



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 01:09 pm GMT

PDB ID : 5TB4
EMDB ID: : EMD-8395
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-11
Resolution : 4.50 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

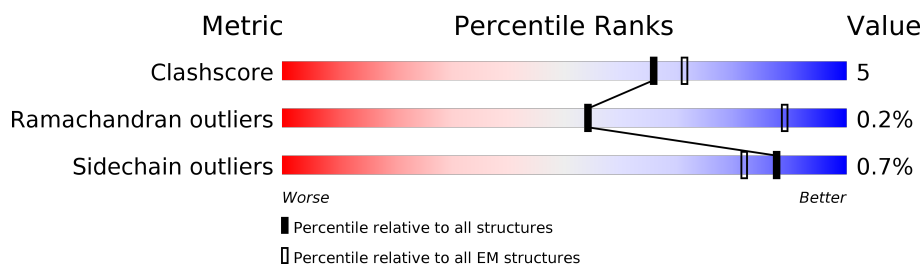
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	84% 15% .
1	F	108	81% 19% .
1	H	108	85% 14% .
1	J	108	83% 16% .
2	B	4416	84% 10% 5%
2	E	4416	84% 10% 5%
2	G	4416	84% 10% 5%
2	I	4416	84% 10% 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.

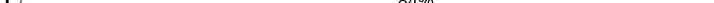
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

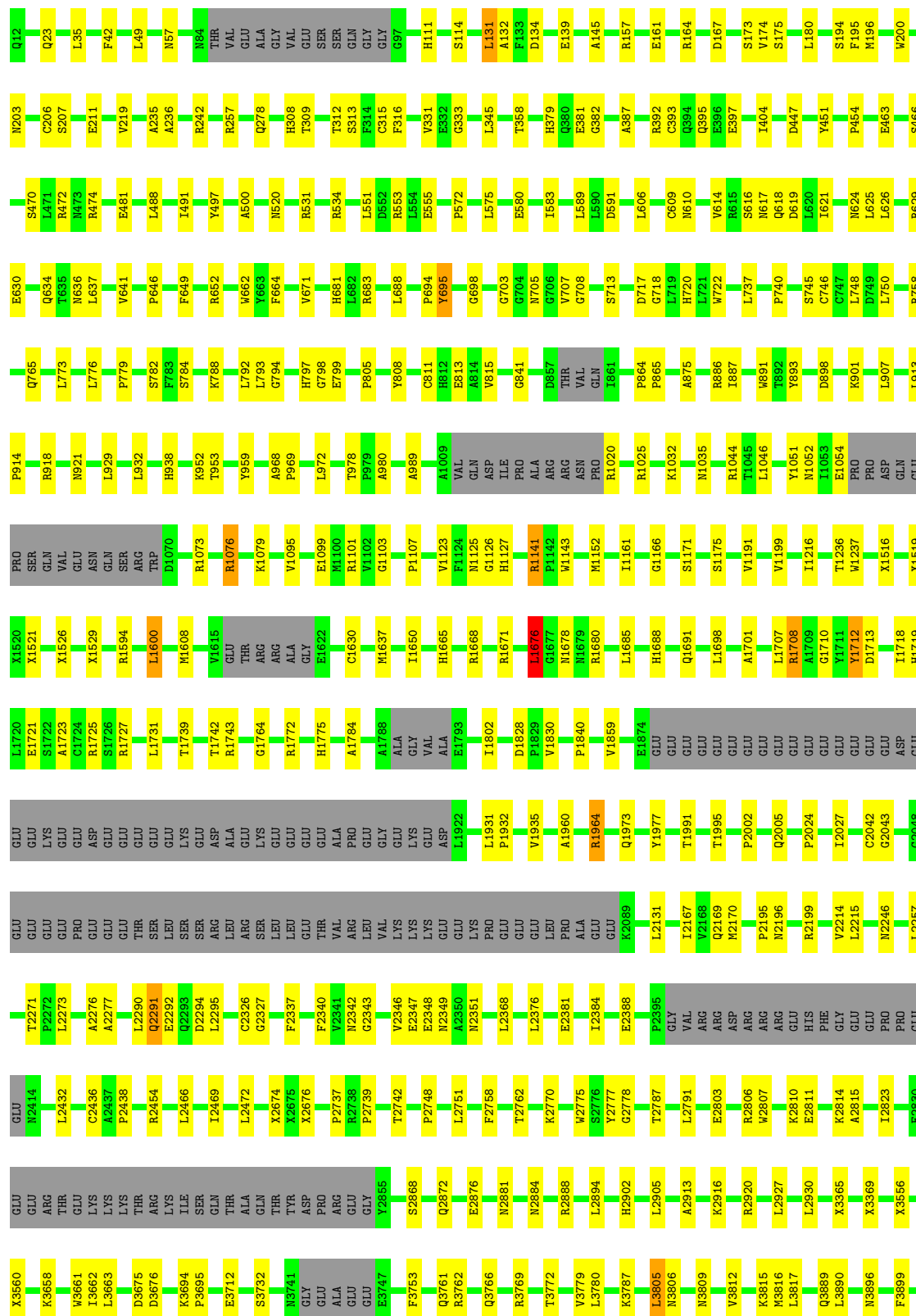
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	

