



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 01:11 pm GMT

PDB ID : 5TB1
EMDB ID: : EMD-8392
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

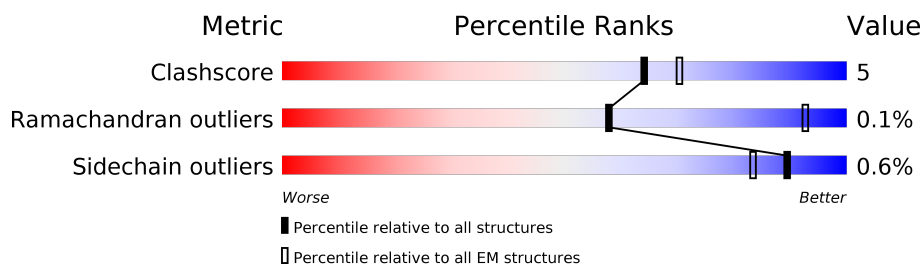
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	108	74% 25% .
1	F	108	73% 26% .
1	H	108	76% 23% .
1	J	108	77% 22% .
2	B	4416	84% 11% 5%
2	E	4416	84% 11% 5%
2	G	4416	84% 11% 5%
2	I	4416	84% 11% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

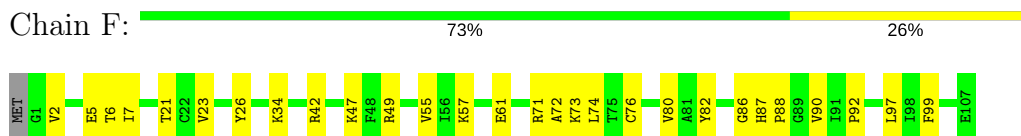
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

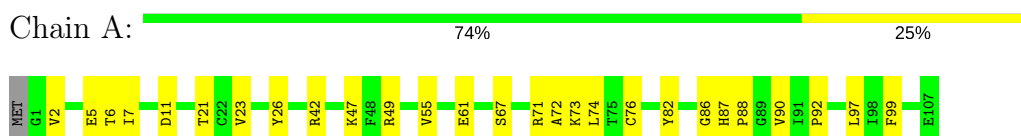
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

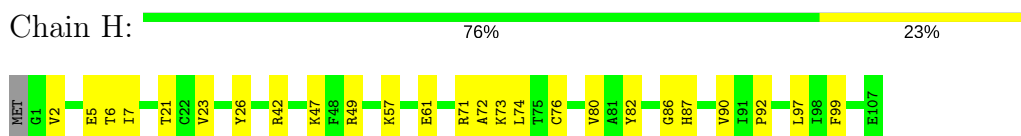
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



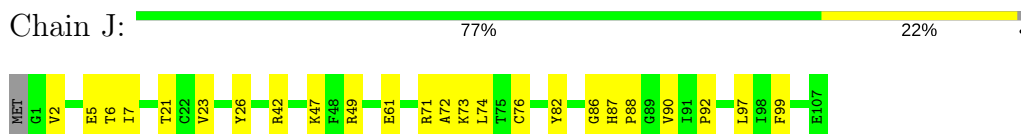
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



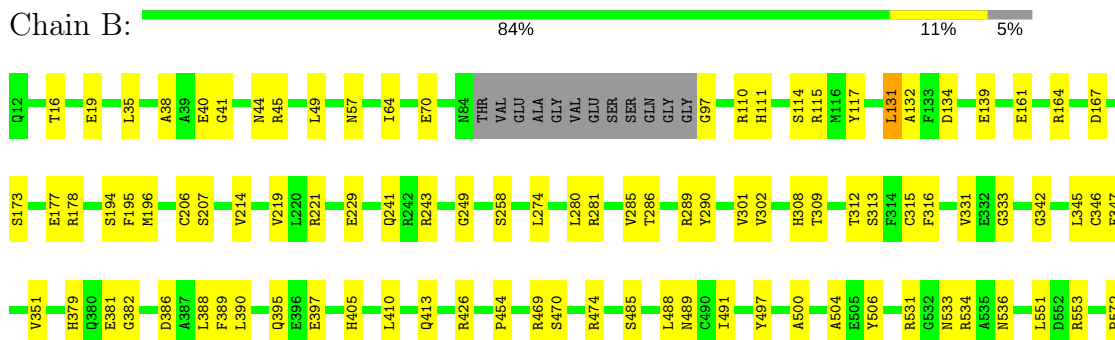
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



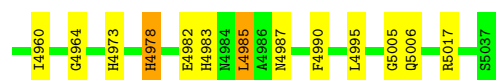
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

