



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 02:36 PM EDT

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 wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

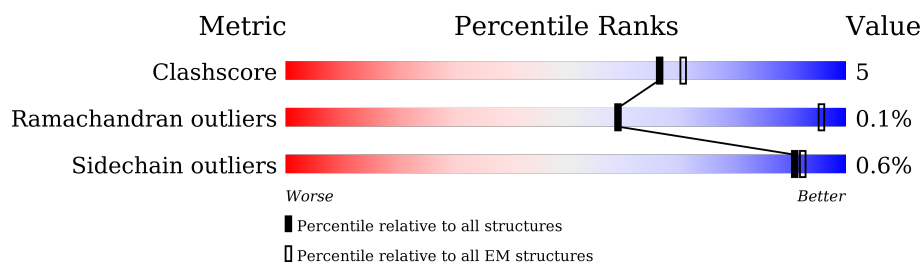
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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		

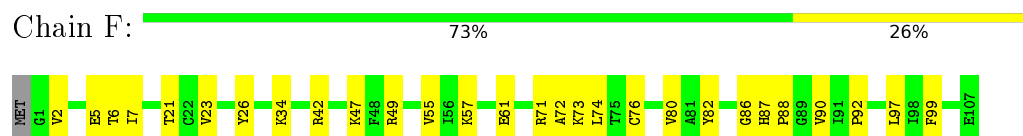
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	

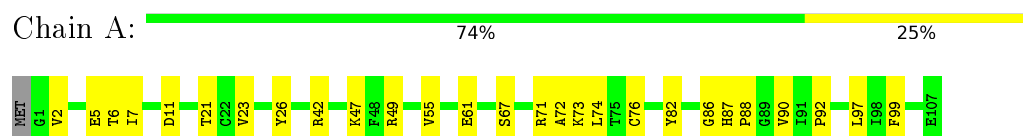
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

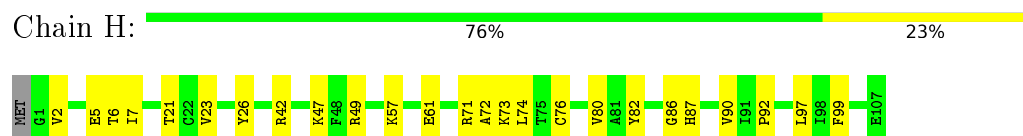
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



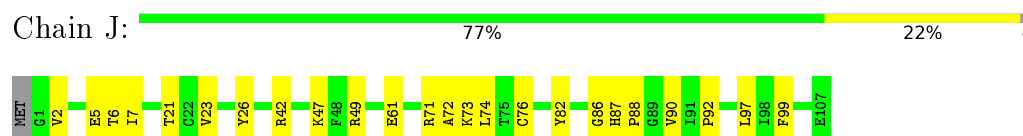
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



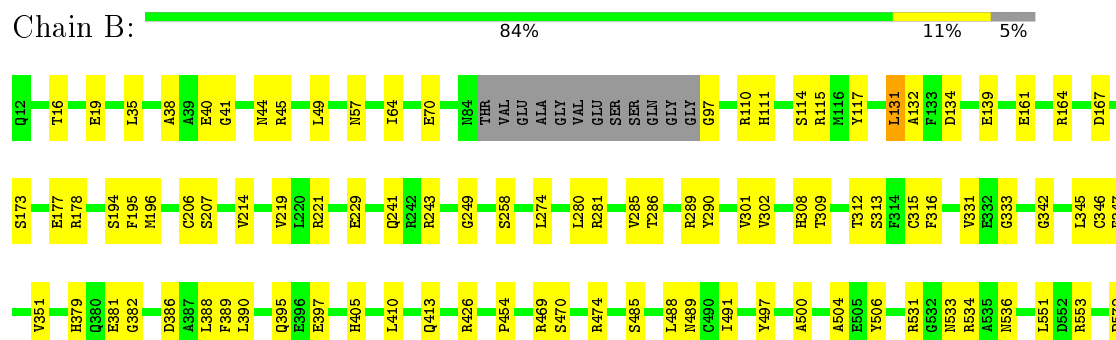
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