M4864	T4148	Q3927	K3658	GLU	W2414	T2271	GLU	ASP	T1742	V1615	R1076	Y959	F783	F649
E4871	E4152	S3931	W3661	THR	L2432	P2272	GLU	ALA	R1743	GLU	A1077	Y959	S784	F649
C4876	H4156	S3937	I3662	GLU	L2273	L2273	THR	GLU	G1764	THR	K1078	A968	K788	R652
H4886	L4166	Y3937	I3662	LYS	A2276	A2276	LEU	GLU	R1772	ALA	S1080	P969	L792	V662
C4890	A4167	K3948	F3669	LYS	P2438	A2277	SER	GLU	H1775	GLY	V1095	L872	L793	V663
Y4909	P4176	M3955	D3675	THR	R2454	L2290	SER	GLU	A1788	E1622	V1095	T978	G794	F664
I4925	Y4177	V3961	D3676	ARG	Q2291	Q2291	ARG	ALA	A1784	C1630	R1101	P979	H797	V671
L4929	L4178	V3961	E3712	ILE	E2292	E2292	ARG	PRO	A1784	C1630	R1101	A980	G798	V671
F4959	I4181	F3962	S3732	SER	D2294	D2294	SER	GLY	A1788	M1637	G1103	A859	E799	H681
I4960	I4193	N3963	N3741	GLN	L2469	L2295	LEU	LEU	ALA	I1650	P1107	A859	P805	H682
F4968	I4194	G3971	GLY	THR	L2472	C3236	GLU	LYS	GLY	I1650	P1107	A859	P805	H683
H4978	Y4194	A3981	GLU	ALA	X2674	G2327	THR	ASP	VAL	H1665	E1109	VAL	Y808	L688
E4982	R4202	A3981	ALA	ASP	X2676	F2337	ARG	L1922	E1793	H1665	E1109	VAL	Y808	L688
H4983	E4227	R3984	GLU	PRO	P2737	F2340	VAL	L1931	I1802	R1668	L1120	ASP	C811	P694
N4984	A4228	L3985	GLU	ARG	R2738	V2341	LYS	P1932	D1828	L1676	V1123	PRO	H812	Y695
L4985	E4229	W3986	GLU	GLU	P2739	G2343	LYS	V1935	P1829	L1677	F1124	ALA	E813	G699
A4986	K4230	F3753	GLY	GLY	Y2855	G2343	GLU	K1936	V1830	G1677	G1126	ARG	V815	G703
W4987	F3992	F3753	Y2855	GLU	V2346	V2346	GLU	C1940	P1840	M1678	R1141	ASN	G841	G704
Y4988	L3993	Q3761	S2868	LYS	E2347	E2347	LYS	C1940	P1840	R1680	P1142	PRO	D857	N705
C5027	X4344	R3762	Q2872	PRO	E2348	E2348	PRO	D1948	V1859	R1680	P1142	PRO	D857	G706
L5036	N4553	Q3766	E2876	GLU	A2350	A2350	GLU	A1960	E1874	L1685	W1143	R1025	THR	V707
S5037	M4558	R3769	E2876	LEU	N2351	N2351	LEU	R1964	GLU	H1688	M1152	K1032	GLN	G708
	S4008	T3772	N2881	PRO	L2368	L2368	PRO	R1964	GLU	Q1691	I1161	N1035	I861	S713
	L4019	V3779	N2884	ALA	L2376	L2376	ALA	Q1973	GLU	L1698	G1166	N1035	A875	D717
	N4034	L3780	R2888	GLU	E2381	E2381	GLU	Y1977	GLU	L1698	G1166	R1044	R886	G718
	E4056	K3787	L2894	LEU	E2381	E2381	LEU	T1991	GLU	A1701	V1199	L1046	I887	L719
	L4059	L3805	H2902	PRO	L2384	L2384	PRO	T1991	GLU	L1707	V1199	L1046	W891	H720
	K4060	N3806	L2905	ALA	E2388	E2388	ALA	T1995	GLU	R1708	I1216	M1052	T892	L721
	D4063	N3809	L2905	GLY	P2395	P2395	GLY	P2002	GLU	Y1711	T1235	N1053	Y893	W722
	D4083	V3812	A2913	VAL	P2395	P2395	VAL	Q2005	GLU	Y1712	W1237	E1054	D898	P740
	P4084	K3915	K2916	ARG	V2166	V2166	ARG	Q2005	GLU	D1713	X1516	PRO	K901	S745
	R4085	M3815	K2916	ASP	Q2169	Q2169	ASP	P2022	GLU	I1718	X1519	GLN	L907	C746
	G4086	L3817	R2920	ARG	M2170	M2170	ARG	P2024	ASP	H1719	X1519	GLU	L907	C746
	K4090	L3817	L2927	ARG	P2195	P2195	ARG	T2027	GLU	L1720	X1520	PRO	L913	L748
	Q4094	Q3889	L2930	ARG	N2196	N2196	ARG	R2028	GLU	E1721	X1521	SER	R918	L750
	Q4094	L3890	L2930	HIS	R2199	R2199	HIS	C2042	LYS	A1723	X1526	VAL	N921	R758
	T4104	N3896	X3365	PHE	V2214	V2214	PHE	G2043	GLU	C1724	X1526	GLU	N921	R758
	G4105	G4105	K2814	GLY	V2214	V2214	GLY	G2043	ASP	R1725	X1529	ASN	L929	Q765
	P4106	F3899	A2815	GLU	L2215	L2215	GLU	G2048	GLU	S1728	X1529	GLN	L929	Q765
	E4107	T3907	I2823	PRO	PRO	PRO	PRO	G2048	GLU	R1727	R1594	TRP	L932	L773
	N4120	L3923	E2830	GLU	E2830	E2830	GLU	G2048	GLU	L1731	L1600	D1070	H838	L776
				GLU			GLU			T1739	M1608	R1073	K952	P779
													T953	S782