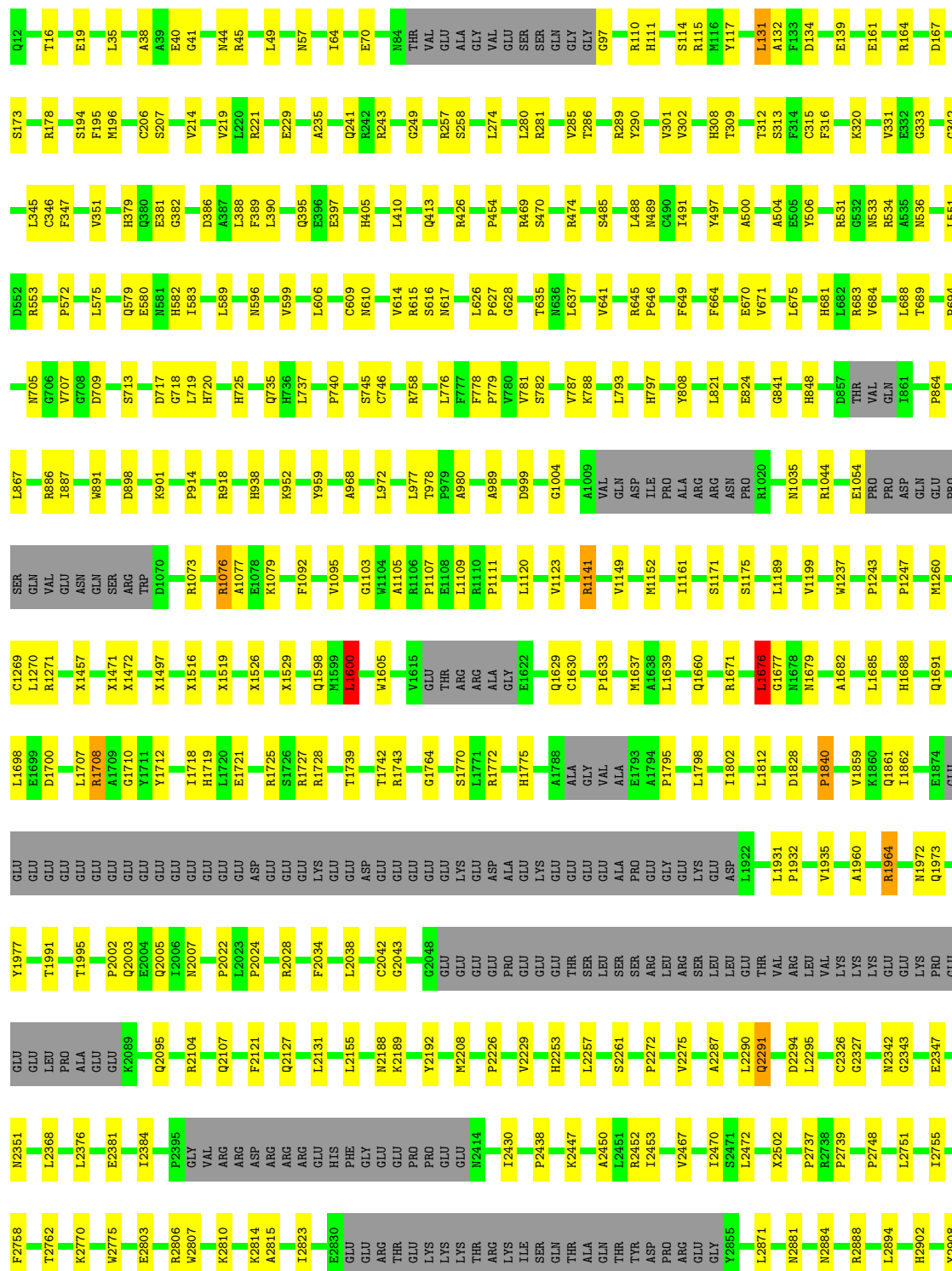


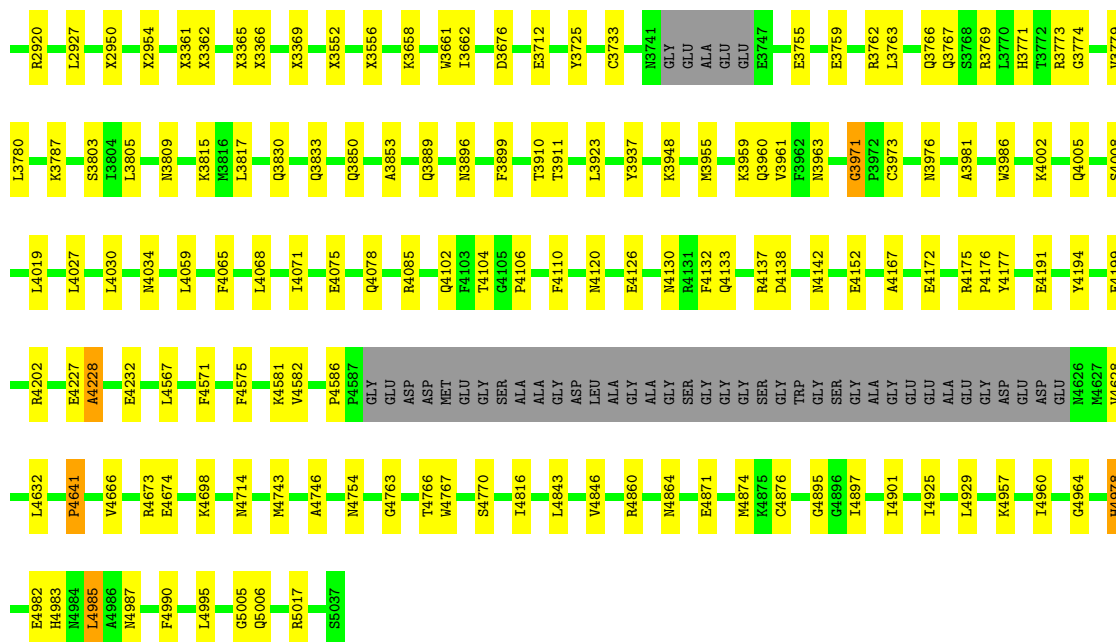


• Molecule 2: Ryanodine receptor 1

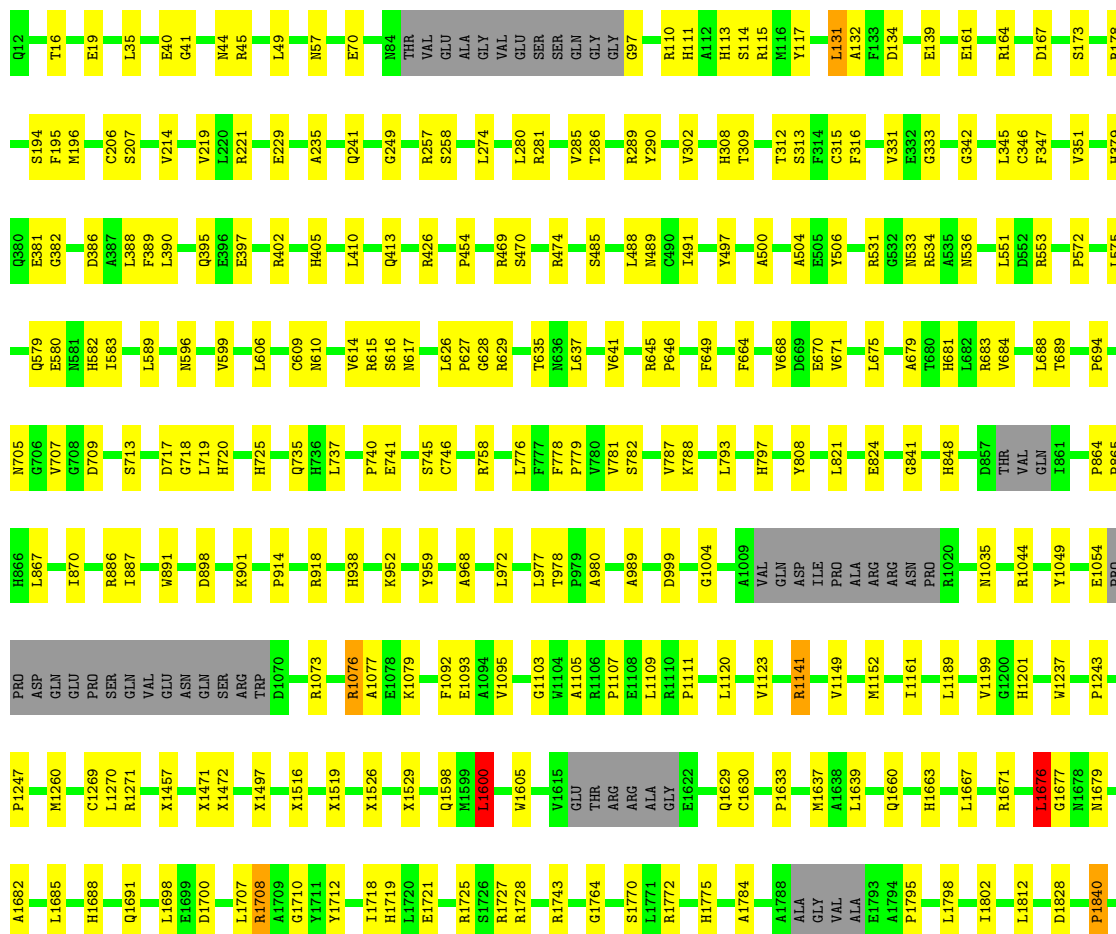
Chain I: 84% 11% 5%

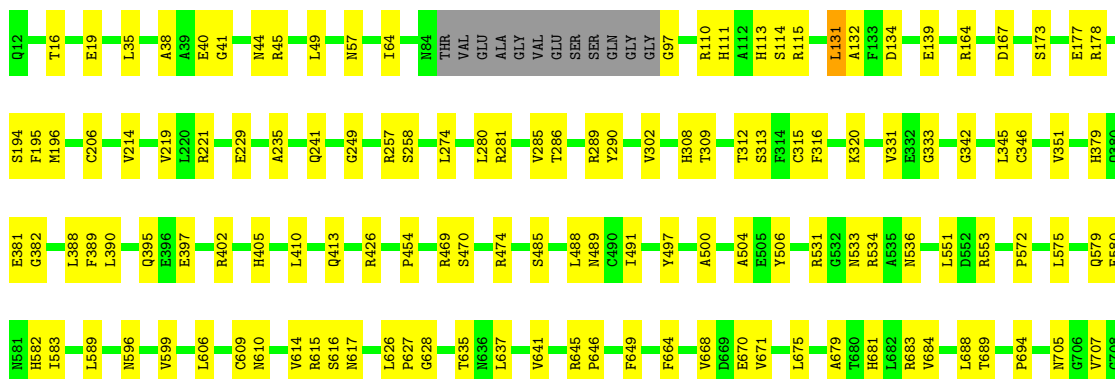




• Molecule 2: Ryanodine receptor 1

Chain E: 84% 11% 5%





N4987	R4673	F4551	L4059	X3365	K2810	GLY	R2104	Q2003	L1707	X1457	TRP	D709
F4990	E4674	L4567	F4065	X3366	K2814	VAL	Q2107	E2004	R1708	X1471	D1070	S713
L4995	K4698	F4571	F4068	X3369	A2815	ARG	F2121	L2006	G1710	X1472	R1073	D717
G5005	N4714	F4575	L4068	X3552	I2823	ARG	Q2127	P2022	Y1712	X1497	R1076	G718
Q5006	M4743	K4581	I4071	X3556	E2830	ARG	L2131	L2023	I1718	X1516	A1077	L719
R5017	V4582	V4582	E4075	K3658	E2830	GLU	L2155	P2024	H1719	X1519	K1079	H720
S5037	A4746	P4586	Q4078	X3658	E2830	HIS	L2155	R2028	L1720	X1519	F1092	H725
	N4754	P4587	Q4078	X3661	E2830	GLY	L2155	R2028	E1721	X1526	E1093	Q735
	G4763	GLY	R4085	I3662	E2830	GLY	N2188	C2042	R1725	X1526	A1094	H736
	V4767	ASP	Q4102	D3676	E2830	GLY	K2189	G2043	S1726	X1529	V1095	L737
	S4770	ASP	F4103	T3911	E2830	PRO	Y2192	G2048	R1727	Q1598	G1103	P740
	I4816	GLY	T4104	L3923	E2830	PRO	W2208	GLY	R1728	M1599	A1104	E741
	L4843	SER	G4105	Y3937	E2830	GLY	P2226	GLY	R1743	L1600	A1105	S745
	R4860	ALA	P4106	N3741	E2830	GLY	V2229	GLY	G1764	W1605	R1106	C746
	N4864	GLY	F4110	N3741	E2830	GLY	H2253	GLY	S1770	V1615	E1108	R758
	E4871	GLY	N4120	GLY	E2830	GLY	L2257	GLY	L1771	GLY	R1110	L776
	R4874	ASP	E4126	ALA	E2830	GLY	P2272	GLY	R1772	THR	P1111	L776
	C4876	GLY	K3959	GLY	E2830	GLY	V2275	GLY	H1775	ARG	L1120	F777
	R4892	GLY	Q3960	GLY	E2830	GLY	A2287	GLY	G1775	ALA	G1004	P779
	I4897	TRP	V3961	GLY	E2830	GLY	S2261	GLY	A1788	E1622	V1123	V780
	I4901	SER	F3962	GLY	E2830	GLY	P2272	GLY	ALA	VAL	R1141	S782
	I4925	ALA	C3971	GLY	E2830	GLY	V2275	GLY	GLY	Q1629	R1141	S782
	L4928	GLY	P3972	GLY	E2830	GLY	L2290	GLY	VAL	C1630	V1149	V787
	L4929	GLY	C3973	GLY	E2830	GLY	D2294	GLY	ALA	P1633	M1152	K788
	K4957	GLY	L3763	GLY	E2830	GLY	L2295	GLY	PRO	M1637	M1152	L793
	I4960	ASP	E3765	GLY	E2830	GLY	C2326	GLY	ALA	I1161	I1161	L793
	G4964	GLY	E3766	GLY	E2830	GLY	Q2327	GLY	ARG	ARG	S1171	H797
	H4973	GLY	Q3767	GLY	E2830	GLY	D2294	GLY	ASN	ARG	G1171	Y808
	H4978	GLY	R3768	GLY	E2830	GLY	L2295	GLY	PRO	ARG	S1175	Y808
	E4982	GLY	N2881	GLY	E2830	GLY	C2326	GLY	VAL	Q1660	R1020	L821
	N4983	GLY	N2884	GLY	E2830	GLY	Q2342	GLY	L1812	R1671	L1189	L821
	L4985	GLY	N2888	GLY	E2830	GLY	E2347	GLY	L1932	R1671	P1190	E824
	L4986	GLY	R2889	GLY	E2830	GLY	N2342	GLY	L1935	R1671	P1190	E824
		GLY	R2890	GLY	E2830	GLY	C2343	GLY	P1840	L1677	V1199	G841
		GLY	R2902	GLY	E2830	GLY	L2751	GLY	P1840	N1678	G1200	G841
