:173:VAL:HG22	1.90	0.54
1:O:88:LEU:HD22	1:O:130:SER:HB2	1.89	0.54
1:B:135:SER:O	1:B:139:ARG:HG3	2.07	0.54
1:F:93:MET:HE1	1:F:131:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:HIS:O	1:G:15:VAL:HG23	2.08	0.54
1:H:23:LEU:HD11	1:H:78:LEU:HD22	1.89	0.54
1:D:44:THR:HG23	1:D:54:LEU:HD11	1.90	0.54
1:I:42:HIS:CE1	1:O:45:GLU:HG3	2.43	0.54
1:K:93:MET:HE1	1:K:131:VAL:HG21	1.90	0.54
1:A:113:HIS:HB2	1:A:115:VAL:HG23	1.90	0.54
1:E:53:ASP:OD1	1:E:55:ALA:HB3	2.07	0.54
1:M:92:LYS:O	1:M:94:LYS:HG3	2.07	0.54
1:O:53:ASP:OD1	1:O:55:ALA:CB	2.56	0.54
1:D:112:HIS:ND1	4:D:3334:HOH:O	2.34	0.54
1:L:113:HIS:N	1:L:113:HIS:CD2	2.75	0.54
1:N:207:GLN:HE22	1:O:208:ASN:HD21	1.55	0.54
1:I:14:LEU:HB2	1:I:20:GLU:HG2	1.91	0.53
1:J:24:ARG:HG3	1:N:53:ASP:HA	1.90	0.53
1:K:79:ASP:C	1:K:81:ALA:H	2.16	0.53
1:B:106:LEU:HD23	1:B:106:LEU:C	2.33	0.53
1:E:183:LYS:HG3	1:E:190:ALA:HA	1.91	0.53
1:I:200:GLY:O	1:I:203:PHE:HB2	2.08	0.53
1:L:106:LEU:HD23	1:L:107:THR:N	2.22	0.53
1:L:111:GLU:HG2	1:L:150:VAL:HG23	1.90	0.53
1:N:139:ARG:NH1	3:N:3358:CL:CL	2.78	0.53
1:C:57:ASP:HA	1:C:60:MET:HE2	1.91	0.53
1:F:19:LEU:CD2	1:G:93:MET:HA	2.38	0.53
1:H:153:ARG:O	1:H:157:GLN:HG3	2.09	0.53
1:M:50:LEU:O	1:M:51:ASN:HB2	2.09	0.53
1:M:153:ARG:HB2	1:N:93:MET:HG2	1.90	0.53
1:O:98:MET:HE1	1:O:213:PHE:HA	1.91	0.53
1:J:24:ARG:HH12	1:N:48:GLN:NE2	2.05	0.53
1:F:54:LEU:HB2	1:M:24:ARG:NH2	2.24	0.53
1:K:44:THR:HG23	1:K:54:LEU:HD13	1.91	0.53
1:D:70:TYR:O	1:D:75:PHE:HB2	2.07	0.53
1:F:113:HIS:CB	1:M:69:MET:HE1	2.39	0.53
1:I:100:THR:HG23	1:I:124:ALA:HB2	1.90	0.53
1:O:113:HIS:N	1:O:113:HIS:CD2	2.76	0.53
1:A:208:ASN:CG	1:E:207:GLN:HE22	2.17	0.53
1:G:106:LEU:HD23	1:G:106:LEU:O	2.09	0.53
1:M:185:ARG:NH1	1:M:185:ARG:HG2	2.24	0.53
1:C:212:GLU:HA	1:C:215:ARG:NH1	2.24	0.52
1:G:101:VAL:CG1	1:G:104:ILE:HD11	2.40	0.52
1:K:62:THR:HB	1:K:63:PRO:HD3	1.90	0.52
1:K:98:MET:HE1	1:K:213:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:152:GLU:OE1	1:M:152:GLU:N	2.37	0.52
1:A:6:GLU:H	1:A:6:GLU:CD	2.17	0.52
1:F:156:GLN:O	1:F:160:ILE:HG12	2.09	0.52
1:I:168:THR:HG22	1:I:169:ASN:N	2.24	0.52
1:N:109:THR:CG2	1:N:114:PHE:HA	2.40	0.52
1:I:44:THR:HG23	1:I:54:LEU:HD13	1.90	0.52
1:J:62:THR:HB	1:J:63:PRO:HD3	1.90	0.52
1:N:136:LYS:O	1:N:140:ILE:HG13	2.09	0.52
1:O:212:GLU:HG2	1:O:215:ARG:HH22	1.75	0.52
1:B:11:HIS:O	1:B:15:VAL:HG23	2.10	0.52
1:F:217:VAL:HG12	1:F:218:ARG:N	2.23	0.52
1:A:93:MET:H	1:A:93:MET:HE2	1.73	0.52
1:I:62:THR:HB	1:I:63:PRO:HD3	1.92	0.52
1:I:194:THR:HG21	1:J:134:LEU:CD2	2.40	0.52
1:K:207:GLN:HE22	1:L:208:ASN:ND2	2.07	0.52
1:C:217:VAL:HG12	1:C:218:ARG:N	2.23	0.52
1:E:132:ILE:HB	1:E:166:LEU:HD21	1.92	0.52
1:E:217:VAL:HG12	1:E:218:ARG:N	2.24	0.52
1:I:14:LEU:CB	1:I:20:GLU:HG2	2.40	0.52
1:M:137:ILE:O	1:M:141:VAL:HG23	2.09	0.52
1:O:6:GLU:CD	1:O:6:GLU:N	2.66	0.52
1:F:20:GLU:OE1	1:F:21:THR:N	2.41	0.52
1:G:97:GLU:OE1	1:G:97:GLU:HA	2.09	0.52
1:H:69:MET:CE	1:K:113:HIS:HB3	2.39	0.52
1:J:21:THR:O	1:J:23:LEU:HD13	2.10	0.52
1:M:98:MET:HE1	1:M:213:PHE:HA	1.92	0.52
1:H:172:ALA:HB1	1:H:199:LEU:HD23	1.91	0.52
1:I:24:ARG:HH12	1:O:48:GLN:NE2	2.07	0.52
1:K:92:LYS:C	1:K:94:LYS:H	2.17	0.52
1:E:35:ARG:O	1:E:39:ILE:HG13	2.09	0.52
1:E:185:ARG:HG2	1:E:186:GLY:N	2.24	0.52
1:I:125:TYR:CD2	1:I:166:LEU:HD13	2.45	0.52
1:J:73:GLU:OE2	1:N:185:ARG:NH1	2.43	0.52
1:M:79:ASP:C	1:M:81:ALA:H	2.18	0.52
1:J:43:MET:HE2	1:J:66:ILE:CD1	2.40	0.52
1:J:185:ARG:HH11	1:J:185:ARG:HG3	1.75	0.52
1:A:112:HIS:HB2	4:A:3331:HOH:O	2.10	0.51
1:F:79:ASP:OD2	1:F:81:ALA:HB3	2.10	0.51
1:I:102:ARG:HG3	1:I:102:ARG:NH1	2.25	0.51
1:J:46:ILE:HG23	1:N:39:ILE:HG23	1.90	0.51
1:L:11:HIS:O	1:L:15:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:56:ASP:O	1:N:58:SER:N	2.42	0.51
1:G:185:ARG:CG	1:G:185:ARG:NH1	2.71	0.51
1:J:217:VAL:HG12	1:J:218:ARG:N	2.24	0.51
1:B:217:VAL:HG12	1:B:218:ARG:N	2.26	0.51
1:E:43:MET:HE2	1:E:66:ILE:CD1	2.39	0.51
1:G:24:ARG:NH2	1:L:54:LEU:H	2.08	0.51
1:J:174:SER:CB	1:J:197:THR:HG22	2.40	0.51
1:E:6:GLU:CD	1:E:6:GLU:H	2.17	0.51
1:J:106:LEU:C	1:J:106:LEU:CD2	2.83	0.51
1:L:22:PRO:C	1:L:23:LEU:HD12	2.36	0.51