- Molecule 2: Ryanodine receptor 1

Chain E:  84% 10% 5%



T3907	M4120	GLY	E4871
L5923	T4148	SER	C4876
Q3927	E4152	GLY	H4886
S3931	H4156	SER	G4890
Y3937	L4166	TRP	Y4909
K3948	A4167	GLY	I4925
M3955	P4176	ALA	L4929
Q3960	Y4177	GLY	L4935
V3961	L4178	GLU	F4959
F3962	I4181	GLU	I4960
N3963	I4193	GLY	F4969
G3971	Y4194	ASP	H4978
A3981	R4202	ASP	E4982
R3984	E4227	GLU	H4983
L3985	A4228	GLN	N4984
W3986	E4229	SER	A4985
F3992	K4230	GLY	A4986
L3993	Q4250	GLY	N4987
X4344	X4344	VAL	Y4988
F3996	M4553	GLU	C5027
K4002	F4571	GLY	L5036
S4008	F4575	GLY	S5037
L4019	I4576		
M4034	L4577		
E4056	Y4580		
L4059	K4581		
K4060	V4582		
D4063	P4587		
D4083	GLY		
P4084	GLU		
R4085	ASP		
G4086	MET		
K4090	GLU		
Q4094	GLY		
T4104	ALA		
G4105	F4195		
P4106	S4770		
	M4833		
	R4860		
	N4864		

• Molecule 2: Ryanodine receptor 1

Chain I:  84% 10% 5%

Q12	E211	S485	L637	L776	L932	D1070	R1594	R1727	GLU
Q23	V219	L488	V641	P779	K952	R1073	L1600	L1731	GLU
L35	F232	M489	F646	S782	T953	O1077	M1608	T1739	GLU
F42	I233	I491	F649	F784	Y959	E1078	V1615	T1742	LYS
L49	S234	Y497	R652	K788	A968	E1079	GLU	R1743	ASP
N57	A236	A500	R652	L792	P969	S1080	THR	G1764	ALA
N84	R242	N520	V662	L793	L972	Y1081	ARG	R1772	GLY
THR	R257	R531	F664	G794	T978	V1095	GLY	H1775	GLU
GLU	Q278	G532	V671	H797	P979	E1099	E1622	A1784	ALA
VAL	L4935	N533	H681	G798	A980	M1100	C1630	A1788	ALA
ALA	H308	R534	L682	E799	A989	R1101	M1637	A1788	VAL
GLY	T309	A535	R683	P805	A1009	G1103	I1650	ALA	GLY
VAL	T312	N536	L688	Y808	VAL	P1107	I1668	I1802	GLY
GLU	S313	L551	P694	C811	ASP	E1108	H1665	D1828	VAL
GLN	C315	R553	Y695	H812	ILE	L1109	R1671	P1829	GLU
GLY	F316	L554	G688	E813	PRO	L1120	R1671	V1830	LYS
G97	V331	E555	G703	A814	ALA	V1123	R1671	P1840	LYS
H111	E332	P572	G704	V815	ARG	F1124	L1676	P1859	GLU
S114	G333	L575	N705	G841	ASN	M1125	G1677	A1874	GLU
L131	L345	E580	G706	D857	R1020	G1126	N1679	GLU	ALA
A132	T358	I583	G708	THR	R1025	H1127	R1680	GLU	GLU
D134	H379	L589	S713	VAL	K1032	R1141	L1685	GLU	GLU
E139	Q380	D591	D717	GLM	N1035	P1142	H1688	GLU	GLU
A145	E381	L606	G718	A875	R1044	W1143	Q1691	GLU	GLU
R157	G382	C609	H720	R886	T1045	M1152	L1698	GLU	GLU
E161	A387	N610	W722	I887	L1046	I1161	A1701	GLU	GLU
R164	Q393	R392	L737	W891	Y1051	G1166	L1707	GLU	GLU
D167	E395	C393	V614	T892	N1052	V1191	R1708	GLU	GLU
S173	E396	Q394	R615	Y893	E1054	V1199	A1709	GLU	GLU
V174	E397	D447	N617	D898	PRO	I1216	G1710	GLU	GLU
S175	D447	Y451	Q618	K901	ASP	T1236	Y1711	GLU	GLU
S194	S470	P454	D619	L907	GLM	W1237	Y1712	GLU	GLU
F195	L471	L625	L620	L913	GLU	X1516	D1713	GLU	GLU
M196	R472	L626	L621	P914	PRO	X1519	I1718	ASP	GLU
N203	N474	R629	L621	L750	GLM	X1520	H1719	GLU	GLU
C206	R474	E530	L626	L750	VAL	X1521	L1720	GLU	GLU
S207	R474	L626	L626	L750	GLU	X1526	E1721	GLU	GLU
					ASN	X1526	S1722	LYS	GLU
					GLN	X1529	A1723	GLU	GLU
					ARG	X1529	C1725	ASP	GLU
					TRP		S1726	GLU	GLU