		GLY	R2908	GLY	E2830	GLY	L2755	GLY	V1859	N1679	H1201	H848
		GLY	R2920	GLY	E2830	GLY	F2758	GLY	K1860	A1682	W1237	D857
		GLY	R2927	GLY	E2830	GLY	T2762	GLY	I1862	A1682	P1243	VAL
		GLY	L2927	GLY	E2830	GLY	L2368	GLY	L1685	L1685	P1243	VAL
		GLY	L2950	GLY	E2830	GLY	K2770	GLY	GLY	H1688	P1247	GLN
		GLY	X2954	GLY	E2830	GLY	W2775	GLY	GLY	Q1691	M1260	P864
		GLY	X2954	GLY	E2830	GLY	E2803	GLY	GLY	L1698	C1269	L867
		GLY	X3361	GLY	E2830	GLY	I2384	GLY	GLY	E1699	L1270	L867
		GLY	X3362	GLY	E2830	GLY	R2806	GLY	GLY	D1700	R1271	R886
		GLY	X3362	GLY	E2830	GLY	R2807	GLY	GLY	D1700	R1271	R886

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.53	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.29	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	24/142628 (0.0%)

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
2	B	0	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	64

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.01	133.72	115.30
2	B	131	LEU	CA-CB-CG	8.00	133.69	115.30
2	E	131	LEU	CA-CB-CG	7.99	133.68	115.30
2	I	131	LEU	CA-CB-CG	7.99	133.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4985	LEU	CA-CB-CG	7.25	131.97	115.30
2	I	4985	LEU	CA-CB-CG	7.25	131.97	115.30
2	E	4985	LEU	CA-CB-CG	7.25	131.96	115.30
2	G	4985	LEU	CA-CB-CG	7.24	131.95	115.30
2	B	1600	LEU	CA-CB-CG	6.59	130.46	115.30
2	I	1600	LEU	CA-CB-CG	6.59	130.46	115.30
2	E	1600	LEU	CA-CB-CG	6.59	130.45	115.30
2	G	1600	LEU	CA-CB-CG	6.58	130.42	115.30
2	E	1676	LEU	CA-CB-CG	6.56	130.38	115.30
2	I	1676	LEU	CA-CB-CG	6.55	130.38	115.30
2	B	1676	LEU	CA-CB-CG	6.55	130.37	115.30
2	G	1676	LEU	CA-CB-CG	6.55	130.36	115.30
2	E	977	LEU	CA-CB-CG	5.71	128.43	115.30
2	I	977	LEU	CA-CB-CG	5.70	128.41	115.30
2	G	977	LEU	CA-CB-CG	5.70	128.40	115.30
2	B	977	LEU	CA-CB-CG	5.69	128.39	115.30
2	I	688	LEU	CA-CB-CG	5.09	127.02	115.30
2	E	688	LEU	CA-CB-CG	5.08	126.99	115.30
2	B	688	LEU	CA-CB-CG	5.07	126.97	115.30
2	G	688	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4228	ALA	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4228	ALA	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4228	ALA	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	I	4228	ALA	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	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	818	0	824	16	0
1	F	818	0	824	18	0
1	H	818	0	824	15	0
1	J	818	0	824	14	0
2	B	29499	0	24746	268	0
2	E	29499	0	24746	273	0
2	G	29499	0	24746	261	0
2	I	29499	0	24746	262	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121272	0	102280	1100	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 5.