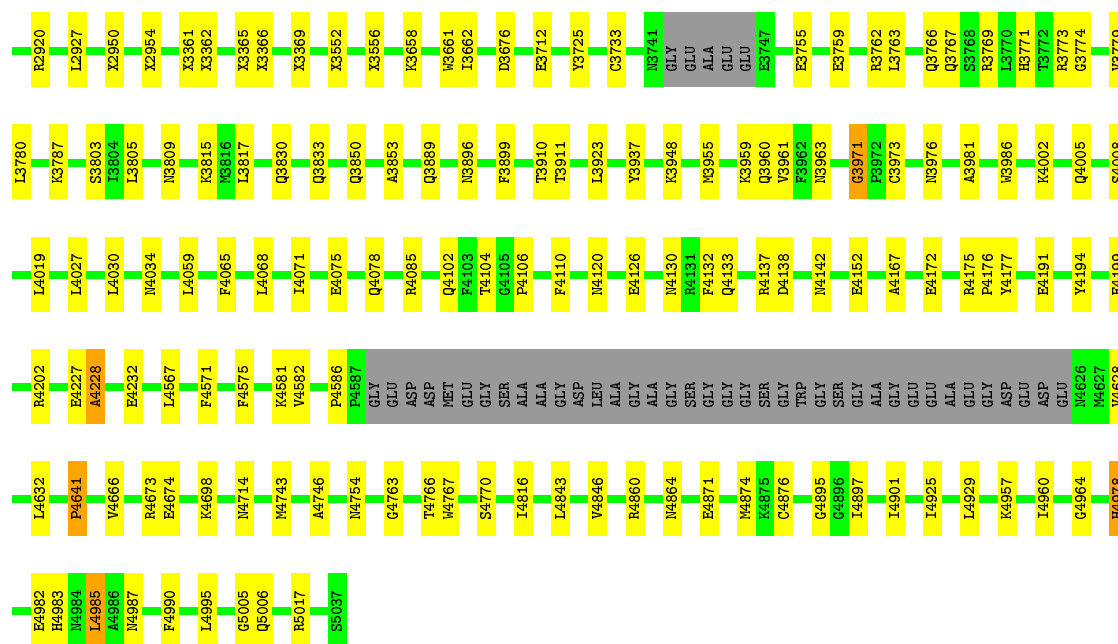
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