Category A	GLN	R918	R758	R629	L471	N203	Q12
	VAL	N921	Q765	E630	R472	C206	Q23
	ASN	L929	L773	D634	R474	S207	L35
	GLN	L932	L776	N636	E481	E211	F42
	SER	L938	L779	L637	L488	V219	L49
	TRP	H938	P779	V641	I491	A235	N57
	D1070	K952	P646	P646	Y497	A236	N64
	R1073	T953	F782	F649	A500	R242	THR
	R1076	Y959	S784	R652	N520	R257	VAL
	K1079	A968	K788	H662	R531	H308	ALA
Category B	V1095	P969	L792	V663	G532	T309	GLY
	E1099	L972	G794	F664	N533	T312	VAL
	M1100	P978	H797	V671	R634	S313	GLU
	R1101	P979	G798	H681	A535	F314	SER
	V1102	A980	E799	L682	N536	C315	GLN
	G1103	A989	P805	R683	L551	F316	GLY
	P1107	A1009	Y808	L688	R552	V331	GLY
	V1123	VAL	C811	G694	L554	E332	H111
	N1125	GLN	H812	V695	E555	G333	S114
	G1126	ASP	E813	G696	P572	L345	L131
Category C	H1127	PRO	A814	G698	L575	T358	A132
	R1141	ALA	V815	G703	E580	H379	F133
	V1142	ARG	G841	G704	G380	G381	D134
	W1143	ARG	G841	G705	E583	G382	E139
	M1152	ASN	D857	G706	I583	A387	A145
	I1161	PRO	THR	V707	L589	R392	R157
	G1166	R1020	VAL	G708	L590	C393	E161
	V1191	R1025	GLN	S713	D591	G394	R164
	V1199	N1035	A875	D717	L606	Q395	D167
	I1216	R1044	R886	G718	C609	E396	S173
Category D	T1236	T1045	I887	H719	N610	D447	V174
	W1237	L1046	L721	W722	V614	Y451	S175
	X1516	X1053	D898	P740	Q618	D619	L180
	X1519	X1054	K901	S745	L620	P454	S194
	X1520	PRO	I892	G746	I621	E463	M196
	X1521	ASP	L907	G747	N624	S466	W200
	X1526	GLU	L913	D749	L625	S470	
	X1526	GLN	P914	L750	L626		
	X1529	PRO					
	X1529	PRO					




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	0.31	0/834	0.51	0/1123
1	F	0.31	0/834	0.51	0/1123
1	H	0.31	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.55	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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	695	TYR	C-N	5.28	1.44	1.34
2	I	695	TYR	C-N	5.28	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	695	TYR	C-N	5.28	1.44	1.34
2	E	695	TYR	C-N	5.26	1.44	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	E	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	G	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	I	131	LEU	CA-CB-CG	8.21	134.18	115.30
2	I	1600	LEU	CA-CB-CG	6.73	130.78	115.30
2	B	1600	LEU	CA-CB-CG	6.71	130.75	115.30
2	E	1600	LEU	CA-CB-CG	6.71	130.75	115.30
2	G	1600	LEU	CA-CB-CG	6.70	130.71	115.30
2	G	1676	LEU	CA-CB-CG	6.39	130.01	115.30
2	B	1676	LEU	CA-CB-CG	6.39	130.00	115.30
2	I	1676	LEU	CA-CB-CG	6.39	130.00	115.30
2	E	1676	LEU	CA-CB-CG	6.38	129.98	115.30
2	I	2290	LEU	CA-CB-CG	5.65	128.30	115.30
2	B	2290	LEU	CA-CB-CG	5.65	128.30	115.30
2	E	2290	LEU	CA-CB-CG	5.65	128.30	115.30
2	G	2290	LEU	CA-CB-CG	5.62	128.23	115.30
2	B	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	E	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	I	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	G	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	B	4985	LEU	CA-CB-CG	5.37	127.66	115.30
2	E	4985	LEU	CA-CB-CG	5.37	127.66	115.30
2	I	4985	LEU	CA-CB-CG	5.37	127.66	115.30
2	G	4985	LEU	CA-CB-CG	5.37	127.66	115.30