All (1100) 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)
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.68
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.66
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.61	0.65
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.61	0.65
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.62	0.64
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.61	0.64
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.79	0.64
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.61	0.64
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.79	0.64
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.81	0.63
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.81	0.63
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.81	0.63
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.79	0.62
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.79	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.81	0.62
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.62
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.32	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.32	0.61
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.65	0.61
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.82	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.82	0.61
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.32	0.61
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.82	0.61
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.82	0.61
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.83	0.61
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.61
2:G:3755:GLU:O	2:G:3762:ARG:NH2	2.34	0.61
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.61
2:I:3755:GLU:O	2:I:3762:ARG:NH2	2.34	0.61
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.83	0.60
2:B:3755:GLU:O	2:B:3762:ARG:NH2	2.34	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.60
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.83	0.60
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.83	0.60
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.82	0.60
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.82	0.60
2:E:3755:GLU:O	2:E:3762:ARG:NH2	2.34	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.82	0.60
2:I:683:ARG:NH1	2:I:707:VAL:O	2.34	0.60
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.35	0.60
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.35	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.60
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.59
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.84	0.59
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.59
2:I:331:VAL:HG12	2:I:333:GLY:H	1.66	0.59
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.83	0.59
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.83	0.59
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.82	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
2:E:683:ARG:NH1	2:E:707:VAL:O	2.34	0.59
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.85	0.59
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.85	0.58
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.85	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.35	0.58
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.84	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.58
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.85	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.58
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.86	0.58
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.37	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.57
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.37	0.57
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.85	0.57
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.37	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.57
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.69	0.57
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.87	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.57
2:E:132:ALA:HA	2:E:194:SER:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:614:VAL:HG22	2:G:616:SER:H	1.69	0.57
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.37	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.69	0.56
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.86	0.56
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.69	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.69	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.87	0.56
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.69	0.56
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.87	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.88	0.56
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.87	0.56
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.86	0.56
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.39	0.56
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.88	0.56
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.39	0.56
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.86	0.56
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.39	0.56
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.39	0.56
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.87	0.56
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.39	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.87	0.56
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.88	0.56
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.39	0.56
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.88	0.56
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.87	0.56
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.87	0.56
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.88	0.56
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.88	0.56
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.88	0.56
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.87	0.56
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.88	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.56
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.88	0.56
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.88	0.56
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.88	0.56
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.87	0.55
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.87	0.55
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.89	0.55
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.88	0.55
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.88	0.55
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.39	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.39	0.55
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.88	0.55
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.55
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.89	0.55
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.39	0.55
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.40	0.55
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.39	0.55
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.38	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.87	0.55
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.88	0.55
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.89	0.55
2:B:683:ARG:NH1	2:B:707:VAL:O	2.34	0.55
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.39	0.55
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.55
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.72	0.55
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.89	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.55
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.89	0.55
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.40	0.55
2:E:614:VAL:HG22	2:E:616:SER:H	1.69	0.55
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.88	0.55
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.39	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.39	0.55
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.69	0.55
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.88	0.55
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.40	0.55
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.89	0.55
2:I:241:GLN:O	2:I:289:ARG:NH1	2.37	0.55
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.88	0.55
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.72	0.55
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.40	0.55
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.40	0.55
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.89	0.55
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.89	0.55
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.72	0.55
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.88	0.55
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.72	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.33	0.54
2:I:164:ARG:N	2:I:167:ASP:OD2	2.41	0.54
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.88	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.88	0.54
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.40	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.54
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.89	0.54
2:E:4763:GLY:H	2:E:4767:TRP:HE1	1.56	0.54
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.41	0.54
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.88	0.54
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.90	0.54
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.41	0.54
2:B:4763:GLY:H	2:B:4767:TRP:HE1	1.56	0.54
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.89	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.80	0.54
2:G:4763:GLY:H	2:G:4767:TRP:HE1	1.56	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.89	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.72	0.54
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.40	0.54
2:G:164:ARG:N	2:G:167:ASP:OD2	2.41	0.54
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.90	0.54
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.88	0.54
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.54
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.54
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.54
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.90	0.53
2:G:241:GLN:O	2:G:289:ARG:NH1	2.37	0.53
2:G:609:CYS:SG	2:G:610:ASN:N	2.80	0.53
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.53
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.73	0.53
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.41	0.53
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.53
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.41	0.53
2:B:609:CYS:SG	2:B:610:ASN:N	2.80	0.53
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.91	0.53
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.73	0.53
2:I:2347:GLU:O	2:I:2351:ASN:N	2.39	0.53
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.73	0.53
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.53
2:E:164:ARG:N	2:E:167:ASP:OD2	2.41	0.53
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.53
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.90	0.53
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.73	0.53
2:I:4763:GLY:H	2:I:4767:TRP:HE1	1.56	0.53
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.53
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.53
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.82	0.53
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.53
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.41	0.53
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.82	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.39	0.53
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.73	0.53
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.91	0.53
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.53
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.42	0.53
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.91	0.53
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.53
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.53
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.91	0.53
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.41	0.53
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.82	0.53
2:B:164:ARG:N	2:B:167:ASP:OD2	2.41	0.52
2:G:290:TYR:O	2:G:302:VAL:N	2.43	0.52
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.90	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.40	0.52
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.74	0.52
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.74	0.52
2:G:645:ARG:N	2:G:824:GLU:O	2.40	0.52
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.74	0.52
2:B:2347:GLU:O	2:B:2351:ASN:N	2.39	0.52
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.75	0.52
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.73	0.52
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.91	0.52
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.52
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.91	0.52
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.42	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.92	0.52
2:E:290:TYR:O	2:E:302:VAL:N	2.42	0.52
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.75	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.41	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.92	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.92	0.52
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.43	0.52
2:E:1660:GLN:HG3	2:E:1707:LEU:HD13	1.92	0.52
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.82	0.52
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.43	0.52
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.43	0.52
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.91	0.52
2:I:290:TYR:O	2:I:302:VAL:N	2.42	0.52
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.74	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.52
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.42	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.74	0.52
2:B:1660:GLN:HG3	2:B:1707:LEU:HD13	1.92	0.52
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.91	0.52
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.74	0.52