1:A:218:ARG:O	1:A:218:ARG:HG3	2.10	0.51
1:D:217:VAL:CG1	1:D:218:ARG:N	2.72	0.51
1:F:48:GLN:HG2	1:M:24:ARG:NH1	2.25	0.51
1:F:136:LYS:NZ	3:F:3355:CL:CL	2.80	0.51
1:G:87:THR:HG23	1:G:136:LYS:CE	2.41	0.51
1:F:192:SER:HB3	1:G:104:ILE:HA	1.92	0.51
1:G:24:ARG:NE	1:L:53:ASP:HA	2.25	0.51
1:G:214:LEU:HD13	1:H:215:ARG:HH22	1.76	0.51
1:H:6:GLU:HB3	1:H:165:LEU:HD21	1.93	0.51
1:I:24:ARG:HG3	1:O:53:ASP:HA	1.92	0.51
1:I:53:ASP:HA	1:O:24:ARG:NE	2.26	0.51
1:L:106:LEU:C	1:L:106:LEU:CD2	2.84	0.51
1:H:115:VAL:HG21	1:K:69:MET:HE1	1.93	0.51
1:O:109:THR:HG22	1:O:114:PHE:HA	1.92	0.51
1:I:185:ARG:NH2	3:J:3354:CL:CL	2.81	0.50
1:K:187:ILE:O	1:K:188:ARG:HB2	2.10	0.50
1:M:19:LEU:HD21	1:N:93:MET:HA	1.92	0.50
1:H:34:THR:O	1:H:38:LEU:HG	2.10	0.50
1:B:109:THR:CG2	1:B:114:PHE:HA	2.41	0.50
1:J:106:LEU:HA	1:J:142:GLN:OE1	2.11	0.50
1:M:142:GLN:O	1:M:146:GLN:HG2	2.12	0.50
1:O:97:GLU:HA	1:O:97:GLU:OE1	2.11	0.50
1:C:217:VAL:O	1:C:218:ARG:HB3	2.11	0.50
1:D:138:ASN:H	1:D:138:ASN:HD22	1.57	0.50
1:G:44:THR:HG23	1:G:54:LEU:HD13	1.94	0.50
1:N:159:LEU:HD22	1:N:198:SER:HB3	1.93	0.50
1:N:217:VAL:CG1	1:N:218:ARG:N	2.75	0.50
1:E:185:ARG:CG	1:E:185:ARG:NH1	2.71	0.50
1:K:215:ARG:HH12	1:O:214:LEU:HD13	1.76	0.50
1:F:217:VAL:CG1	1:F:218:ARG:N	2.74	0.50
1:I:45:GLU:HG3	1:O:42:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:HIS:O	1:J:114:PHE:HB2	2.11	0.50
1:H:180:TYR:CE2	1:H:183:LYS:HD3	2.46	0.50
1:K:217:VAL:O	1:K:218:ARG:HB3	2.12	0.50
1:N:6:GLU:CD	1:N:6:GLU:N	2.65	0.50
1:O:151:GLN:HG2	1:O:196:THR:OG1	2.12	0.50
1:B:50:LEU:O	1:B:51:ASN:HB2	2.11	0.49
1:B:70:TYR:O	1:B:75:PHE:HB2	2.12	0.49
1:F:180:TYR:CE2	1:F:183:LYS:HD3	2.47	0.49
1:I:24:ARG:NH1	1:O:48:GLN:HG2	2.27	0.49
1:C:44:THR:HG23	1:C:54:LEU:CD1	2.41	0.49
1:G:138:ASN:HD22	1:G:138:ASN:H	1.60	0.49
1:H:24:ARG:HH12	1:K:48:GLN:HE21	1.60	0.49
1:I:185:ARG:HD2	1:O:69:MET:HE2	1.94	0.49
1:N:56:ASP:C	1:N:58:SER:N	2.69	0.49
1:O:44:THR:HG23	1:O:54:LEU:HD13	1.94	0.49
1:F:93:MET:HE3	1:J:152:GLU:HB3	1.93	0.49
1:M:109:THR:CG2	1:M:114:PHE:HA	2.42	0.49
1:B:112:HIS:ND1	4:B:3332:HOH:O	2.31	0.49
1:I:194:THR:HG21	1:J:134:LEU:HD22	1.95	0.49
1:K:153:ARG:O	1:K:157:GLN:HG3	2.12	0.49
1:C:210:ARG:NH2	1:D:97:GLU:OE1	2.45	0.49
1:E:187:ILE:HG13	1:E:187:ILE:O	2.12	0.49
1:I:185:ARG:NH1	1:O:73:GLU:OE1	2.46	0.49
1:I:218:ARG:HG2	1:I:218:ARG:HH11	1.76	0.49
1:D:152:GLU:HB3	1:E:95:VAL:HG21	1.94	0.49
1:A:44:THR:HG23	1:A:54:LEU:HD13	1.93	0.49
1:B:109:THR:HG22	1:B:114:PHE:HA	1.94	0.49
1:G:53:ASP:OD1	1:G:55:ALA:HB3	2.12	0.49
1:H:6:GLU:CD	1:H:6:GLU:H	2.21	0.49
1:L:88:LEU:HD22	1:L:130:SER:HB2	1.93	0.49
1:D:156:GLN:O	1:D:160:ILE:HG12	2.13	0.49
1:F:185:ARG:HD2	1:M:69:MET:CE	2.28	0.49
1:J:24:ARG:NH2	1:N:54:LEU:CB	2.64	0.49
1:K:109:THR:HG22	1:K:114:PHE:HA	1.94	0.49
1:O:6:GLU:O	1:O:7:ALA:C	2.56	0.49
1:I:6:GLU:HB3	1:I:165:LEU:HD21	1.94	0.49
1:J:73:GLU:OE1	1:N:185:ARG:NH1	2.46	0.49
1:F:48:GLN:HE21	1:M:24:ARG:NH1	2.06	0.49
1:H:35:ARG:O	1:H:39:ILE:HG13	2.13	0.49
1:I:185:ARG:CG	1:I:185:ARG:NH1	2.73	0.49
1:J:35:ARG:HD2	1:N:49:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:217:VAL:HG12	1:M:218:ARG:N	2.27	0.49
1:A:200:GLY:O	1:A:203:PHE:HB2	2.13	0.48
1:G:102:ARG:HG3	1:G:102:ARG:NH1	2.28	0.48
1:H:62:THR:HB	1:H:63:PRO:HD3	1.96	0.48
1:D:113:HIS:N	1:D:113:HIS:CD2	2.80	0.48
1:D:152:GLU:OE1	1:D:152:GLU:N	2.37	0.48
1:F:113:HIS:HB3	1:M:69:MET:CE	2.42	0.48
1:J:22:PRO:C	1:J:23:LEU:HD12	2.37	0.48
1:M:44:THR:HG23	1:M:54:LEU:CD1	2.43	0.48
1:A:70:TYR:O	1:A:75:PHE:HB2	2.13	0.48
1:B:136:LYS:O	1:B:140:ILE:HG13	2.14	0.48
1:F:70:TYR:O	1:F:75:PHE:HB2	2.13	0.48
1:H:150:VAL:HG12	1:H:153:ARG:H	1.77	0.48
1:L:5:LYS:HB2	1:L:6:GLU:OE2	2.13	0.48
1:M:185:ARG:HH11	1:M:185:ARG:HG3	1.77	0.48
1:O:43:MET:HE2	1:O:66:ILE:CD1	2.43	0.48
1:A:150:VAL:HG12	1:A:153:ARG:H	1.78	0.48
1:J:92:LYS:C	1:J:94:LYS:H	2.22	0.48
1:L:111:GLU:HG2	1:L:149:GLN:O	2.14	0.48
1:N:185:ARG:CG	1:N:185:ARG:NH1	2.72	0.48
1:H:207:GLN:HE22	1:I:208:ASN:CG	2.22	0.48
1:I:207:GLN:OE1	1:I:211:HIS:CE1	2.66	0.48
1:L:42:HIS:O	1:L:46:ILE:HG13	2.14	0.48
1:N:112:HIS:HB2	4:N:3344:HOH:O	2.13	0.48