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	624	ASN	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	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	4666	VAL	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	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	4666	VAL	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
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
2	I	4666	VAL	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	11	0
1	F	818	0	824	12	0
1	H	818	0	824	9	0
1	J	818	0	824	11	0
2	B	29499	0	24757	259	0
2	E	29499	0	24757	259	0
2	G	29499	0	24757	251	0
2	I	29499	0	24757	256	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	102324	1040	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 (1040) 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:G:2291:GLN:HB3	2:G:2294:ASP:H	1.51	0.76
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.51	0.76
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.51	0.75
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.51	0.74
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.57	0.70
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.57	0.69
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.57	0.69
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.57	0.68
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.76	0.67
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.76	0.66
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.31	0.66
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.31	0.66
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.31	0.65
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.76	0.65
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.31	0.65
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.76	0.65
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.80	0.63
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.82	0.62
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.82	0.62
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.82	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.82	0.62
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.73	0.62
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.73	0.62
1:J:35:LYS:HD3	2:I:636:ASN:HD21	1.65	0.62
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.82	0.61
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.73	0.61
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.82	0.61
1:F:35:LYS:HD3	2:E:636:ASN:HD21	1.65	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.82	0.61
1:H:35:LYS:HD3	2:G:636:ASN:HD21	1.65	0.61
2:I:379:HIS:HD2	2:I:382:GLY:H	1.49	0.61
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.82	0.61
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.82	0.61
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.82	0.61
1:A:35:LYS:HD3	2:B:636:ASN:HD21	1.65	0.61
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.73	0.60
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.83	0.60
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.82	0.60
2:B:379:HIS:HD2	2:B:382:GLY:H	1.49	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:E:2347:GLU:O	2:E:2351:ASN:N	2.32	0.60
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:HIS:HD2	2:E:382:GLY:H	1.49	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.67	0.60
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.84	0.60
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.82	0.60
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.82	0.59
2:B:2347:GLU:O	2:B:2351:ASN:N	2.32	0.59
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.84	0.59
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.84	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.59
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.68	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.83	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.68	0.59
2:I:331:VAL:HG12	2:I:333:GLY:H	1.67	0.59
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.68	0.59
2:E:626:LEU:HD23	2:E:630:GLU:H	1.68	0.59
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.36	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.68	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.58
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.84	0.58
2:E:331:VAL:HG12	2:E:333:GLY:H	1.67	0.58
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.84	0.58
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.84	0.58
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.84	0.58
2:G:2347:GLU:O	2:G:2351:ASN:N	2.32	0.58
2:I:626:LEU:HD23	2:I:630:GLU:H	1.68	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.67	0.58
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.84	0.58
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.86	0.58
2:G:379:HIS:HD2	2:G:382:GLY:H	1.49	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.36	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.86	0.58
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.85	0.58
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.36	0.57
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.86	0.57
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.39	0.57
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.40	0.57
2:G:626:LEU:HD23	2:G:630:GLU:H	1.68	0.57
2:B:626:LEU:HD23	2:B:630:GLU:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.78	0.57
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.86	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.78	0.57
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.40	0.57
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.86	0.57
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.38	0.57
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.57
2:B:652:ARG:HD3	2:B:773:LEU:HD13	1.87	0.57
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.86	0.57
2:G:315:CYS:SG	2:G:316:PHE:N	2.78	0.57
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.57
2:I:315:CYS:SG	2:I:316:PHE:N	2.78	0.57
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.73	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.57
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.38	0.57
2:I:652:ARG:HD3	2:I:773:LEU:HD13	1.87	0.57
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.87	0.56
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.87	0.56
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.87	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.38	0.56
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.36	0.56
2:E:652:ARG:HD3	2:E:773:LEU:HD13	1.87	0.56
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.39	0.56
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.38	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.86	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.86	0.56
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.87	0.56
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.56
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.88	0.56
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.56
2:E:1076:ARG:HB3	2:E:1191:VAL:HG23	1.89	0.55
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.55
2:G:652:ARG:HD3	2:G:773:LEU:HD13	1.87	0.55
2:I:1671:ARG:HH21	2:I:1713:ASP:HB3	1.71	0.55