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.74	0.52
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.92	0.51
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.92	0.51
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.44	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.51
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.91	0.51
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.91	0.51
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.93	0.51
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.43	0.51
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.43	0.51
2:B:290:TYR:O	2:B:302:VAL:N	2.43	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.43	0.51
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.51
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.91	0.51
2:B:3984:ARG:HH22	2:I:161:GLU:HG2	1.74	0.51
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.93	0.51
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.75	0.51
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.43	0.51
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.93	0.51
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.93	0.51
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.51
2:I:645:ARG:N	2:I:824:GLU:O	2.40	0.51
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.92	0.51
2:B:241:GLN:O	2:B:289:ARG:NH1	2.37	0.51
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.44	0.51
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.39	0.51
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.92	0.51
2:G:1660:GLN:HG3	2:G:1707:LEU:HD13	1.92	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.51
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.91	0.51
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:I:2452:ARG:HH12	2:G:177:GLU:HG3	1.76	0.51
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.93	0.51
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.41	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.93	0.51
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.43	0.51
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.93	0.51
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.75	0.51
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.75	0.51
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.44	0.51
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.43	0.51
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.93	0.51
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.93	0.51
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.92	0.50
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.43	0.50
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.93	0.50
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.92	0.50
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.50
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.50
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.92	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.50
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.42	0.50
2:G:470:SER:O	2:G:474:ARG:NE	2.40	0.50
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.75	0.50
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.93	0.50
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.75	0.50
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.92	0.50
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.94	0.50
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.92	0.50
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.93	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.92	0.50
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.91	0.50
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.92	0.50
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.94	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.92	0.50
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.93	0.50
2:E:4065:PHE:HB3	2:E:4132:PHE:CE2	2.47	0.50
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.45	0.50
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.93	0.50
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.92	0.50
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.94	0.50
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.93	0.50
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.94	0.50
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.45	0.50
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.50
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.94	0.50
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.50
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.93	0.50
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.93	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.44	0.50
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.50
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.50
2:G:4065:PHE:HB3	2:G:4132:PHE:CE2	2.47	0.50
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.45	0.50
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.50
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.44	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.92	0.50
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.50
2:B:4065:PHE:HB3	2:B:4132:PHE:CE2	2.47	0.50
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.93	0.50
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.92	0.50
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.93	0.50
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.50
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.77	0.50
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.94	0.50
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.93	0.50
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.93	0.50
2:I:1660:GLN:HG3	2:I:1707:LEU:HD13	1.92	0.50
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	1.94	0.50
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	1.94	0.49
2:B:470:SER:O	2:B:474:ARG:NE	2.40	0.49
2:E:173:SER:HB3	2:E:178:ARG:H	1.77	0.49
2:E:241:GLN:O	2:E:289:ARG:NH1	2.37	0.49
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.93	0.49
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.49
2:I:3762:ARG:H	2:I:4754:ASN:HA	1.77	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.77	0.49
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.45	0.49
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.93	0.49
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.77	0.49
2:B:3762:ARG:H	2:B:4754:ASN:HA	1.77	0.49
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.46	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.92	0.49
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.46	0.49
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.45	0.49
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.49
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.44	0.49
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.93	0.49
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	1.94	0.49
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.92	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.49
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.46	0.49
2:B:309:THR:O	2:B:313:SER:OG	2.31	0.49
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.49
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.94	0.49
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	1.94	0.49
2:G:309:THR:O	2:G:313:SER:OG	2.31	0.49
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.78	0.49
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.94	0.49
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.94	0.49
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.44	0.49
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.94	0.49
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.94	0.49
2:B:286:THR:HA	2:B:405:HIS:HB2	1.95	0.49
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.44	0.49
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.49
2:I:286:THR:HA	2:I:405:HIS:HB2	1.95	0.49
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.78	0.49
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:B:999:ASP:O	2:B:1004:GLY:N	2.46	0.49
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.78	0.49
2:B:645:ARG:N	2:B:824:GLU:O	2.40	0.49
2:E:999:ASP:O	2:E:1004:GLY:N	2.46	0.49
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.94	0.49
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.94	0.49
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.45	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.49
2:E:3762:ARG:H	2:E:4754:ASN:HA	1.77	0.49
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.45	0.49
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.78	0.49
2:I:309:THR:O	2:I:313:SER:OG	2.31	0.49
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.78	0.49
2:B:173:SER:HB3	2:B:178:ARG:H	1.77	0.49
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.46	0.49
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.49
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.46	0.49
2:E:309:THR:O	2:E:313:SER:OG	2.31	0.49
2:E:286:THR:HA	2:E:405:HIS:HB2	1.95	0.49
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.78	0.49
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.45	0.49
1:H:6:THR:HA	1:H:72:ALA:HA	1.94	0.49
2:I:999:ASP:O	2:I:1004:GLY:N	2.46	0.49
2:I:134:ASP:OD1	2:I:134:ASP:N	2.46	0.49
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.94	0.49
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.30	0.49
2:G:286:THR:HA	2:G:405:HIS:HB2	1.95	0.49
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.46	0.49
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.94	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.93	0.49
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.93	0.49
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.94	0.49
2:G:999:ASP:O	2:G:1004:GLY:N	2.46	0.49
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.77	0.49
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.44	0.49
2:I:16:THR:OG1	2:I:97:GLY:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:173:SER:HB3	2:I:178:ARG:H	1.77	0.49
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.95	0.49
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.46	0.49
2:I:4065:PHE:HB3	2:I:4132:PHE:CE2	2.47	0.49
1:A:6:THR:HA	1:A:72:ALA:HA	1.94	0.48
2:E:3767:GLN:NE2	2:E:3803:SER:O	2.46	0.48
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.78	0.48
2:E:606:LEU:O	2:E:617:ASN:ND2	2.46	0.48
2:I:4138:ASP:O	2:I:4142:ASN:ND2	2.46	0.48
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.42	0.48
2:E:4987:ASN:HA	2:E:4990:PHE:HD2	1.78	0.48
1:F:6:THR:HA	1:F:72:ALA:HA	1.94	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:I:3767:GLN:NE2	2:I:3803:SER:O	2.46	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.46	0.48
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.47	0.48
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.48
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.79	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.85	0.48
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.46	0.48
2:G:4138:ASP:O	2:G:4142:ASN:ND2	2.47	0.48
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.47	0.48
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.48
2:I:4987:ASN:HA	2:I:4990:PHE:HD2	1.78	0.48
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.95	0.48
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.79	0.48
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.79	0.48
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.94	0.48
2:G:1270:LEU:O	2:G:1472:UNK:N	2.47	0.48
2:G:3762:ARG:H	2:G:4754:ASN:HA	1.77	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:E:1270:LEU:O	2:E:1472:UNK:N	2.47	0.48
2:E:4138:ASP:O	2:E:4142:ASN:ND2	2.47	0.48
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.39	0.48
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.95	0.48
2:I:1270:LEU:O	2:I:1472:UNK:N	2.47	0.48
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.46	0.48
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.79	0.48
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.96	0.48
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.79	0.48
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.48
2:I:606:LEU:O	2:I:617:ASN:ND2	2.46	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.48
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.78	0.48
2:B:606:LEU:O	2:B:617:ASN:ND2	2.46	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.48
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.95	0.48
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.48
2:G:606:LEU:O	2:G:617:ASN:ND2	2.46	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.48
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.96	0.48
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.78	0.48
2:G:16:THR:OG1	2:G:97:GLY:O	2.31	0.48
2:G:4987:ASN:HA	2:G:4990:PHE:HD2	1.78	0.48
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.30	0.48
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.96	0.48
1:J:6:THR:HA	1:J:72:ALA:HA	1.94	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.48
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.95	0.48
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.96	0.48
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.79	0.48
2:B:1270:LEU:O	2:B:1472:UNK:N	2.47	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.46	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.48
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.48
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.48
2:G:134:ASP:OD1	2:G:134:ASP:N	2.46	0.48
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.48
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.96	0.47
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.77	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.96	0.47
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.96	0.47
2:G:173:SER:HB3	2:G:178:ARG:H	1.77	0.47
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.96	0.47
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.78	0.47
2:B:134:ASP:OD1	2:B:134:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3767:GLN:NE2	2:B:3803:SER:O	2.46	0.47
2:G:1171:SER:HG	2:G:1175:SER:H	1.59	0.47
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.96	0.47
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.47