1:A:113:HIS:CD2	1:A:113:HIS:N	2.81	0.48
1:A:159:LEU:O	1:A:163:GLN:HG3	2.14	0.48
1:F:180:TYR:C	1:F:182:VAL:H	2.22	0.48
1:G:207:GLN:HA	1:G:207:GLN:NE2	2.29	0.48
1:L:19:LEU:HD13	1:L:156:GLN:HB3	1.95	0.48
1:M:112:HIS:CG	4:M:3343:HOH:O	2.66	0.48
1:M:135:SER:O	1:M:139:ARG:HG3	2.14	0.48
1:C:109:THR:CG2	1:C:114:PHE:HA	2.44	0.48
1:N:119:GLY:HA3	1:N:177:ALA:HB2	1.96	0.48
1:O:36:LYS:HG2	1:O:71:VAL:HG21	1.96	0.48
1:G:182:VAL:HG12	1:G:182:VAL:O	2.14	0.47
1:H:217:VAL:O	1:H:218:ARG:HB3	2.15	0.47
1:J:6:GLU:CD	1:J:6:GLU:H	2.20	0.47
1:L:159:LEU:HD22	1:L:198:SER:HB3	1.95	0.47
1:D:199:LEU:HD12	1:D:210:ARG:NH1	2.29	0.47
1:H:160:ILE:HA	1:H:163:GLN:HE21	1.79	0.47
1:H:180:TYR:O	1:H:184:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:ARG:CG	1:J:185:ARG:NH1	2.70	0.47
1:L:125:TYR:CD2	1:L:166:LEU:HD13	2.49	0.47
1:O:132:ILE:CG2	1:O:166:LEU:HD21	2.43	0.47
1:C:132:ILE:HB	1:C:166:LEU:HD21	1.96	0.47
1:E:119:GLY:HA3	1:E:177:ALA:HB2	1.97	0.47
1:J:24:ARG:HG3	1:N:53:ASP:CA	2.44	0.47
1:N:154:LEU:HD12	1:N:154:LEU:O	2.14	0.47
1:F:112:HIS:HB2	4:F:3336:HOH:O	2.13	0.47
1:H:153:ARG:HG2	1:H:157:GLN:NE2	2.29	0.47
1:J:156:GLN:HA	1:J:156:GLN:OE1	2.15	0.47
1:L:217:VAL:CG1	1:L:218:ARG:N	2.77	0.47
1:B:98:MET:HE1	1:B:213:PHE:HA	1.96	0.47
1:E:146:GLN:HE21	1:E:146:GLN:HA	1.80	0.47
1:K:97:GLU:OE2	1:O:204:LYS:NZ	2.48	0.47
1:A:6:GLU:O	1:A:10:VAL:HG23	2.14	0.47
1:B:162:LEU:O	1:B:166:LEU:HD12	2.14	0.47
1:I:92:LYS:O	1:I:94:LYS:HG3	2.15	0.47
1:O:93:MET:HE2	1:O:93:MET:HB2	1.74	0.47
1:A:14:LEU:HD23	1:A:160:ILE:HG21	1.96	0.47
1:A:144:PHE:O	1:A:149:GLN:NE2	2.38	0.47
1:B:53:ASP:OD1	1:B:55:ALA:HB3	2.15	0.47
1:B:217:VAL:O	1:B:218:ARG:HB3	2.14	0.47
1:F:185:ARG:CG	1:F:185:ARG:HH11	2.27	0.47
1:I:69:MET:CE	1:O:185:ARG:HD2	2.45	0.47
1:J:102:ARG:HG3	1:J:102:ARG:HH11	1.78	0.47
1:J:187:ILE:O	1:J:187:ILE:HG13	2.14	0.47
1:K:102:ARG:O	1:O:192:SER:HA	2.15	0.47
1:L:185:ARG:HH11	1:L:185:ARG:CG	2.28	0.47
1:B:62:THR:HB	1:B:63:PRO:HD3	1.97	0.47
1:I:142:GLN:NE2	1:O:188:ARG:NH2	2.63	0.47
1:C:102:ARG:HG3	1:C:102:ARG:HH11	1.80	0.47
1:D:50:LEU:O	1:D:51:ASN:HB2	2.15	0.47
1:E:61:GLU:HB2	1:E:65:ARG:CZ	2.45	0.47
1:E:106:LEU:HD23	1:E:106:LEU:O	2.15	0.47
1:I:24:ARG:HH12	1:O:48:GLN:HE21	1.62	0.47
1:K:115:VAL:CG1	1:K:116:THR:N	2.78	0.47
1:M:108:SER:HB3	1:M:117:ILE:HB	1.96	0.47
1:N:207:GLN:OE1	1:N:210:ARG:HD3	2.15	0.47
1:O:92:LYS:C	1:O:94:LYS:N	2.73	0.47
1:F:153:ARG:O	1:F:157:GLN:HG3	2.15	0.47
1:H:42:HIS:HE1	1:K:45:GLU:OE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:92:LYS:C	1:M:94:LYS:H	2.23	0.47
1:C:155:THR:HG22	1:C:198:SER:OG	2.14	0.46
1:E:80:TYR:C	1:E:82:ASN:N	2.69	0.46
1:H:153:ARG:HG2	1:H:157:GLN:HE21	1.80	0.46
1:I:180:TYR:CD2	1:O:116:THR:HG21	2.50	0.46
1:K:185:ARG:HG2	1:K:185:ARG:NH1	2.29	0.46
1:E:109:THR:CG2	1:E:114:PHE:HA	2.45	0.46
1:E:185:ARG:HG2	1:E:185:ARG:NH1	2.30	0.46
1:F:6:GLU:H	1:F:6:GLU:CD	2.23	0.46
1:J:93:MET:HB2	1:J:95:VAL:HG23	1.97	0.46
1:K:218:ARG:O	1:K:218:ARG:HG3	2.16	0.46
1:M:44:THR:O	1:M:48:GLN:HG3	2.15	0.46
1:O:88:LEU:HD23	1:O:132:ILE:CA	2.43	0.46
1:A:53:ASP:OD1	1:A:53:ASP:C	2.59	0.46
1:F:142:GLN:OE1	1:F:142:GLN:HA	2.14	0.46
1:I:185:ARG:HD2	1:O:69:MET:CE	2.45	0.46
1:M:77:GLY:O	1:M:147:ARG:NE	2.43	0.46
1:A:93:MET:HE3	1:A:93:MET:HB2	1.77	0.46
1:C:162:LEU:HA	1:C:162:LEU:HD23	1.79	0.46
1:F:24:ARG:HH22	1:M:54:LEU:HB2	1.78	0.46
1:G:24:ARG:HE	1:L:53:ASP:HA	1.81	0.46
1:G:132:ILE:HB	1:G:166:LEU:HD21	1.97	0.46
1:I:50:LEU:O	1:I:51:ASN:HB2	2.16	0.46
1:K:185:ARG:NH1	1:K:185:ARG:CG	2.78	0.46
1:I:53:ASP:C	1:I:55:ALA:H	2.23	0.46
1:A:98:MET:HE1	1:A:213:PHE:HA	1.98	0.46
1:A:185:ARG:HH11	1:A:185:ARG:HG3	1.80	0.46
1:F:113:HIS:HB3	1:M:69:MET:HE1	1.97	0.46
1:G:24:ARG:NH2	1:L:54:LEU:CB	2.79	0.46
1:I:24:ARG:HH21	1:O:54:LEU:HB2	1.78	0.46
1:J:24:ARG:NH1	1:N:48:GLN:HG2	2.31	0.46
1:K:92:LYS:C	1:K:94:LYS:N	2.71	0.46
1:M:202:LEU:HA	1:M:205:SER:OG	2.16	0.46
1:O:20:GLU:OE2	1:O:80:TYR:OH	2.33	0.46
1:B:102:ARG:HG3	1:B:102:ARG:HH11	1.81	0.46
1:G:212:GLU:CG	1:G:215:ARG:HH22	2.25	0.46
1:I:54:LEU:H	1:O:24:ARG:CZ	2.29	0.46
1:J:24:ARG:HE	1:N:53:ASP:HA	1.78	0.46