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.88	0.55
2:E:3993:LEU:HA	2:E:3996:PHE:HB2	1.88	0.55
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.87	0.55
2:I:2347:GLU:O	2:I:2351:ASN:N	2.32	0.55
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.87	0.55
2:G:1076:ARG:HB3	2:G:1191:VAL:HG23	1.89	0.55
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.89	0.55
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.55
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.89	0.55
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.55
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.89	0.55
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.55
2:I:1076:ARG:HB3	2:I:1191:VAL:HG23	1.88	0.55
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.89	0.55
2:I:3993:LEU:HA	2:I:3996:PHE:HB2	1.89	0.55
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.75	0.55
2:G:3993:LEU:HA	2:G:3996:PHE:HB2	1.89	0.55
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.88	0.55
2:B:1076:ARG:HB3	2:B:1191:VAL:HG23	1.88	0.55
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.75	0.55
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.40	0.55
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.40	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.40	0.55
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.55
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.40	0.55
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.88	0.55
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.55
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.40	0.55
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.89	0.54
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.72	0.54
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.89	0.54
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.40	0.54
2:E:1671:ARG:HH21	2:E:1713:ASP:HB3	1.71	0.54
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.88	0.54
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.88	0.54
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.88	0.54
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.75	0.54
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.40	0.54
2:G:1671:ARG:HH21	2:G:1713:ASP:HB3	1.71	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.40	0.54
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3993:LEU:HA	2:B:3996:PHE:HB2	1.88	0.54
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.40	0.54
2:E:161:GLU:OE2	2:G:3984:ARG:NH2	2.41	0.54
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.88	0.54
2:B:1671:ARG:HH21	2:B:1713:ASP:HB3	1.71	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.41	0.54
2:E:3732:SER:O	2:E:3766:GLN:NE2	2.41	0.54
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.41	0.54
2:G:4960:ILE:HG21	2:G:4988:TYR:HE2	1.73	0.54
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.72	0.54
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.89	0.54
2:G:3732:SER:O	2:G:3766:GLN:NE2	2.41	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.80	0.53
2:I:3732:SER:O	2:I:3766:GLN:NE2	2.41	0.53
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.41	0.53
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.40	0.53
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.40	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.91	0.53
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.72	0.53
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.72	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.91	0.53
2:B:1052:ASN:ND2	2:B:1054:GLU:OE2	2.42	0.53
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.91	0.53
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.41	0.53
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.90	0.53
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.91	0.53
2:B:3732:SER:O	2:B:3766:GLN:NE2	2.41	0.53
2:B:4056:GLU:O	2:B:4060:LYS:N	2.36	0.53
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.42	0.53
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.53
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.89	0.53
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.53
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.53
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.90	0.53
2:B:161:GLU:OE2	2:E:3984:ARG:NH2	2.42	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.91	0.53
2:I:4960:ILE:HG21	2:I:4988:TYR:HE2	1.73	0.53
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.74	0.53
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.42	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.91	0.53
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.91	0.52
2:E:4960:ILE:HG21	2:E:4988:TYR:HE2	1.73	0.52
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.42	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.52
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:E:1052:ASN:ND2	2:E:1054:GLU:OE2	2.42	0.52
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.91	0.52
2:G:1052:ASN:ND2	2:G:1054:GLU:OE2	2.42	0.52
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.90	0.52
2:I:1052:ASN:ND2	2:I:1054:GLU:OE2	2.42	0.52
2:B:173:SER:OG	2:B:174:VAL:N	2.43	0.52
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.42	0.52
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.74	0.52
2:I:4056:GLU:O	2:I:4060:LYS:N	2.36	0.52
2:G:4090:LYS:O	2:G:4094:GLN:N	2.42	0.52
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.42	0.52
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.92	0.52
2:B:4960:ILE:HG21	2:B:4988:TYR:HE2	1.73	0.52
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.52
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.90	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:I:173:SER:OG	2:I:174:VAL:N	2.43	0.52
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.43	0.52
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.80	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:G:4056:GLU:O	2:G:4060:LYS:N	2.36	0.52
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.92	0.52
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.41	0.51
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.51
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.43	0.51
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.74	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.80	0.51
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.92	0.51
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.41	0.51
2:E:173:SER:OG	2:E:174:VAL:N	2.43	0.51
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.90	0.51
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.43	0.51
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.92	0.51
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.92	0.51
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.43	0.51
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.92	0.51
2:B:3984:ARG:NH2	2:I:161:GLU:OE2	2.43	0.51
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.93	0.51
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.43	0.51
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.93	0.51
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.92	0.51
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.92	0.51
2:B:2195:PRO:HB3	2:B:2246:ASN:HD21	1.76	0.51
2:E:2195:PRO:HB3	2:E:2246:ASN:HD21	1.76	0.51