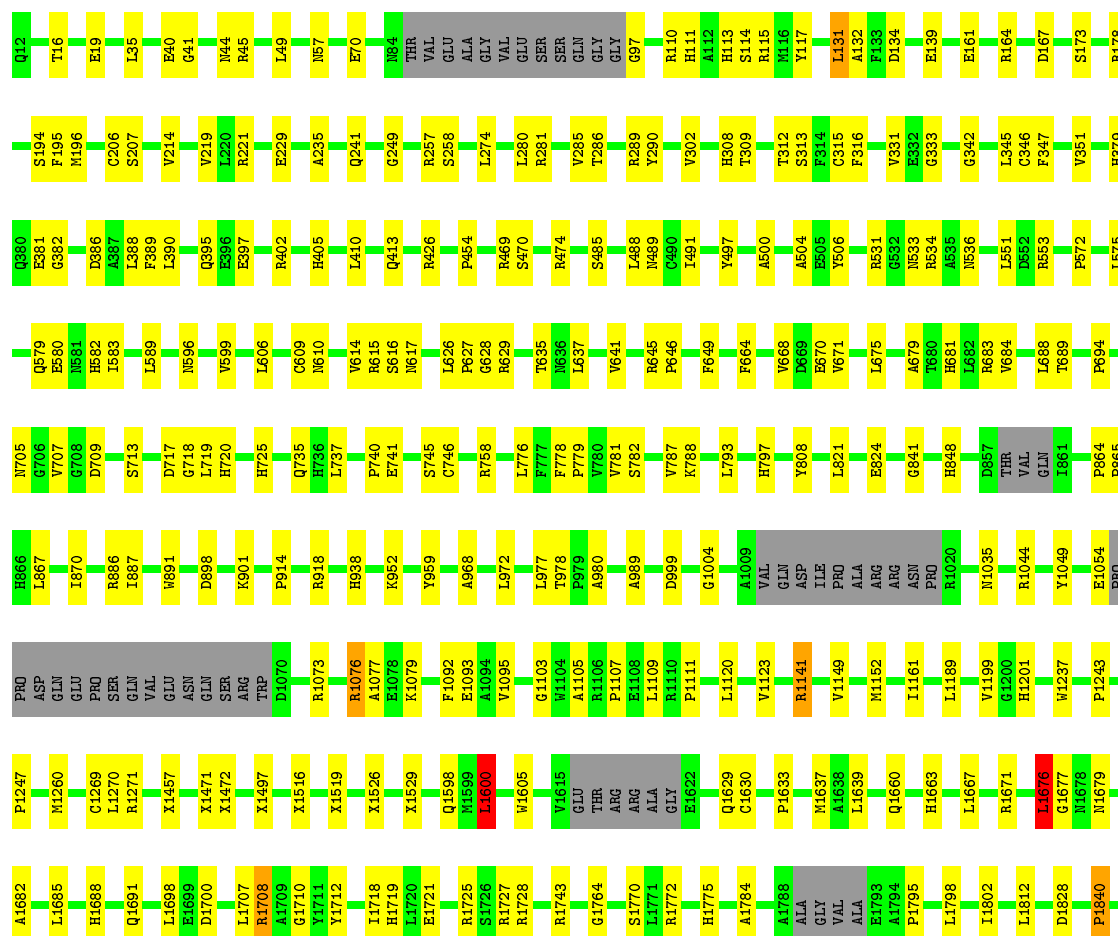





• Molecule 2: Ryanodine receptor 1

Chain E: 84% 11% 5%



V1859	C1940	L2295	X2493	L2871	Q3766	N3976	E4152	TRP	G4895
K1860	A1960	L2296	X2502	N2881	Q3767	N3981	A4167	GLY	I4925
Q1861	A1960	C2327	X2502	N2881	S3768	A3981	A4167	SER	L4925
I1862	A1960	G2327	X2502	N2881	R3769	A3981	E4168	GLY	L4928
E1874	R1964	N2342	E2737	N2884	R3770	R3984	S4169	GLY	L4929
GLU	R1964	G2343	E2738	N2888	H3771	I3985	E4172	GLU	K4957
GLU	N1972	E2347	E2748	R2888	T3772	W3986	E4172	GLU	A4978
GLU	Q1973	N2351	L2751	L2894	G3774	K4002	R4175	GLU	I4960
GLU	Y1977	N2351	L2751	H2902	G3774	Q4005	P4176	GLY	G4964
GLU	T1991	L2368	L2755	E2908	V3779	Q4005	Y4177	ASP	H4973
GLU	T1995	L2376	L2758	Y2908	L3780	S4008	E4191	ASP	H4973
GLU	P2002	E2381	T2762	R2920	K3787	L4019	Y4194	GLU	H4978
GLU	Q2003	E2381	T2762	R2920	S3803	L4019	Y4194	GLU	E4982
GLU	P2004	L2384	K2770	L2927	I3804	L4027	E4199	GLU	H4983
GLU	Q2005	L2384	K2770	X2960	L3805	L4030	R4202	GLU	L4985
GLU	L2006	P2395	W2775	X2960	N3809	L4030	R4202	GLU	A4986
ASP	N2007	VAL	E2803	X2954	K3815	N4034	E4227	GLU	N4987
GLU	P2022	ARG	E2803	X3361	N3816	L4059	A4228	GLU	V4666
GLU	P2024	ASP	R2806	X3362	L3817	L4059	E4232	GLU	F4990
LYS	R2028	ARG	W2807	X3365	Q3830	D4063	L4567	GLU	L4995
ASP	F2034	ARG	K2810	X3366	Q3833	F4065	F4571	GLY	G5005
GLU	L2038	GLU	K2814	X3369	Q3850	L4068	F4575	GLU	Q5006
GLU	C2042	GLU	A2815	X3562	A3853	I4071	F4575	GLU	R5017
GLU	G2043	GLU	L2823	X3556	Q3889	E4075	K4581	GLY	S5037
LYS	G2048	PRO	E2830	K3658	Q3889	Q4078	V4582	GLY	
ASP	GLU	PRO	GLU	K3661	N3896	R4085	P4586	GLY	
ALA	GLU	GLU	ARG	I3662	F3899	R4085	P4587	GLU	
GLU	GLU	GLU	THR	I3662	F3899	Q4102	ASP	ASP	
LYS	PRO	PRO	LYS	D8676	T3910	F4103	ASP	GLY	
GLU	GLU	H2420	LYS	E3712	T3911	T4104	MET	GLY	
GLU	GLU	L2430	LYS	E3712	G4105	P4106	GLY	GLY	
GLU	GLU	L2430	THR	Y3725	L3923	F4110	SER	SER	
ALA	THR	H2253	ANG	Y3725	Y3937	F4110	ALA	ALA	
ALA	THR	L2257	LYS	N3741	Y3937	N4120	ALA	ALA	
PRO	LEU	L2257	ILE	GLY	K3948	N4120	GLY	GLY	
GLY	SER	S2261	GLN	GLU	M3955	E4126	ASP	ASP	
GLY	SER	S2261	THR	GLU	M3955	E4126	LEU	LEU	
LYS	ANG	P2272	ALA	GLU	K3959	N4130	ALA	ALA	
LEU	LEU	V2275	GLN	E3747	Q3960	R4131	ALA	ALA	
ASP	ARG	V2275	THR	E3747	V3961	F4132	GLY	GLY	
LYS	LEU	A2287	TYR	E3755	F3962	Q4133	SER	SER	
L1923	LEU	V2467	ASP	E3755	N3963	Q4133	GLY	GLY	
L1931	LEU	A2287	PRO	E3755	N3963	Q4133	GLY	GLY	
P1932	GLU	L2290	ARG	E3759	G3971	R4137	GLY	GLY	
V1935	THR	L2290	GLY	E3759	P3972	D4138	GLY	GLY	
ARG	VAL	Q2291	GLY	R3762	C3973	N4142	SER	SER	
		D2294	ARG	L3763			GLY	GLY	