1:N:90:GLU:OE2	1:N:92:LYS:HG2	2.15	0.46
1:N:211:HIS:HE2	1:O:212:GLU:HG3	1.81	0.46
1:E:146:GLN:HA	1:E:146:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:VAL:HG12	1:L:124:ALA:N	2.30	0.46
1:M:75:PHE:CE1	1:M:148:PRO:HG3	2.50	0.46
1:D:214:LEU:HD13	1:E:215:ARG:HH22	1.79	0.46
1:I:6:GLU:CD	1:I:6:GLU:H	2.23	0.46
1:L:88:LEU:HD23	1:L:132:ILE:HA	1.97	0.46
1:M:5:LYS:O	1:M:9:LEU:HB2	2.16	0.46
1:O:142:GLN:O	1:O:146:GLN:HG2	2.16	0.46
1:A:217:VAL:O	1:A:218:ARG:HB3	2.16	0.46
1:B:25:PRO:O	1:B:26:PRO:C	2.59	0.46
1:C:185:ARG:HG2	1:C:185:ARG:NH1	2.30	0.46
1:G:125:TYR:CD2	1:G:166:LEU:HD13	2.50	0.46
1:K:176:ASP:OD2	1:L:102:ARG:NH2	2.42	0.46
1:L:21:THR:HG22	1:L:23:LEU:CD1	2.46	0.46
1:O:213:PHE:O	1:O:217:VAL:HG23	2.15	0.46
1:B:187:ILE:HD13	1:C:139:ARG:HG2	1.98	0.45
1:L:93:MET:HE2	1:L:93:MET:HB2	1.81	0.45
1:N:70:TYR:O	1:N:75:PHE:HB2	2.15	0.45
1:O:20:GLU:OE1	1:O:20:GLU:HA	2.15	0.45
1:A:87:THR:HG23	1:A:136:LYS:HE3	1.98	0.45
1:B:92:LYS:C	1:B:94:LYS:H	2.23	0.45
1:B:150:VAL:HG12	1:B:153:ARG:H	1.81	0.45
1:F:119:GLY:HA3	1:F:177:ALA:CB	2.47	0.45
1:K:117:ILE:O	1:K:117:ILE:HG22	2.14	0.45
1:N:98:MET:HE3	1:N:124:ALA:HB1	1.97	0.45
1:O:88:LEU:HD21	1:O:132:ILE:HB	1.98	0.45
1:G:24:ARG:HH12	1:L:48:GLN:NE2	2.14	0.45
1:K:123:VAL:HG22	1:K:173:VAL:HG22	1.98	0.45
1:N:214:LEU:HD13	1:O:215:ARG:HH22	1.81	0.45
1:O:111:GLU:CD	1:O:150:VAL:HG23	2.41	0.45
1:H:139:ARG:NH1	3:H:3352:CL:CL	2.87	0.45
1:I:185:ARG:HH11	1:I:185:ARG:HG3	1.81	0.45
1:I:217:VAL:CG1	1:I:218:ARG:N	2.79	0.45
1:L:133:GLY:O	1:L:134:LEU:C	2.58	0.45
1:M:56:ASP:OD2	1:M:58:SER:HB3	2.17	0.45
1:B:93:MET:HE3	1:B:95:VAL:HG23	1.98	0.45
1:C:4:SER:O	1:C:5:LYS:C	2.58	0.45
1:C:93:MET:HE2	1:C:93:MET:HB2	1.68	0.45
1:F:93:MET:HE2	1:F:93:MET:HB2	1.65	0.45
1:J:71:VAL:HG12	1:J:72:ASP:OD1	2.16	0.45
1:M:79:ASP:C	1:M:81:ALA:N	2.75	0.45
1:A:43:MET:HE2	1:A:66:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:VAL:CG1	1:C:218:ARG:N	2.79	0.45
1:H:152:GLU:OE1	1:H:152:GLU:N	2.31	0.45
1:J:218:ARG:O	1:J:218:ARG:HG3	2.16	0.45
1:L:185:ARG:HG2	1:L:186:GLY:N	2.32	0.45
1:C:168:THR:HG22	1:C:169:ASN:N	2.31	0.45
1:E:88:LEU:HD23	1:E:132:ILE:HA	1.98	0.45
1:F:48:GLN:HG2	1:M:24:ARG:HH12	1.80	0.45
1:N:163:GLN:HG2	1:N:169:ASN:HA	1.98	0.45
1:O:53:ASP:C	1:O:55:ALA:H	2.24	0.45
1:O:182:VAL:HG12	1:O:182:VAL:O	2.16	0.45
1:F:185:ARG:HH11	1:M:73:GLU:CD	2.24	0.45
1:I:10:VAL:C	1:I:12:GLU:N	2.74	0.45
1:I:48:GLN:HE21	1:O:24:ARG:NH1	2.15	0.45
1:M:217:VAL:CG1	1:M:218:ARG:N	2.80	0.45
1:F:111:GLU:OE2	1:M:58:SER:OG	2.26	0.45
1:F:115:VAL:HG12	1:F:116:THR:N	2.32	0.45
1:K:169:ASN:O	1:K:200:GLY:C	2.60	0.45
1:A:44:THR:HG23	1:A:54:LEU:CD1	2.47	0.45
1:B:218:ARG:HH11	1:B:218:ARG:HG2	1.81	0.45
1:D:44:THR:O	1:D:48:GLN:HG3	2.16	0.45
1:E:217:VAL:CG1	1:E:218:ARG:N	2.80	0.45
1:F:25:PRO:O	1:F:26:PRO:C	2.58	0.45
1:J:14:LEU:HB2	1:J:20:GLU:HG2	1.98	0.45
1:J:113:HIS:CD2	1:J:113:HIS:N	2.85	0.45
1:J:217:VAL:CG1	1:J:218:ARG:N	2.80	0.45
1:K:79:ASP:C	1:K:81:ALA:N	2.75	0.45
1:M:112:HIS:HE1	1:M:150:VAL:HG22	1.81	0.45
1:N:15:VAL:HG22	1:N:20:GLU:HG3	1.99	0.45
1:N:175:ILE:O	1:N:195:THR:HA	2.17	0.45
1:F:218:ARG:O	1:F:218:ARG:HG3	2.17	0.44
1:J:56:ASP:HB3	1:J:59:LEU:HB2	1.98	0.44
1:K:104:ILE:HG23	1:K:138:ASN:OD1	2.17	0.44
1:C:139:ARG:NH1	3:C:3347:CL:CL	2.88	0.44
1:F:202:LEU:HD23	1:F:202:LEU:HA	1.75	0.44
1:I:150:VAL:HG12	1:I:153:ARG:H	1.82	0.44
1:J:92:LYS:C	1:J:94:LYS:N	2.72	0.44
1:M:119:GLY:HA3	1:M:177:ALA:HB2	2.00	0.44
1:M:207:GLN:NE2	1:M:207:GLN:HA	2.32	0.44
1:N:174:SER:OG	1:N:197:THR:HG22	2.17	0.44
1:H:50:LEU:O	1:H:51:ASN:HB2	2.18	0.44
1:B:92:LYS:C	1:B:94:LYS:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ILE:O	1:C:138:ASN:C	2.61	0.44
1:E:213:PHE:O	1:E:217:VAL:HG23	2.17	0.44
1:F:20:GLU:OE2	1:F:80:TYR:OH	2.26	0.44
1:F:93:MET:HE2	1:F:95:VAL:HG23	2.00	0.44
1:F:192:SER:HA	1:G:102:ARG:O	2.17	0.44
1:H:73:GLU:O	1:H:76:SER:OG	2.34	0.44
1:J:53:ASP:C	1:J:55:ALA:H	2.25	0.44
1:J:73:GLU:CD	1:N:185:ARG:NH1	2.76	0.44
1:K:113:HIS:CD2	1:K:113:HIS:N	2.86	0.44
1:M:135:SER:HA	1:M:138:ASN:HD22	1.81	0.44
1:M:152:GLU:HB3	1:N:95:VAL:HG21	2.00	0.44