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.93	0.51
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.93	0.51
2:G:173:SER:OG	2:G:174:VAL:N	2.43	0.51
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.44	0.51
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.50
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.43	0.50
2:I:3984:ARG:NH2	2:G:161:GLU:OE2	2.43	0.50
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.44	0.50
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.92	0.50
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.94	0.50
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.41	0.50
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.92	0.50
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.94	0.50
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.42	0.50
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.50
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.50
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.93	0.50
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.94	0.50
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.94	0.50
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.77	0.50
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.77	0.50
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.94	0.50
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.94	0.50
2:E:4059:LEU:O	2:E:4063:ASP:N	2.45	0.50
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.50
2:I:2195:PRO:HB3	2:I:2246:ASN:HD21	1.76	0.50
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.94	0.50
2:E:4056:GLU:O	2:E:4060:LYS:N	2.36	0.49
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:913:LEU:O	2:I:918:ARG:NH2	2.45	0.49
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.49
2:B:913:LEU:O	2:B:918:ARG:NH2	2.45	0.49
2:E:609:CYS:SG	2:E:610:ASN:N	2.85	0.49
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.94	0.49
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.76	0.49
2:G:2195:PRO:HB3	2:G:2246:ASN:HD21	1.76	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:G:609:CYS:SG	2:G:610:ASN:N	2.85	0.49
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.44	0.49
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.49
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.43	0.49
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.94	0.49
2:I:4059:LEU:O	2:I:4063:ASP:N	2.45	0.49
2:B:4059:LEU:O	2:B:4063:ASP:N	2.45	0.49
2:B:451:TYR:O	2:B:474:ARG:NH1	2.43	0.49
2:B:3753:PHE:HE2	2:B:4718:LYS:HB2	1.77	0.49
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.95	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.49
2:E:1991:THR:O	2:E:1995:THR:OG1	2.30	0.49
2:E:4090:LYS:O	2:E:4094:GLN:N	2.42	0.49
2:G:1991:THR:O	2:G:1995:THR:OG1	2.30	0.49
2:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.77	0.49
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.77	0.49
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.49
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.49
2:E:913:LEU:O	2:E:918:ARG:NH2	2.45	0.49
2:G:913:LEU:O	2:G:918:ARG:NH2	2.45	0.49
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.94	0.49
2:I:3992:PHE:O	2:I:3996:PHE:N	2.43	0.49
2:I:609:CYS:SG	2:I:610:ASN:N	2.85	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.49
2:E:4978:HIS:HE1	2:E:5027:CYS:SG	2.36	0.49
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.93	0.49
2:G:132:ALA:HA	2:G:194:SER:HB2	1.95	0.49
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.93	0.49
2:I:132:ALA:HA	2:I:194:SER:HB2	1.95	0.49
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.76	0.49
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.94	0.49
2:E:2868:SER:O	2:E:2872:GLN:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.95	0.49
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.49
2:I:4090:LYS:O	2:I:4094:GLN:N	2.42	0.49
2:I:683:ARG:NH1	2:I:707:VAL:O	2.44	0.49
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.49
2:G:4059:LEU:O	2:G:4063:ASP:N	2.45	0.49
2:G:4978:HIS:HE1	2:G:5027:CYS:SG	2.36	0.49
2:I:3753:PHE:HE2	2:I:4718:LYS:HB2	1.77	0.49
2:B:1991:THR:O	2:B:1995:THR:OG1	2.30	0.49
2:B:4978:HIS:HE1	2:B:5027:CYS:SG	2.36	0.49
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.49
2:E:3753:PHE:HE2	2:E:4718:LYS:HB2	1.77	0.49
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.44	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.95	0.49
2:I:1991:THR:O	2:I:1995:THR:OG1	2.30	0.49
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.94	0.48
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.44	0.48
2:G:683:ARG:NH1	2:G:707:VAL:O	2.44	0.48
2:I:4978:HIS:HE1	2:I:5027:CYS:SG	2.36	0.48
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.94	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.48
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.48
2:B:609:CYS:SG	2:B:610:ASN:N	2.85	0.48
2:G:3753:PHE:HE2	2:G:4718:LYS:HB2	1.78	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:E:132:ALA:HA	2:E:194:SER:HB2	1.95	0.48
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.95	0.48
2:B:132:ALA:HA	2:B:194:SER:HB2	1.95	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.47	0.48
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.79	0.48
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.79	0.48
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.29	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.48
2:E:4571:PHE:O	2:E:4575:PHE:N	2.46	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.46	0.48
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4571:PHE:O	2:B:4575:PHE:N	2.46	0.48
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.42	0.48
2:B:683:ARG:NH1	2:B:707:VAL:O	2.44	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.79	0.48
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.47	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.79	0.48
2:I:1973:GLN:HE22	2:I:2005:GLN:HE22	1.62	0.48
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.42	0.48
2:I:395:GLN:HG3	2:I:397:GLU:H	1.79	0.48
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.41	0.48
2:B:4090:LYS:O	2:B:4094:GLN:N	2.42	0.48
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.79	0.48
2:B:929:LEU:HD23	2:B:932:LEU:HD12	1.96	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.47	0.48
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.44	0.48
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.96	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.39	0.48
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.79	0.48
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.47	0.48
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.96	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.47	0.47
2:B:395:GLN:HG3	2:B:397:GLU:H	1.79	0.47
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.44	0.47
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.47
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.47	0.47
2:B:1973:GLN:HE22	2:B:2005:GLN:HE22	1.62	0.47
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.32	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:1973:GLN:HE22	2:G:2005:GLN:HE22	1.62	0.47
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.47	0.47
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.32	0.47