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.96	0.47
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.96	0.47
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.79	0.47
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.47
2:B:4138:ASP:O	2:B:4142:ASN:ND2	2.46	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.97	0.47
2:B:4987:ASN:HA	2:B:4990:PHE:HD2	1.78	0.47
2:B:16:THR:OG1	2:B:97:GLY:O	2.31	0.47
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.97	0.47
2:E:134:ASP:N	2:E:134:ASP:OD1	2.46	0.47
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.47	0.47
2:I:485:SER:O	2:I:489:ASN:N	2.43	0.47
2:I:579:GLN:H	2:I:582:HIS:HD2	1.63	0.47
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.96	0.47
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.47
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.96	0.47
2:G:1457:UNK:N	2:G:1497:UNK:O	2.47	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.48	0.47
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.95	0.47
2:I:1457:UNK:N	2:I:1497:UNK:O	2.47	0.47
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.96	0.47
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.47
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.96	0.47
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.42	0.47
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.78	0.47
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.88	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.43	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.88	0.47
2:I:2342:ASN:N	2:I:2342:ASN:OD1	2.48	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.96	0.47
2:G:3767:GLN:NE2	2:G:3803:SER:O	2.46	0.47
2:I:4571:PHE:O	2:I:4575:PHE:N	2.48	0.47
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.96	0.47
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.80	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.48	0.47
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.78	0.47
2:B:1457:UNK:N	2:B:1497:UNK:O	2.47	0.47
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.97	0.47
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.97	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.80	0.47
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.47
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.97	0.47
2:B:342:GLY:N	2:B:390:LEU:O	2.48	0.47
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.47
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.96	0.47
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.30	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.47
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.79	0.47
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.96	0.47
2:E:16:THR:OG1	2:E:97:GLY:O	2.31	0.47
2:E:670:GLU:HG3	2:E:787:VAL:HG13	1.97	0.47
2:G:579:GLN:H	2:G:582:HIS:HD2	1.63	0.47
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.80	0.47
2:B:4892:ARG:NH2	2:I:4895:GLY:O	2.39	0.47
1:A:11:ASP:OD1	1:A:67:SER:OG	2.30	0.47
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.88	0.47
2:B:579:GLN:H	2:B:582:HIS:HD2	1.63	0.47
2:B:670:GLU:HG3	2:B:787:VAL:HG13	1.97	0.47
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.96	0.47
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.96	0.47
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.97	0.46
2:G:342:GLY:N	2:G:390:LEU:O	2.48	0.46
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.46
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.85	0.46
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.80	0.46
2:E:161:GLU:HG2	2:G:3984:ARG:HH22	1.80	0.46
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.88	0.46
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.25	0.46
2:B:2208:MET:SD	2:B:2253:HIS:ND1	2.85	0.46
2:E:1457:UNK:N	2:E:1497:UNK:O	2.47	0.46
2:E:2208:MET:SD	2:E:2253:HIS:ND1	2.85	0.46
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.97	0.46
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.48	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.48	0.46
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.97	0.46
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.48	0.46
2:E:579:GLN:H	2:E:582:HIS:HD2	1.63	0.46
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.80	0.46
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.80	0.46
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.98	0.46
2:B:221:ARG:NE	2:B:258:SER:OG	2.43	0.46
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.46	0.46
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.48	0.46
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.96	0.46
2:I:3771:HIS:O	2:I:3774:GLY:N	2.45	0.46
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.98	0.46
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.98	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.98	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.85	0.46
2:E:4227:GLU:OE2	2:G:4973:HIS:ND1	2.49	0.46
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.81	0.46
2:B:2810:LYS:O	2:B:2814:LYS:N	2.45	0.46
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.98	0.46
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.81	0.46
2:E:342:GLY:N	2:E:390:LEU:O	2.48	0.46
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.96	0.46
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.46
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.80	0.46
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.98	0.46
2:E:221:ARG:NE	2:E:258:SER:OG	2.44	0.46
2:E:3759:GLU:OE1	2:E:3762:ARG:NH2	2.43	0.46
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.98	0.46
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.97	0.46
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.46
2:G:689:THR:H	2:G:778:PHE:HE2	1.64	0.46
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.48	0.46
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.48	0.46
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.48	0.46
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.81	0.46
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.46	0.46
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.98	0.46
2:G:3759:GLU:OE1	2:G:3762:ARG:NH2	2.43	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.97	0.46
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.48	0.46
2:B:4005:GLN:HE21	2:B:4110:PHE:HE1	1.64	0.45
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.98	0.45
2:E:485:SER:O	2:E:489:ASN:N	2.43	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.82	0.45
2:G:395:GLN:HG3	2:G:397:GLU:H	1.81	0.45
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.49	0.45
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.46	0.45
2:I:346:CYS:N	2:I:388:LEU:O	2.49	0.45
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.98	0.45
2:E:395:GLN:HG3	2:E:397:GLU:H	1.81	0.45
2:E:4005:GLN:HE21	2:E:4110:PHE:HE1	1.64	0.45
2:G:346:CYS:N	2:G:388:LEU:O	2.49	0.45
2:G:4005:GLN:HE21	2:G:4110:PHE:HE1	1.64	0.45
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.98	0.45
2:I:2208:MET:SD	2:I:2253:HIS:ND1	2.85	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.98	0.45
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.98	0.45
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.45
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.80	0.45
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.52	0.45
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.81	0.45
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	1.99	0.45
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.81	0.45
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.45
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.98	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.30	0.45
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.97	0.45
2:I:689:THR:H	2:I:778:PHE:HE2	1.64	0.45
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.99	0.45
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.49	0.45
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.98	0.45
2:E:689:THR:H	2:E:778:PHE:HE2	1.64	0.45
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.45
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:TYR:O	1:H:86:GLY:N	2.43	0.45
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.99	0.45
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:B:346:CYS:N	2:B:388:LEU:O	2.49	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.98	0.45
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.49	0.45
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.98	0.45
2:G:670:GLU:HG3	2:G:787:VAL:HG13	1.97	0.45
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.99	0.45
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.98	0.45
2:E:346:CYS:N	2:E:388:LEU:O	2.49	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.45
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.98	0.45
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.45
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.98	0.45
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.98	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.98	0.45
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	1.99	0.45
2:I:342:GLY:N	2:I:390:LEU:O	2.48	0.45
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.98	0.45
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.82	0.45
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.81	0.45
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.99	0.45
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.48	0.45
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.98	0.45
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.99	0.45
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.52	0.45
2:B:41:GLY:O	2:B:45:ARG:NH1	2.50	0.45
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.97	0.45
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	1.99	0.45
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.99	0.45
2:B:395:GLN:HG3	2:B:397:GLU:H	1.81	0.45
2:E:2810:LYS:O	2:E:2814:LYS:N	2.45	0.45
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.99	0.45
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.98	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.52	0.45
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.99	0.45
2:G:3771:HIS:O	2:G:3774:GLY:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:41:GLY:O	2:G:45:ARG:NH1	2.50	0.45
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.81	0.45
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.44
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.81	0.44
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.44
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.81	0.44
2:G:3759:GLU:HG3	2:G:3763:LEU:HD22	1.99	0.44
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.98	0.44
2:I:395:GLN:HG3	2:I:397:GLU:H	1.81	0.44
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.83	0.44
2:B:689:THR:H	2:B:778:PHE:HE2	1.64	0.44
2:E:645:ARG:N	2:E:824:GLU:O	2.40	0.44
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.99	0.44
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.85	0.44
2:B:2381:GLU:HA	2:B:2384:ILE:HD12	2.00	0.44
2:B:243:ARG:NH1	2:B:301:VAL:O	2.44	0.44
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.99	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.53	0.44
2:E:3766:GLN:HG3	2:E:3769:ARG:HH12	1.83	0.44
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.82	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.44
2:E:41:GLY:O	2:E:45:ARG:NH1	2.50	0.44
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.98	0.44
2:G:3766:GLN:HG3	2:G:3769:ARG:HH12	1.83	0.44
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.53	0.44
2:I:4005:GLN:HE21	2:I:4110:PHE:HE1	1.64	0.44
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.00	0.44
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.98	0.44
2:G:2810:LYS:O	2:G:2814:LYS:N	2.45	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.44
2:I:3759:GLU:HG3	2:I:3763:LEU:HD22	1.99	0.44
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.49	0.44
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.30	0.44
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.98	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.82	0.44
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.44
2:B:3766:GLN:HG3	2:B:3769:ARG:HH12	1.83	0.44
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.99	0.44
2:E:4895:GLY:O	2:G:4892:ARG:NH2	2.43	0.44
2:G:111:HIS:CD2	2:G:114:SER:H	2.36	0.44
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.44
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.98	0.44
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.00	0.44
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.99	0.44
2:E:793:LEU:HD12	2:E:797:HIS:HB2	2.00	0.44
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	1.99	0.44
2:I:2950:UNK:O	2:I:2954:UNK:N	2.51	0.44
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.99	0.44
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.83	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.82	0.44
2:B:2950:UNK:O	2:B:2954:UNK:N	2.51	0.44
2:B:668:VAL:O	2:B:741:GLU:N	2.49	0.44
2:E:2381:GLU:HA	2:E:2384:ILE:HD12	2.00	0.44
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.83	0.44
2:G:2381:GLU:HA	2:G:2384:ILE:HD12	2.00	0.44
2:G:2950:UNK:O	2:G:2954:UNK:N	2.51	0.44
2:B:111:HIS:CD2	2:B:114:SER:H	2.36	0.43
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.53	0.43
2:B:793:LEU:HD12	2:B:797:HIS:HB2	2.00	0.43
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.00	0.43
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.43
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.99	0.43
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.83	0.43
2:E:1936:LYS:O	2:E:1940:CYS:N	2.47	0.43
2:E:2758:PHE:O	2:E:2762:THR:N	2.52	0.43
2:E:626:LEU:HG	2:E:628:GLY:H	1.83	0.43
2:I:111:HIS:CD2	2:I:114:SER:H	2.36	0.43
2:B:626:LEU:HG	2:B:628:GLY:H	1.83	0.43
2:E:2950:UNK:O	2:E:2954:UNK:N	2.51	0.43
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.84	0.43
2:G:793:LEU:HD12	2:G:797:HIS:HB2	2.00	0.43
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.43
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.43
2:G:4065:PHE:HD1	2:G:4068:LEU:HD22	1.83	0.43
2:I:1105:ALA:N	2:I:1189:LEU:O	2.51	0.43
2:I:3766:GLN:HG3	2:I:3769:ARG:HH12	1.83	0.43
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.46	0.43