1:O:106:LEU:HD11	1:O:175:ILE:HD13	1.99	0.44
1:C:168:THR:HG21	1:C:170:ASN:HB2	1.98	0.44
1:F:146:GLN:HE21	1:F:146:GLN:HA	1.81	0.44
1:G:64:HIS:O	1:G:67:ALA:HB3	2.16	0.44
1:J:48:GLN:NE2	1:N:24:ARG:HH12	2.16	0.44
1:J:93:MET:HE1	1:J:131:VAL:HG21	2.00	0.44
1:L:217:VAL:O	1:L:218:ARG:HB3	2.18	0.44
1:O:185:ARG:HH11	1:O:185:ARG:HG3	1.81	0.44
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.82	0.44
1:B:19:LEU:CD2	1:C:93:MET:HA	2.47	0.44
1:E:14:LEU:CB	1:E:20:GLU:HG2	2.47	0.44
1:H:6:GLU:CD	1:H:6:GLU:N	2.75	0.44
1:I:156:GLN:O	1:I:160:ILE:HG12	2.18	0.44
1:K:35:ARG:O	1:K:39:ILE:HG13	2.18	0.44
1:K:93:MET:HE2	1:K:95:VAL:HG23	2.00	0.44
1:L:50:LEU:O	1:L:51:ASN:HB2	2.17	0.44
1:M:151:GLN:NE2	1:M:196:THR:HG23	2.32	0.44
1:N:115:VAL:HG12	1:N:116:THR:N	2.32	0.44
1:E:90:GLU:HB3	1:E:92:LYS:HE3	1.99	0.44
1:J:79:ASP:C	1:J:81:ALA:H	2.26	0.44
1:G:185:ARG:HD2	1:L:69:MET:CE	2.44	0.44
1:K:217:VAL:O	1:K:218:ARG:CB	2.65	0.44
1:O:42:HIS:O	1:O:46:ILE:HG13	2.17	0.44
3:A:3350:CL:CL	1:E:185:ARG:NH2	2.88	0.44
1:B:132:ILE:CG1	1:B:133:GLY:N	2.81	0.44
1:H:113:HIS:O	1:H:114:PHE:HB2	2.18	0.44
1:I:23:LEU:HD12	1:I:23:LEU:HA	1.79	0.44
1:N:88:LEU:HD23	1:N:132:ILE:HA	1.99	0.44
1:O:123:VAL:HG22	1:O:173:VAL:HG22	2.00	0.44
1:A:25:PRO:O	1:A:26:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:ARG:HH12	1:K:48:GLN:NE2	2.16	0.43
1:H:69:MET:HG2	1:H:74:ILE:HG12	2.00	0.43
1:L:180:TYR:O	1:L:184:ALA:HB3	2.17	0.43
1:O:93:MET:HE1	1:O:131:VAL:HG21	1.99	0.43
1:O:160:ILE:HD13	1:O:163:GLN:NE2	2.33	0.43
1:C:152:GLU:HB3	1:D:95:VAL:HG21	1.98	0.43
1:F:24:ARG:NH1	1:M:48:GLN:HG2	2.29	0.43
1:L:163:GLN:HG2	1:L:168:THR:O	2.18	0.43
1:O:79:ASP:C	1:O:81:ALA:H	2.26	0.43
1:I:52:LEU:HD11	1:O:148:PRO:HG2	2.00	0.43
1:J:24:ARG:HH21	1:N:54:LEU:H	1.66	0.43
1:J:40:ALA:O	1:J:41:GLY:C	2.60	0.43
1:N:20:GLU:HA	1:N:20:GLU:OE1	2.18	0.43
1:A:212:GLU:CD	1:E:210:ARG:HE	2.26	0.43
1:E:32:ASN:C	1:E:34:THR:N	2.75	0.43
1:E:93:MET:HE2	1:E:93:MET:HB2	1.79	0.43
1:L:156:GLN:O	1:L:157:GLN:C	2.61	0.43
1:C:112:HIS:HB2	4:C:3333:HOH:O	2.19	0.43
1:H:185:ARG:HG2	1:H:185:ARG:NH1	2.34	0.43
1:M:92:LYS:C	1:M:94:LYS:N	2.76	0.43
1:N:68:LYS:HG3	1:N:72:ASP:OD2	2.17	0.43
1:O:75:PHE:CE1	1:O:148:PRO:HG3	2.54	0.43
1:E:147:ARG:O	1:E:148:PRO:C	2.59	0.43
1:F:54:LEU:HB2	1:M:24:ARG:HH22	1.83	0.43
1:G:50:LEU:O	1:G:51:ASN:HB2	2.18	0.43
1:L:92:LYS:O	1:L:94:LYS:HG3	2.18	0.43
1:G:88:LEU:HD23	1:G:132:ILE:HA	2.00	0.43
1:H:185:ARG:NH1	1:K:73:GLU:OE1	2.52	0.43
1:I:24:ARG:HH12	1:O:48:GLN:CG	2.31	0.43
1:J:93:MET:HE2	1:J:93:MET:H	1.83	0.43
1:K:218:ARG:O	1:K:218:ARG:CG	2.67	0.43
1:O:31:ASP:O	1:O:34:THR:HB	2.18	0.43
1:O:53:ASP:C	1:O:55:ALA:N	2.75	0.43
1:D:125:TYR:CD2	1:D:166:LEU:HD13	2.53	0.43
1:E:61:GLU:HB2	1:E:65:ARG:NH1	2.33	0.43
1:E:62:THR:O	1:E:66:ILE:HG13	2.19	0.43
1:E:68:LYS:NZ	1:E:72:ASP:OD2	2.38	0.43
1:F:53:ASP:HA	1:M:24:ARG:NE	2.34	0.43
1:G:86:ILE:HG13	1:G:165:LEU:HD13	1.99	0.43
1:H:113:HIS:CD2	1:H:113:HIS:N	2.85	0.43
1:H:211:HIS:NE2	1:I:212:GLU:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:46:ILE:HD13	1:O:39:ILE:HG23	2.01	0.43
1:L:163:GLN:HG2	1:L:169:ASN:HA	2.01	0.43
1:N:97:GLU:OE1	1:N:97:GLU:HA	2.17	0.43
1:O:185:ARG:CG	1:O:185:ARG:NH1	2.77	0.43
1:D:187:ILE:HG13	1:D:187:ILE:O	2.18	0.43
1:K:162:LEU:HA	1:K:162:LEU:HD23	1.79	0.43
1:N:109:THR:HG22	1:N:110:CYS:O	2.18	0.43
1:O:50:LEU:O	1:O:51:ASN:HB2	2.19	0.43
1:A:217:VAL:HG12	1:A:218:ARG:N	2.33	0.43
1:D:14:LEU:HB3	1:D:20:GLU:HG2	2.00	0.43
1:F:212:GLU:HG2	1:J:214:LEU:CD1	2.49	0.43
1:I:109:THR:CG2	1:I:114:PHE:HA	2.49	0.43
1:J:79:ASP:O	1:J:81:ALA:N	2.52	0.43
1:J:153:ARG:O	1:J:157:GLN:HG3	2.18	0.43
1:K:99:VAL:O	1:K:124:ALA:HA	2.19	0.43
1:L:168:THR:HG22	1:L:170:ASN:H	1.83	0.43
1:F:80:TYR:C	1:F:82:ASN:N	2.77	0.42
1:M:168:THR:HG22	1:M:169:ASN:N	2.33	0.42
1:C:6:GLU:HB3	1:C:165:LEU:HD21	2.01	0.42
1:L:214:LEU:HB3	1:M:215:ARG:NH2	2.34	0.42
1:N:80:TYR:C	1:N:82:ASN:N	2.75	0.42
1:G:210:ARG:NH2	1:H:97:GLU:OE1	2.50	0.42
1:J:24:ARG:O	1:J:25:PRO:C	2.61	0.42
1:J:50:LEU:O	1:J:51:ASN:HB2	2.20	0.42
1:L:25:PRO:O	1:L:26:PRO:C	2.61	0.42