• Molecule 2: Ryanodine receptor 1

Chain G:  84% 11% 5%

Q12	S194	E381	N581
T16	F195	G382	H582
E19	M196	L388	I583
L35	C206	L388	L589
A38	V214	L390	I596
A39	V219	Q395	V599
E40	L220	E396	L606
G41	R221	E397	L606
N44	E229	R402	C609
R45	E235	H405	I610
L49	Q241	L410	V614
N57	Q241	Q413	R615
I64	G249	R426	S616
N84	R257	P454	I617
THR	S258	R469	L626
VAL	L274	S470	P627
GLU	L280	R474	O628
ALA	R281	S485	T635
GLY	T285	L488	H636
VAL	T286	M489	L637
SER	R289	C490	V641
GLN	Y290	I491	R645
GLY	V302	Y497	P646
G97	H308	A500	F649
R110	T309	A504	F664
H111	T312	E505	V668
H113	S313	Y506	D669
S114	F314	B531	E670
R115	C315	G532	V671
L131	F316	N533	L675
A132	R320	R534	A679
F133	V331	A535	T680
D134	E332	N536	H681
E139	G333	L551	L682
R164	G342	D552	R683
D167	L345	R553	V684
S173	C346	P572	L688
S173	V351	L575	T689
E177	H379	Q579	P694
R178	Q380	E580	N705
			G705
			V707
			G708