1:A:55:VAL:HA	2:B:1784:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2758:PHE:O	2:B:2762:THR:N	2.52	0.43
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.54	0.43
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.53	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.99	0.43
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.00	0.43
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.01	0.43
2:I:4065:PHE:HD1	2:I:4068:LEU:HD22	1.83	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.84	0.43
1:A:21:THR:HA	1:A:49:ARG:HA	2.01	0.43
2:E:1105:ALA:N	2:E:1189:LEU:O	2.51	0.43
2:E:111:HIS:CD2	2:E:114:SER:H	2.36	0.43
2:E:668:VAL:O	2:E:741:GLU:N	2.49	0.43
2:G:2467:VAL:HA	2:G:2470:ILE:HD12	2.01	0.43
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.00	0.43
2:I:313:SER:HB3	2:I:351:VAL:HB	2.01	0.43
2:I:4864:ASN:HA	2:I:4874:MET:HG2	2.01	0.43
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	2.01	0.43
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.84	0.43
2:E:4864:ASN:HA	2:E:4874:MET:HG2	2.01	0.43
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.54	0.43
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	2.01	0.43
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.83	0.43
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	2.01	0.43
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.54	0.43
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	2.01	0.43
2:I:2381:GLU:HA	2:I:2384:ILE:HD12	2.00	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.01	0.43
2:E:3759:GLU:HG3	2:E:3763:LEU:HD22	1.99	0.43
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.43
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.84	0.43
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.01	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:41:GLY:O	2:I:45:ARG:NH1	2.50	0.43
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	2.01	0.43
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.84	0.43
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.54	0.43
2:I:793:LEU:HD12	2:I:797:HIS:HB2	2.00	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.52	0.43
2:B:3771:HIS:O	2:B:3774:GLY:N	2.45	0.43
2:B:4864:ASN:HA	2:B:4874:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.84	0.43
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.00	0.43
2:B:4973:HIS:ND1	2:I:4227:GLU:OE2	2.51	0.43
2:B:3759:GLU:HG3	2:B:3763:LEU:HD22	1.99	0.43
2:B:4065:PHE:HD1	2:B:4068:LEU:HD22	1.83	0.43
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.01	0.43
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.84	0.43
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.84	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
1:F:21:THR:HA	1:F:49:ARG:HA	2.01	0.43
2:G:2257:LEU:O	2:G:2261:SER:N	2.52	0.43
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.83	0.43
1:J:7:ILE:HB	1:J:71:ARG:HB3	2.01	0.43
2:E:615:ARG:NH2	2:E:1677:GLY:O	2.52	0.42
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.00	0.42
2:E:313:SER:HB3	2:E:351:VAL:HB	2.01	0.42
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	2.01	0.42
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	2.01	0.42
2:G:3361:UNK:O	2:G:3365:UNK:N	2.52	0.42
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.38	0.42
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.01	0.42
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.01	0.42
1:A:7:ILE:HB	1:A:71:ARG:HB3	2.01	0.42
2:B:1105:ALA:N	2:B:1189:LEU:O	2.51	0.42
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.84	0.42
2:E:2257:LEU:O	2:E:2261:SER:N	2.52	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.01	0.42
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.83	0.42
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.84	0.42
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	2.02	0.42
1:J:21:THR:HA	1:J:49:ARG:HA	2.01	0.42
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.84	0.42
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.42
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.01	0.42
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	2.01	0.42
2:G:4864:ASN:HA	2:G:4874:MET:HG2	2.01	0.42
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.42
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.02	0.42
2:I:626:LEU:HG	2:I:628:GLY:H	1.83	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	2.01	0.42
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.01	0.42
2:E:4065:PHE:HD1	2:E:4068:LEU:HD22	1.83	0.42
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.01	0.42
2:G:626:LEU:HG	2:G:628:GLY:H	1.83	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.01	0.42
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.84	0.42
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.01	0.42
2:G:2447:LYS:HG3	2:G:2450:ALA:H	1.84	0.42
2:I:2257:LEU:O	2:I:2261:SER:N	2.52	0.42
2:I:2447:LYS:HG3	2:I:2450:ALA:H	1.84	0.42
2:I:221:ARG:NE	2:I:258:SER:OG	2.43	0.42
2:I:3759:GLU:OE1	2:I:3762:ARG:NH2	2.43	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.84	0.42
2:B:1770:SER:OG	2:B:1772:ARG:NE	2.53	0.42
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.02	0.42
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	2.02	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.42
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	2.02	0.42
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.02	0.42
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.84	0.42
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.30	0.42
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.84	0.42
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	2.02	0.42
2:G:668:VAL:O	2:G:741:GLU:N	2.49	0.42
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.02	0.42
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.42
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.00	0.42
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.42
2:B:1171:SER:OG	2:B:1175:SER:N	2.45	0.42
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	2.02	0.42
2:E:788:LYS:HG2	2:E:1629:GLN:HA	2.01	0.42
2:G:221:ARG:NE	2:G:258:SER:OG	2.43	0.42
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.48	0.42
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.02	0.42
2:I:320:LYS:NZ	2:I:381:GLU:O	2.36	0.42
2:B:2447:LYS:HG3	2:B:2450:ALA:H	1.84	0.42
2:B:3361:UNK:O	2:B:3365:UNK:N	2.52	0.42
2:E:2447:LYS:HG3	2:E:2450:ALA:H	1.84	0.42
2:E:3361:UNK:O	2:E:3365:UNK:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.50	0.42
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.02	0.42
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	2.02	0.42
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	2.02	0.42
2:B:313:SER:HB3	2:B:351:VAL:HB	2.01	0.42
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	2.02	0.42
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.02	0.42
2:I:1770:SER:OG	2:I:1772:ARG:NE	2.53	0.42
2:I:4177:TYR:CE1	2:I:4199:GLU:HB3	2.55	0.42
2:E:1663:HIS:O	2:E:1667:LEU:N	2.52	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.45	0.42
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.85	0.42
2:G:788:LYS:HG2	2:G:1629:GLN:HA	2.01	0.42
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.52	0.42
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.84	0.42
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.85	0.42
1:H:21:THR:HA	1:H:49:ARG:HA	2.01	0.42
2:I:788:LYS:HG2	2:I:1629:GLN:HA	2.02	0.42
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.02	0.41
1:F:71:ARG:HH22	2:E:679:ALA:HB2	1.85	0.41
2:G:1105:ALA:N	2:G:1189:LEU:O	2.51	0.41
1:H:7:ILE:HB	1:H:71:ARG:HB3	2.01	0.41
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.02	0.41
2:I:2758:PHE:O	2:I:2762:THR:N	2.52	0.41
2:I:4027:LEU:HA	2:I:4030:LEU:HD12	2.02	0.41
2:I:776:LEU:HG	2:I:848:HIS:HA	2.02	0.41
2:B:3759:GLU:OE1	2:B:3762:ARG:NH2	2.43	0.41
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.01	0.41
1:F:55:VAL:HA	2:E:1784:ALA:HA	2.02	0.41
2:G:1770:SER:OG	2:G:1772:ARG:NE	2.53	0.41
2:G:776:LEU:HG	2:G:848:HIS:HA	2.02	0.41
2:I:615:ARG:NH2	2:I:1677:GLY:O	2.52	0.41
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	2.03	0.41
2:I:684:VAL:HA	2:I:781:VAL:HA	2.02	0.41
2:B:161:GLU:HG2	2:E:3984:ARG:HH22	1.85	0.41
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.48	0.41
2:B:4177:TYR:CE1	2:B:4199:GLU:HB3	2.55	0.41
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	2.01	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.85	0.41
2:E:1770:SER:OG	2:E:1772:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:914:PRO:O	2:E:918:ARG:N	2.49	0.41
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	2.03	0.41
2:G:4547:GLN:O	2:G:4551:PHE:N	2.49	0.41
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.02	0.41
2:I:914:PRO:O	2:I:918:ARG:N	2.49	0.41
2:B:788:LYS:HG2	2:B:1629:GLN:HA	2.01	0.41
2:B:1936:LYS:O	2:B:1940:CYS:N	2.47	0.41
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.01	0.41
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.02	0.41
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	2.03	0.41
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	2.02	0.41
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.93	0.41
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.02	0.41
2:G:2208:MET:SD	2:G:2253:HIS:ND1	2.85	0.41
2:G:4177:TYR:CE1	2:G:4199:GLU:HB3	2.55	0.41
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	2.03	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.01	0.41
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	2.02	0.41
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.85	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.93	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.41
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.02	0.41
2:B:4897:ILE:HG12	2:B:4901:ILE:HD13	2.02	0.41
2:E:2034:PHE:O	2:E:2038:LEU:N	2.54	0.41
2:E:4027:LEU:HA	2:E:4030:LEU:HD12	2.02	0.41
2:E:745:SER:N	2:E:758:ARG:O	2.43	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.52	0.41
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.41
2:E:1973:GLN:O	2:E:1977:TYR:N	2.54	0.41
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.01	0.41
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	2.03	0.41
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.02	0.41
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	2.03	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.41
2:I:347:PHE:HE1	2:I:386:ASP:HB2	1.86	0.41
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	2.02	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.01	0.41
2:B:2874:MET:O	2:B:2878:LEU:N	2.44	0.41
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.02	0.41
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.02	0.41
2:E:4133:GLN:HE22	2:E:4137:ARG:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4177:TYR:CE1	2:E:4199:GLU:HB3	2.55	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.94	0.41
1:F:7:ILE:HB	1:F:71:ARG:HB3	2.01	0.41
2:G:1973:GLN:O	2:G:1977:TYR:N	2.54	0.41
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.02	0.41
2:G:4027:LEU:HA	2:G:4030:LEU:HD12	2.02	0.41
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	2.02	0.41
2:G:4897:ILE:HG12	2:G:4901:ILE:HD13	2.02	0.41
1:H:71:ARG:HH22	2:G:679:ALA:HB2	1.86	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.78	0.41
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.86	0.41
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.48	0.41
2:I:4897:ILE:HG12	2:I:4901:ILE:HD13	2.02	0.41
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.02	0.41
2:B:4133:GLN:HE22	2:B:4137:ARG:HG3	1.86	0.41
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.86	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.42	0.41
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.02	0.41
2:I:4133:GLN:HE22	2:I:4137:ARG:HG3	1.86	0.41
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.86	0.40
2:B:1639:LEU:N	2:B:1648:MET:O	2.54	0.40
2:B:615:ARG:NH2	2:B:1677:GLY:O	2.52	0.40
2:B:206:CYS:SG	2:B:207:SER:N	2.94	0.40
2:E:206:CYS:SG	2:E:207:SER:N	2.94	0.40
2:B:4227:GLU:OE2	2:E:4973:HIS:ND1	2.55	0.40
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.02	0.40
2:G:4053:SER:HA	2:G:4056:GLU:HB2	2.03	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.94	0.40
2:I:4843:LEU:HA	2:I:4846:VAL:HG12	2.03	0.40
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	2.04	0.40
2:E:776:LEU:HG	2:E:848:HIS:HA	2.02	0.40
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.40
2:G:684:VAL:HA	2:G:781:VAL:HA	2.03	0.40
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.04	0.40
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.57	0.40
2:B:347:PHE:HE1	2:B:386:ASP:HB2	1.86	0.40
2:B:38:ALA:HB1	2:B:64:ILE:HG13	2.04	0.40
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	2.03	0.40
2:B:583:ILE:HG13	2:B:583:ILE:H	1.69	0.40
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.57	0.40
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.57	0.40
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.40
2:E:4843:LEU:HA	2:E:4846:VAL:HG12	2.03	0.40
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.57	0.40
2:I:1739:THR:H	2:I:1742:THR:HB	1.87	0.40
2:I:2034:PHE:O	2:I:2038:LEU:N	2.54	0.40
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.93	0.40
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.40
2:B:4547:GLN:O	2:B:4551:PHE:N	2.49	0.40
2:B:684:VAL:HA	2:B:781:VAL:HA	2.03	0.40
2:B:776:LEU:HG	2:B:848:HIS:HA	2.02	0.40
2:E:347:PHE:HE1	2:E:386:ASP:HB2	1.86	0.40
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.77	0.40
2:E:684:VAL:HA	2:E:781:VAL:HA	2.03	0.40
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.04	0.40
2:G:38:ALA:HB1	2:G:64:ILE:HG13	2.04	0.40
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.40
2:I:243:ARG:NH1	2:I:301:VAL:O	2.44	0.40
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	2.04	0.40
2:B:485:SER:O	2:B:489:ASN:N	2.43	0.40
2:B:4885:PHE:HE2	2:B:4901:ILE:HD11	1.87	0.40
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.53	0.40
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.04	0.40
2:G:320:LYS:NZ	2:G:381:GLU:O	2.36	0.40
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.40
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.40
2:I:1973:GLN:O	2:I:1977:TYR:N	2.54	0.40
2:I:38:ALA:HB1	2:I:64:ILE:HG13	2.04	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 PDB entries followed by that with respect to all EM entries.