1:L:115:VAL:HG12	1:L:116:THR:N	2.34	0.42
1:A:135:SER:O	1:A:139:ARG:HG3	2.19	0.42
1:B:113:HIS:CD2	1:B:113:HIS:N	2.87	0.42
1:D:147:ARG:O	1:D:148:PRO:C	2.63	0.42
1:F:212:GLU:HA	1:F:215:ARG:CZ	2.50	0.42
1:J:39:ILE:O	1:J:40:ALA:C	2.61	0.42
1:M:113:HIS:CD2	1:M:113:HIS:N	2.87	0.42
1:B:4:SER:O	1:B:5:LYS:C	2.60	0.42
1:C:207:GLN:OE1	1:C:211:HIS:CE1	2.72	0.42
1:D:4:SER:O	1:D:5:LYS:C	2.62	0.42
1:F:185:ARG:NH2	3:G:3351:CL:CL	2.90	0.42
1:H:217:VAL:CG1	1:H:218:ARG:N	2.82	0.42
1:L:43:MET:HE2	1:L:66:ILE:CD1	2.48	0.42
1:M:72:ASP:O	1:M:76:SER:HB3	2.19	0.42
1:M:218:ARG:HD2	1:M:218:ARG:HA	1.84	0.42
1:O:109:THR:CG2	1:O:114:PHE:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ILE:O	1:E:143:PHE:HB3	2.20	0.42
1:I:53:ASP:C	1:I:55:ALA:N	2.76	0.42
1:K:6:GLU:HG2	1:K:86:ILE:HB	2.02	0.42
1:K:25:PRO:O	1:K:26:PRO:C	2.61	0.42
1:L:100:THR:HG23	1:L:124:ALA:HB2	2.01	0.42
1:M:163:GLN:HG2	1:M:168:THR:O	2.20	0.42
1:N:211:HIS:NE2	1:O:212:GLU:HG3	2.34	0.42
1:O:217:VAL:CG1	1:O:218:ARG:N	2.81	0.42
1:A:53:ASP:OD1	1:A:55:ALA:HB3	2.20	0.42
1:B:44:THR:HG23	1:B:54:LEU:HD11	2.01	0.42
1:D:185:ARG:CG	1:D:185:ARG:HH11	2.31	0.42
1:I:25:PRO:HA	1:I:26:PRO:HD3	1.85	0.42
1:J:185:ARG:HG2	1:J:185:ARG:NH1	2.35	0.42
1:N:119:GLY:HA3	1:N:177:ALA:CB	2.50	0.42
1:E:135:SER:O	1:E:139:ARG:HG3	2.19	0.42
1:I:154:LEU:HD12	1:I:154:LEU:O	2.19	0.42
1:J:139:ARG:NH1	3:J:3354:CL:CL	2.90	0.42
1:O:21:THR:O	1:O:22:PRO:C	2.63	0.42
1:O:150:VAL:O	1:O:151:GLN:C	2.63	0.42
1:F:123:VAL:HG22	1:F:173:VAL:HG22	2.01	0.42
1:G:53:ASP:HA	1:L:24:ARG:HG3	2.01	0.42
1:J:40:ALA:O	1:J:43:MET:N	2.53	0.42
1:K:9:LEU:HD23	1:K:9:LEU:HA	1.87	0.42
1:M:207:GLN:OE1	1:M:211:HIS:CE1	2.73	0.42
1:N:185:ARG:HG2	1:N:185:ARG:NH1	2.35	0.42
1:O:180:TYR:C	1:O:182:VAL:H	2.27	0.42
1:A:213:PHE:O	1:A:217:VAL:HG23	2.20	0.41
1:E:136:LYS:HA	1:E:136:LYS:HD3	1.76	0.41
1:G:22:PRO:O	1:G:23:LEU:HD12	2.19	0.41
1:I:132:ILE:HG12	1:I:133:GLY:N	2.35	0.41
1:J:11:HIS:O	1:J:15:VAL:HG23	2.21	0.41
1:J:24:ARG:CZ	1:N:54:LEU:H	2.32	0.41
1:K:79:ASP:O	1:K:81:ALA:N	2.53	0.41
1:L:109:THR:CG2	1:L:114:PHE:HA	2.49	0.41
1:L:185:ARG:NH1	1:L:185:ARG:CG	2.82	0.41
1:C:108:SER:OG	1:C:109:THR:N	2.52	0.41
1:C:171:VAL:HG12	1:C:172:ALA:N	2.36	0.41
1:G:185:ARG:NH1	1:L:73:GLU:OE1	2.54	0.41
1:K:174:SER:OG	1:K:197:THR:HG22	2.21	0.41
1:B:187:ILE:O	1:B:187:ILE:HG13	2.19	0.41
1:H:48:GLN:HE21	1:K:24:ARG:HH12	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:111:GLU:HB2	1:N:59:LEU:HD21	2.02	0.41
1:O:101:VAL:HG21	1:O:137:ILE:HD12	2.02	0.41
1:D:6:GLU:H	1:D:6:GLU:CD	2.28	0.41
1:D:106:LEU:C	1:D:106:LEU:HD23	2.45	0.41
1:F:185:ARG:NH1	1:F:185:ARG:CG	2.83	0.41
1:H:32:ASN:O	1:H:36:LYS:HG3	2.20	0.41
1:H:159:LEU:CD2	1:H:198:SER:HB3	2.46	0.41
1:O:44:THR:O	1:O:48:GLN:HG3	2.21	0.41
1:A:88:LEU:HD23	1:A:132:ILE:HA	2.03	0.41
1:C:200:GLY:O	1:C:201:GLY:C	2.64	0.41
1:G:59:LEU:CD2	1:L:111:GLU:HB2	2.50	0.41
1:G:147:ARG:O	1:G:148:PRO:C	2.63	0.41
1:J:24:ARG:NH2	1:N:54:LEU:N	2.65	0.41
1:K:156:GLN:O	1:K:160:ILE:HG12	2.20	0.41
1:N:185:ARG:HH11	1:N:185:ARG:HG3	1.83	0.41
1:D:115:VAL:CG1	1:D:116:THR:N	2.84	0.41
1:I:47:MET:HB3	1:I:54:LEU:HD21	2.02	0.41
1:J:53:ASP:C	1:J:55:ALA:N	2.78	0.41
1:D:21:THR:O	1:D:23:LEU:HD22	2.21	0.41
1:E:82:ASN:O	1:E:83:PHE:C	2.64	0.41
1:E:137:ILE:O	1:E:138:ASN:C	2.64	0.41
1:F:109:THR:HG22	1:F:114:PHE:HA	2.02	0.41
1:G:48:GLN:C	1:G:50:LEU:H	2.29	0.41
1:G:90:GLU:OE2	1:G:92:LYS:HG2	2.21	0.41
1:G:93:MET:HE2	1:G:93:MET:HB2	1.87	0.41
1:I:217:VAL:HG12	1:I:218:ARG:H	1.86	0.41
1:J:79:ASP:C	1:J:81:ALA:N	2.77	0.41
1:K:142:GLN:OE1	1:K:142:GLN:HA	2.19	0.41
1:L:149:GLN:HE21	1:L:154:LEU:CD1	2.27	0.41
1:N:62:THR:O	1:N:66:ILE:HG13	2.21	0.41
1:F:113:HIS:O	1:F:114:PHE:HB2	2.20	0.41
1:F:139:ARG:NH1	3:F:3355:CL:CL	2.91	0.41
1:H:211:HIS:O	1:H:215:ARG:HB2	2.21	0.41
1:I:53:ASP:HA	1:O:24:ARG:HG3	2.03	0.41
1:J:39:ILE:HG23	1:N:46:ILE:HG12	2.03	0.41
1:L:112:HIS:HB2	4:L:3342:HOH:O	2.19	0.41
1:N:38:LEU:O	1:N:42:HIS:CD2	2.74	0.41
1:N:98:MET:HE3	1:N:124:ALA:CB	2.50	0.41
1:A:13:ALA:O	1:A:17:ARG:HD3	2.20	0.41
1:A:109:THR:CG2	1:A:114:PHE:HA	2.51	0.41