I4987	R4673	F4551	I4059	Q3830	X3365	K2810	R2104	Q2003	GLU	L1707	X1457	TRP		D709
F4990	E4674	L4567	F4065	Q3833	X3366	K2814	Q2107	E2004	GLU	R1708	X1471	D1070	H891	S713
L4995	K4698	F4571	F4068	Q3850	X3369	A2815	F2121	I2006	GLU	G1710	X1472	R1073	D898	D717
G5005	I4714	F4575	I4071	Q3853	X3552	I2823	Q2127	I2007	GLU	Y1711	X1497	R1076	K901	G718
Q5006	K4743	K4581	E4075	Q3889	X3556	E2830	L2131	P2022	GLU	I1718	X1516	A1077	H938	L719
R5017	A4746	V4582	Q4078	I3896	K3658	GLU	L2155	P2024	ASP	H1719	X1519	K1078	K952	H720
S5037	I4754	P4586	R4085	I3937	K3661	THR	R2028	R2028	GLU	E1721	X1526	F1092	H725	
	G4763	P4587	Q4102	T3910	I3662	GLU	R2188	C2042	LYS	R1725		E1093	Y959	Q735
	K4767	F4103	F4104	T3911	I3676	THR	K2189	G2043	GLU	S1726	X1529	V1095	A968	L737
	S4770	G4105	P4106	I3923	E3712	LYS	Y2192	G2048	GLU	R1743		G1103	L972	P740
	I4846	GLY	F4110	I3937	E3725	LYS	P2226	GLU	GLU	R1770	Q1598	A1104	L977	E741
	L4843	ALA	F4120	K3948	K3741	ILE	V2229	GLU	GLU	L1771	N1599	A1105	L978	S745
	R4860	GLY	R4126	I3955	GLU	ALA	H2253	GLU	GLU	R1772	W1600	R1106	T978	C746
	M4864	LEU	Q4130	K3959	GLU	GLN	L2257	THR	THR	H1775	ARG	E1108	A980	R758
	F4871	ALA	V3961	Q3960	GLY	THR	S2261	SER	LEU	A1788	ALA	R1110	A989	L776
	K4874	ALA	R4131	I3962	GLY	ASP	P2272	ARG	GLY	L1788	E1622	P1111	D999	F778
	C4876	GLY	F4132	I3963	E3755	PRO	Q2290	LEU	GLU	VAL	Q1629	R1141	G1004	P779
	R4892	SER	P4138	I3971	E3759	GLY	V2275	ARG	GLU	ALA	C1630	V1149	A1009	W781
	L4897	TRP	E4152	Q3976	K3762	GLY	A2287	LEU	GLU	E1793	P1633	M1152	VAL	S782
	T4901	GLY	A4167	I3981	I3763	Y2855	Q2291	THR	GLU	A1794	M1637	I1161	ARG	H797
	L4925	ALA	E4172	K3984	I3767	K2881	D2294	ARG	ASP	L1798	L1638	S1171	ASN	W808
	L4928	GLY	R4175	I3985	K3769	K2884	L2295	VAL	PRO	L1812	R1671	L1189	R1020	L821
	L4929	GLU	P4176	K3986	K3771	K2888	C2326	LYS	GLY	D1828		P1190	M1035	E824
	K4957	ALA	Y4177	K4002	K3774	L2894	Q2327	LYS	LYS		L1676	V1199	R1044	G841
	L4960	GLY	E4191	Q4005	V3779	H2902	N2342	GLU	GLU	P1840	G1677	V1200	E1054	H848
	G4964	ASP	Y4194	S4008	I3780	Y2908	G2343	LYS	PRO	V1859	N1679	H1201	PRO	
	H4973	ASP	E4199	I4019	K3787	K2920	E2347	GLU	GLU	K1360	A1682	I1237	ASP	D857
	K4978	GLU	R4202	I4027	S3803	R2927	T2762	LEU	GLU	Q1861	L1685	P1243	GLN	THR
		V4627	E4227	L4030	I3804	L2927	K2770	PRO	Q1973	I1862	H1688	P1247	PRO	VAL
		A4228	O4228	K3809	I3805	X2950	V2775	ALA	GLU		Q1691	M1260	GLN	L861
		L4632		K3815	K3816	Y2954	E2381	GLU	GLU		L1698	C1269	VAL	P864
		P4641	E4232	I3816	X3361	X3361	I2384	THR	T1991		D1700	L1270	ASN	L867
		V4666	Q4547	I3817	X3362	K2806	P2395	Q2095	P2002				SER	R886
						K2807							ARG	L887