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	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	H	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	J	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	55	89
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	55	89
2	G	3235/4416 (73%)	2887 (89%)	344 (11%)	4 (0%)	55	89
2	I	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	55	89
All	All	13360/18096 (74%)	11919 (89%)	1425 (11%)	16 (0%)	58	89

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	I	1932	PRO
2	E	1932	PRO
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	G	1840	PRO
2	G	4641	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 PDB entries followed by that with respect to all EM entries.

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2477 (99%)	16 (1%)	89	94
2	E	2493/3022 (82%)	2477 (99%)	16 (1%)	89	94
2	G	2493/3022 (82%)	2477 (99%)	16 (1%)	89	94
2	I	2493/3022 (82%)	2477 (99%)	16 (1%)	89	94
All	All	10324/12444 (83%)	10260 (99%)	64 (1%)	89	94

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4978	HIS
2	B	4983	HIS
2	B	4995	LEU
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN

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Mol	Chain	Res	Type
2	I	4085	ARG
2	I	4120	ASN
2	I	4978	HIS
2	I	4983	HIS
2	I	4995	LEU
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4978	HIS
2	E	4983	HIS
2	E	4995	LEU
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4978	HIS
2	G	4983	HIS
2	G	4995	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS

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Mol	Chain	Res	Type
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	151	HIS
2	B	273	HIS
2	B	379	HIS
2	B	412	ASN
2	B	413	GLN
2	B	479	GLN
2	B	582	HIS
2	B	949	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	1972	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	3767	GLN
2	B	3781	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3976	ASN
2	B	4034	ASN
2	B	4102	GLN
2	B	4120	ASN
2	B	4130	ASN
2	B	4133	GLN
2	B	4142	ASN
2	I	57	ASN
2	I	111	HIS

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Mol	Chain	Res	Type
2	I	113	HIS
2	I	151	HIS
2	I	273	HIS
2	I	379	HIS
2	I	412	ASN
2	I	413	GLN
2	I	582	HIS
2	I	949	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1972	ASN
2	I	2005	GLN
2	I	2127	GLN
2	I	3700	GLN
2	I	3767	GLN
2	I	3781	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3976	ASN
2	I	4034	ASN
2	I	4102	GLN
2	I	4120	ASN
2	I	4130	ASN
2	I	4133	GLN
2	I	4142	ASN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	151	HIS
2	E	273	HIS
2	E	379	HIS
2	E	412	ASN

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Mol	Chain	Res	Type
2	E	413	GLN
2	E	479	GLN
2	E	582	HIS
2	E	949	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	3767	GLN
2	E	3781	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	4034	ASN
2	E	4102	GLN
2	E	4120	ASN
2	E	4130	ASN
2	E	4133	GLN
2	E	4142	ASN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	151	HIS
2	G	273	HIS
2	G	379	HIS
2	G	412	ASN
2	G	413	GLN
2	G	582	HIS
2	G	949	ASN
2	G	1598	GLN
2	G	1679	ASN

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Mol	Chain	Res	Type
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	3767	GLN
2	G	3781	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4102	GLN
2	G	4120	ASN
2	G	4130	ASN
2	G	4133	GLN
2	G	4142	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.36
1	I	4345:UNK	C	4540:PHE	N	73.36
1	E	4345:UNK	C	4540:PHE	N	73.36
1	G	4345:UNK	C	4540:PHE	N	73.36
1	B	3613:UNK	C	3639:THR	N	46.46
1	I	3613:UNK	C	3639:THR	N	46.46
1	E	3613:UNK	C	3639:THR	N	46.46
1	G	3613:UNK	C	3639:THR	N	46.46
1	B	4253:GLU	C	4320:UNK	N	27.46
1	I	4253:GLU	C	4320:UNK	N	27.46
1	E	4253:GLU	C	4320:UNK	N	27.46
1	G	4253:GLU	C	4320:UNK	N	27.46
1	B	3163:UNK	C	3170:UNK	N	15.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3163:UNK	C	3170:UNK	N	15.87
1	E	3163:UNK	C	3170:UNK	N	15.87
1	G	3163:UNK	C	3170:UNK	N	15.87
1	B	3063:UNK	C	3134:UNK	N	14.92
1	I	3063:UNK	C	3134:UNK	N	14.92
1	E	3063:UNK	C	3134:UNK	N	14.92
1	G	3063:UNK	C	3134:UNK	N	14.92
1	B	3468:UNK	C	3511:UNK	N	14.79
1	I	3468:UNK	C	3511:UNK	N	14.79
1	E	3468:UNK	C	3511:UNK	N	14.79
1	G	3468:UNK	C	3511:UNK	N	14.79
1	B	2703:UNK	C	2734:ASN	N	13.42
1	I	2703:UNK	C	2734:ASN	N	13.42
1	E	2703:UNK	C	2734:ASN	N	13.42
1	G	2703:UNK	C	2734:ASN	N	13.42
1	B	3236:UNK	C	3241:UNK	N	13.13
1	I	3236:UNK	C	3241:UNK	N	13.13
1	E	3236:UNK	C	3241:UNK	N	13.13
1	G	3236:UNK	C	3241:UNK	N	13.13
1	B	1564:UNK	C	1573:MET	N	12.39
1	I	1564:UNK	C	1573:MET	N	12.39
1	E	1564:UNK	C	1573:MET	N	12.39
1	G	1564:UNK	C	1573:MET	N	12.39
1	B	2976:UNK	C	2995:UNK	N	12.28
1	I	2976:UNK	C	2995:UNK	N	12.28
1	E	2976:UNK	C	2995:UNK	N	12.28
1	G	2976:UNK	C	2995:UNK	N	12.28
1	B	3254:UNK	C	3261:UNK	N	8.43
1	I	3254:UNK	C	3261:UNK	N	8.43
1	E	3254:UNK	C	3261:UNK	N	8.43
1	G	3254:UNK	C	3261:UNK	N	8.43
1	B	1297:UNK	C	1430:UNK	N	6.02
1	I	1297:UNK	C	1430:UNK	N	6.02
1	E	1297:UNK	C	1430:UNK	N	6.02
1	G	1297:UNK	C	1430:UNK	N	6.02
1	B	2939:ARG	C	2942:UNK	N	3.58
1	I	2939:ARG	C	2942:UNK	N	3.58
1	E	2939:ARG	C	2942:UNK	N	3.58
1	G	2939:ARG	C	2942:UNK	N	3.58
1	B	2479:LEU	C	2487:UNK	N	3.25
1	I	2479:LEU	C	2487:UNK	N	3.25
1	E	2479:LEU	C	2487:UNK	N	3.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2479:LEU	C	2487:UNK	N	3.25