1:A:208:ASN:CG	1:E:207:GLN:NE2	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HG2	1:B:186:GLY:N	2.36	0.41
1:C:210:ARG:HH22	1:D:97:GLU:CD	2.28	0.41
1:D:109:THR:HG22	1:D:114:PHE:HA	2.00	0.41
1:E:175:ILE:O	1:E:195:THR:HA	2.21	0.41
1:I:88:LEU:HD23	1:I:132:ILE:HA	2.03	0.41
1:I:128:LYS:HB2	1:I:168:THR:OG1	2.20	0.41
1:K:185:ARG:HG2	1:K:185:ARG:HH11	1.85	0.41
1:L:160:ILE:O	1:L:161:ALA:C	2.63	0.41
1:M:14:LEU:HA	1:M:14:LEU:HD23	1.90	0.41
1:N:115:VAL:CG1	1:N:116:THR:N	2.83	0.41
1:N:135:SER:O	1:N:139:ARG:HG3	2.20	0.41
1:E:218:ARG:HA	1:E:218:ARG:HD2	1.96	0.41
1:K:44:THR:O	1:K:48:GLN:HG3	2.21	0.41
1:K:215:ARG:NH1	1:O:214:LEU:HB3	2.36	0.41
1:C:6:GLU:O	1:C:7:ALA:C	2.64	0.40
1:D:62:THR:N	1:D:63:PRO:CD	2.84	0.40
1:D:158:ILE:HG22	1:D:173:VAL:HG21	2.03	0.40
1:F:45:GLU:OE1	1:M:42:HIS:HE1	2.03	0.40
1:G:13:ALA:O	1:G:17:ARG:HD3	2.21	0.40
1:J:44:THR:HG23	1:J:54:LEU:HD13	2.04	0.40
1:J:54:LEU:HB2	1:N:24:ARG:HH22	1.86	0.40
1:K:212:GLU:HG3	1:O:211:HIS:NE2	2.36	0.40
1:L:126:ILE:HA	1:L:127:PRO:HD3	1.86	0.40
1:L:136:LYS:HD3	1:L:136:LYS:HA	1.77	0.40
1:M:53:ASP:OD1	1:M:55:ALA:HB3	2.22	0.40
1:A:126:ILE:HA	1:A:127:PRO:HD3	1.89	0.40
1:G:138:ASN:H	1:G:138:ASN:ND2	2.19	0.40
1:I:24:ARG:HG3	1:O:53:ASP:CA	2.51	0.40
1:I:58:SER:OG	1:O:112:HIS:HE1	2.04	0.40
1:B:155:THR:HG22	1:B:198:SER:OG	2.21	0.40
1:G:24:ARG:HG3	1:L:53:ASP:HA	2.03	0.40
1:G:109:THR:CG2	1:G:114:PHE:HA	2.52	0.40
1:L:119:GLY:C	1:L:120:LYS:HD2	2.46	0.40
1:N:199:LEU:HD12	1:N:210:ARG:NH1	2.36	0.40
1:A:86:ILE:HG13	1:A:165:LEU:HD13	2.04	0.40
1:D:79:ASP:OD1	1:D:79:ASP:C	2.64	0.40
1:H:53:ASP:C	1:H:53:ASP:OD1	2.65	0.40
1:M:160:ILE:O	1:M:161:ALA:C	2.64	0.40
1:N:150:VAL:HG13	1:N:152:GLU:OE1	2.22	0.40
1:O:80:TYR:C	1:O:82:ASN:H	2.28	0.40
1:O:92:LYS:C	1:O:94:LYS:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:HIS:O	1:O:114:PHE:HB2	2.20	0.40
1:A:106:LEU:HD11	1:A:154:LEU:HD21	2.04	0.40
1:C:56:ASP:O	1:C:60:MET:HB2	2.22	0.40
1:K:48:GLN:HG2	1:K:54:LEU:HD12	2.03	0.40
1:K:183:LYS:HG3	1:K:190:ALA:HA	2.03	0.40
1:N:168:THR:HG21	1:N:170:ASN:HB2	2.04	0.40
1:O:79:ASP:C	1:O:81:ALA:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/221 (99%)	206 (94%)	9 (4%)	4 (2%)	6	23
1	B	219/221 (99%)	204 (93%)	11 (5%)	4 (2%)	6	23
1	C	219/221 (99%)	200 (91%)	13 (6%)	6 (3%)	4	15
1	D	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	9	30
1	E	219/221 (99%)	199 (91%)	14 (6%)	6 (3%)	4	15
1	F	219/221 (99%)	196 (90%)	17 (8%)	6 (3%)	4	15
1	G	219/221 (99%)	195 (89%)	20 (9%)	4 (2%)	6	23
1	H	219/221 (99%)	202 (92%)	11 (5%)	6 (3%)	4	15
1	I	219/221 (99%)	197 (90%)	16 (7%)	6 (3%)	4	15
1	J	219/221 (99%)	196 (90%)	18 (8%)	5 (2%)	5	18
1	K	219/221 (99%)	201 (92%)	14 (6%)	4 (2%)	6	23
1	L	219/221 (99%)	191 (87%)	24 (11%)	4 (2%)	6	23
1	M	219/221 (99%)	199 (91%)	14 (6%)	6 (3%)	4	15
1	N	219/221 (99%)	196 (90%)	16 (7%)	7 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	219/221 (99%)	197 (90%)	16 (7%)	6 (3%)	4	15
All	All	3285/3315 (99%)	2979 (91%)	229 (7%)	77 (2%)	5	18

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	218	ARG
1	B	27	VAL
1	F	27	VAL
1	K	27	VAL
1	A	29	GLU
1	B	29	GLU
1	C	26	PRO
1	C	27	VAL
1	C	220	HIS
1	D	27	VAL
1	D	220	HIS
1	E	27	VAL
1	E	220	HIS
1	F	29	GLU
1	F	31	ASP
1	F	220	HIS
1	G	27	VAL
1	G	218	ARG
1	G	220	HIS
1	H	27	VAL
1	H	29	GLU
1	H	218	ARG
1	H	220	HIS
1	I	29	GLU
1	I	220	HIS
1	J	27	VAL
1	J	29	GLU
1	K	29	GLU
1	K	218	ARG
1	L	27	VAL
1	L	29	GLU
1	M	27	VAL
1	M	29	GLU
1	M	220	HIS
1	N	27	VAL

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Mol	Chain	Res	Type
1	N	29	GLU
1	N	57	ASP
1	O	29	GLU
1	C	29	GLU
1	C	218	ARG
1	E	29	GLU
1	E	218	ARG
1	G	29	GLU
1	I	5	LYS
1	I	27	VAL
1	J	220	HIS
1	K	80	TYR
1	L	220	HIS
1	N	22	PRO
1	N	26	PRO
1	N	220	HIS
1	O	27	VAL
1	O	218	ARG
1	O	220	HIS
1	B	218	ARG
1	H	54	LEU
1	J	80	TYR
1	M	80	TYR
1	O	22	PRO
1	B	220	HIS
1	D	218	ARG
1	F	218	ARG
1	J	218	ARG
1	M	22	PRO
1	M	218	ARG
1	N	201	GLY
1	O	80	TYR
1	C	22	PRO
1	E	57	ASP
1	I	54	LEU
1	I	22	PRO
1	E	22	PRO
1	F	22	PRO
1	H	22	PRO
1	L	22	PRO
1	A	22	PRO

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	194/194 (100%)	186 (96%)	8 (4%)	27	62