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:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.61
2:I:745:SER:HB2	2:I:758:ARG:HB3	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: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
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.87	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:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.53
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.41	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:345:LEU:HD23	2:G:389:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.75	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: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:2452:ARG:HH12	2:G:177:GLU:HG3	1.76	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:646:PRO:HD2	2:B:779:PRO:HB2	1.93	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.92	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: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:3762:ARG:H	2:I:4754:ASN:HA	1.77	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:345:LEU:HD23	2:B:389:PHE:HB3	1.93	0.49
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.44	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: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:B:999:ASP:O	2:B:1004:GLY:N	2.46	0.49
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.94	0.49
2:E:999:ASP:O	2:E:1004:GLY:N	2.46	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:286:THR:HA	2:E:405:HIS:HB2	1.95	0.49
2:E:309:THR:O	2:E:313:SER:OG	2.31	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:134:ASP:OD1	2:I:134:ASP:N	2.46	0.49
2:I:999:ASP:O	2:I:1004:GLY: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: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:G:999:ASP:O	2:G:1004:GLY:N	2.46	0.49
2:I:173:SER:HB3	2:I:178:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:16:THR:OG1	2:I:97:GLY:O	2.31	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: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:I:972:LEU:O	2:I:1044:ARG:NH2	2.47	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:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.48
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.79	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:4071:ILE:HD11	2:E:4102:GLN:HE21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.48
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.47	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:4987:ASN:HA	2:G:4990:PHE:HD2	1.78	0.48
2:G:16:THR:OG1	2:G:97:GLY:O	2.31	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:841:GLY:HA2	2:E: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: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: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
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.96	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:4571:PHE:O	2:E:4575:PHE:N	2.48	0.47
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.80	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:670:GLU:HG3	2:E:787:VAL:HG13	1.97	0.47
2:E:16:THR:OG1	2:E:97:GLY:O	2.31	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:4191:GLU:OE1	2:E:5006:GLN:NE2	2.48	0.46
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.97	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:4227:GLU:OE2	2:G:4973:HIS:ND1	2.49	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: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:649:PHE:HB3	2:B:776:LEU:HD13	1.98	0.46
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.80	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:3959:LYS:O	2:G:3963:ASN:ND2	2.49	0.45
2:G:395:GLN:HG3	2:G:397:GLU:H	1.81	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:689:THR:H	2:I:778:PHE:HE2	1.64	0.45
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.97	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:346:CYS:N	2:B:388:LEU:O	2.49	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	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:177:GLU:HG3	2:E:2452:ARG:HH12	1.81	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	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:2131:LEU:HD23	2:I:3662:ILE:HB	1.99	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: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:2467:VAL:HA	2:I:2470:ILE:HD12	2.01	0.43
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.00	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:4586:PRO:HA	2:I:4628:VAL:HG11	2.01	0.43
2:I:41:GLY:O	2:I:45:ARG:NH1	2.50	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:3971:GLY:H	2:B:5005:GLY:HA3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4864:ASN:HA	2:B:4874:MET:HG2	2.01	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:4063:ASP:OD1	2:E:4169:SER:OG	2.30	0.42
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.84	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:57:ASN:HD22	2:E:308:HIS:HB2	1.85	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.45	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
2:G:788:LYS:HG2	2:G:1629:GLN:HA	2.01	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: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:B:788:LYS:HG2	2:B:1629:GLN:HA	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:71: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%)	56	90
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	56	90
2	G	3235/4416 (73%)	2887 (89%)	344 (11%)	4 (0%)	56	90
2	I	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	56	90
All	All	13360/18096 (74%)	11919 (89%)	1425 (11%)	16 (0%)	59	90

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%)	90	95
2	E	2493/3022 (82%)	2477 (99%)	16 (1%)	90	95
2	G	2493/3022 (82%)	2477 (99%)	16 (1%)	90	95
2	I	2493/3022 (82%)	2477 (99%)	16 (1%)	90	95
All	All	10324/12444 (83%)	10260 (99%)	64 (1%)	91	95

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 [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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