1	B	194/194 (100%)	185 (95%)	9 (5%)	24	58
1	C	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	D	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	E	194/194 (100%)	180 (93%)	14 (7%)	13	39
1	F	194/194 (100%)	189 (97%)	5 (3%)	40	75
1	G	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	H	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	I	194/194 (100%)	179 (92%)	15 (8%)	12	36
1	J	194/194 (100%)	187 (96%)	7 (4%)	31	66
1	K	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	L	194/194 (100%)	187 (96%)	7 (4%)	31	66
1	M	194/194 (100%)	180 (93%)	14 (7%)	13	39
1	N	194/194 (100%)	184 (95%)	10 (5%)	21	53
1	O	194/194 (100%)	183 (94%)	11 (6%)	18	49
All	All	2910/2910 (100%)	2755 (95%)	155 (5%)	20	52

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	23	LEU
1	A	93	MET
1	A	113	HIS
1	A	130	SER
1	A	150	VAL
1	A	168	THR
1	A	185	ARG
1	B	23	LEU
1	B	37	SER

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Mol	Chain	Res	Type
1	B	93	MET
1	B	113	HIS
1	B	120	LYS
1	B	130	SER
1	B	150	VAL
1	B	168	THR
1	B	185	ARG
1	C	23	LEU
1	C	31	ASP
1	C	93	MET
1	C	107	THR
1	C	110	CYS
1	C	113	HIS
1	C	130	SER
1	C	150	VAL
1	C	185	ARG
1	C	197	THR
1	C	199	LEU
1	D	4	SER
1	D	21	THR
1	D	23	LEU
1	D	93	MET
1	D	113	HIS
1	D	130	SER
1	D	150	VAL
1	D	168	THR
1	D	185	ARG
1	D	197	THR
1	D	208	ASN
1	E	20	GLU
1	E	23	LEU
1	E	57	ASP
1	E	93	MET
1	E	98	MET
1	E	113	HIS
1	E	130	SER
1	E	131	VAL
1	E	139	ARG
1	E	150	VAL
1	E	168	THR
1	E	185	ARG
1	E	197	THR

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Mol	Chain	Res	Type
1	E	208	ASN
1	F	20	GLU
1	F	93	MET
1	F	113	HIS
1	F	150	VAL
1	F	185	ARG
1	G	9	LEU
1	G	23	LEU
1	G	93	MET
1	G	113	HIS
1	G	120	LYS
1	G	130	SER
1	G	150	VAL
1	G	164	THR
1	G	168	THR
1	G	185	ARG
1	G	197	THR
1	H	20	GLU
1	H	23	LEU
1	H	31	ASP
1	H	63	PRO
1	H	109	THR
1	H	113	HIS
1	H	120	LYS
1	H	130	SER
1	H	139	ARG
1	H	150	VAL
1	H	185	ARG
1	I	9	LEU
1	I	17	ARG
1	I	23	LEU
1	I	37	SER
1	I	87	THR
1	I	93	MET
1	I	100	THR
1	I	107	THR
1	I	113	HIS
1	I	130	SER
1	I	139	ARG
1	I	150	VAL
1	I	163	GLN
1	I	185	ARG

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Mol	Chain	Res	Type
1	I	194	THR
1	J	93	MET
1	J	106	LEU
1	J	113	HIS
1	J	150	VAL
1	J	168	THR
1	J	185	ARG
1	J	208	ASN
1	K	20	GLU
1	K	23	LEU
1	K	93	MET
1	K	107	THR
1	K	113	HIS
1	K	120	LYS
1	K	146	GLN
1	K	150	VAL
1	K	168	THR
1	K	176	ASP
1	K	185	ARG
1	L	20	GLU
1	L	93	MET
1	L	113	HIS
1	L	130	SER
1	L	139	ARG
1	L	150	VAL
1	L	185	ARG
1	M	9	LEU
1	M	20	GLU
1	M	23	LEU
1	M	30	MET
1	M	93	MET
1	M	107	THR
1	M	113	HIS
1	M	130	SER
1	M	139	ARG
1	M	155	THR
1	M	163	GLN
1	M	168	THR
1	M	185	ARG
1	M	208	ASN
1	N	23	LEU
1	N	72	ASP

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Mol	Chain	Res	Type
1	N	93	MET
1	N	107	THR
1	N	113	HIS
1	N	150	VAL
1	N	163	GLN
1	N	185	ARG
1	N	199	LEU
1	N	208	ASN
1	O	9	LEU
1	O	20	GLU
1	O	22	PRO
1	O	23	LEU
1	O	93	MET
1	O	107	THR
1	O	113	HIS
1	O	131	VAL
1	O	163	GLN
1	O	168	THR
1	O	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	138	ASN
1	B	113	HIS
1	B	138	ASN
1	B	207	GLN
1	B	211	HIS
1	C	112	HIS
1	C	113	HIS
1	C	138	ASN
1	C	207	GLN
1	D	113	HIS
1	D	138	ASN
1	D	156	GLN
1	D	163	GLN
1	E	113	HIS
1	E	146	GLN
1	E	163	GLN
1	E	207	GLN
1	E	208	ASN

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Mol	Chain	Res	Type
1	F	48	GLN
1	F	113	HIS
1	F	138	ASN
1	F	146	GLN
1	F	207	GLN
1	F	211	HIS
1	G	48	GLN
1	G	113	HIS
1	G	138	ASN
1	G	163	GLN
1	H	48	GLN
1	H	113	HIS
1	H	157	GLN
1	H	163	GLN
1	H	170	ASN
1	H	207	GLN
1	I	48	GLN
1	I	113	HIS
1	I	146	GLN
1	I	163	GLN
1	J	42	HIS
1	J	48	GLN
1	J	113	HIS
1	J	146	GLN
1	J	163	GLN
1	J	207	GLN
1	J	208	ASN
1	K	48	GLN
1	K	64	HIS
1	K	113	HIS
1	K	207	GLN
1	L	48	GLN
1	L	113	HIS
1	L	157	GLN
1	L	163	GLN
1	M	48	GLN
1	M	113	HIS
1	M	138	ASN
1	M	146	GLN
1	M	151	GLN
1	M	163	GLN
1	N	48	GLN

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Mol	Chain	Res	Type
1	N	113	HIS
1	N	163	GLN
1	N	207	GLN
1	O	48	GLN
1	O	112	HIS
1	O	113	HIS
1	O	138	ASN
1	O	146	GLN
1	O	163	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.