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.79	0.47
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.97	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.46	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.96	0.47
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.96	0.47
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.79	0.47
2:I:929:LEU:HD23	2:I:932:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.47
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.97	0.47
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.47	0.47
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.79	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.47
2:B:2810:LYS:HB3	2:B:2814:LYS:HE3	1.97	0.47
2:E:1723:ALA:HB1	2:E:1775:HIS:HD2	1.80	0.47
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.79	0.47
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.96	0.47
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.32	0.47
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.47
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.32	0.47
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.97	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:219:VAL:O	2:B:392:ARG:NH1	2.48	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.79	0.47
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.47	0.47
2:G:219:VAL:O	2:G:392:ARG:NH1	2.48	0.47
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.97	0.47
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.29	0.47
2:E:1973:GLN:HE22	2:E:2005:GLN:HE22	1.62	0.47
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.42	0.47
2:I:345:LEU:HD22	2:I:387:ALA:HB1	1.97	0.47
2:I:219:VAL:O	2:I:392:ARG:NH1	2.48	0.47
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.47
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.88	0.47
2:E:2810:LYS:HB3	2:E:2814:LYS:HE3	1.97	0.47
2:E:345:LEU:HD22	2:E:387:ALA:HB1	1.97	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.88	0.47
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.79	0.47
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.97	0.47
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.73	0.47
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.79	0.47
2:B:1723:ALA:HB1	2:B:1775:HIS:HD2	1.80	0.46
2:B:1701:ALA:HB1	2:B:1830:VAL:HG22	1.97	0.46
2:B:345:LEU:HD22	2:B:387:ALA:HB1	1.97	0.46
2:B:3806:ASN:HA	2:B:3890:LEU:HD13	1.98	0.46
2:G:164:ARG:N	2:G:167:ASP:OD2	2.47	0.46
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.49	0.46
2:G:345:LEU:HD22	2:G:387:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.46
2:I:1701:ALA:HB1	2:I:1830:VAL:HG22	1.97	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.80	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.39	0.46
2:B:792:LEU:HD22	2:B:799:GLU:H	1.80	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.46
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.98	0.46
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.79	0.46
2:E:929:LEU:HD23	2:E:932:LEU:HD12	1.96	0.46
2:G:792:LEU:HD22	2:G:799:GLU:H	1.80	0.46
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.96	0.46
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.39	0.46
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.98	0.46
2:E:1701:ALA:HB1	2:E:1830:VAL:HG22	1.97	0.46
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.97	0.46
2:E:2913:ALA:HA	2:E:2916:LYS:HB2	1.98	0.46
2:E:219:VAL:O	2:E:392:ARG:NH1	2.48	0.46
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.79	0.46
2:E:463:GLU:O	2:E:466:SER:OG	2.30	0.46
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.97	0.46
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.73	0.46
2:G:2913:ALA:HA	2:G:2916:LYS:HB2	1.98	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.47	0.46
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.97	0.46
2:G:2810:LYS:HB3	2:G:2814:LYS:HE3	1.97	0.46
2:I:4982:GLU:HB3	2:I:4983:HIS:CD2	2.51	0.46
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.98	0.46
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.49	0.46
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.88	0.46
2:B:2913:ALA:HA	2:B:2916:LYS:HB2	1.98	0.46
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.28	0.46
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.98	0.46
2:G:1723:ALA:HB1	2:G:1775:HIS:HD2	1.80	0.46
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	3.04	0.46
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.97	0.46
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.98	0.46
2:B:1516:UNK:N	2:B:1529:UNK:O	2.49	0.46
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.79	0.46
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.98	0.46
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.48	0.46
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.98	0.46
2:G:929:LEU:HD23	2:G:932:LEU:HD12	1.96	0.46
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.98	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.51	0.46
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.46
2:I:3927:GLN:O	2:I:3931:SER:N	2.47	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.51	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.80	0.46
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.46
2:E:683:ARG:NH1	2:E:707:VAL:O	2.44	0.46
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.49	0.46
2:G:1516:UNK:N	2:G:1529:UNK:O	2.49	0.46
2:G:1701:ALA:HB1	2:G:1830:VAL:HG22	1.97	0.46
2:G:2758:PHE:O	2:G:2762:THR:N	2.47	0.46
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.46
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	3.04	0.46
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.88	0.46
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.79	0.46
2:G:978:THR:HB	2:G:980:ALA:H	1.80	0.46
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.46
2:B:195:PHE:HB3	2:B:196:MET:HG2	1.98	0.46
2:B:2381:GLU:HA	2:B:2384:ILE:HD12	1.98	0.46
2:B:3992:PHE:O	2:B:3996:PHE:N	2.43	0.46
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.46
2:I:1516:UNK:N	2:I:1529:UNK:O	2.49	0.46
2:I:2913:ALA:HA	2:I:2916:LYS:HB2	1.98	0.46
2:E:4344:UNK:N	2:I:4909:TYR:OH	2.49	0.46
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.96	0.46
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.81	0.45
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.81	0.45
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.45
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.45
2:I:2810:LYS:HB3	2:I:2814:LYS:HE3	1.97	0.45
2:E:1516:UNK:N	2:E:1529:UNK:O	2.49	0.45
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.49	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.43	0.45
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.99	0.45
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.80	0.45
2:I:3806:ASN:HA	2:I:3890:LEU:HD13	1.98	0.45
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	3.04	0.45
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.45
2:B:4982:GLU:HB3	2:B:4983:HIS:CD2	2.51	0.45
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.80	0.45
2:E:4982:GLU:HB3	2:E:4983:HIS:CD2	2.51	0.45
2:G:2346:VAL:HG13	2:G:2349:ASN:H	1.82	0.45
2:G:2381:GLU:HA	2:G:2384:ILE:HD12	1.99	0.45
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.52	0.45
2:E:195:PHE:HB3	2:E:196:MET:HG2	1.98	0.45
2:E:2381:GLU:HA	2:E:2384:ILE:HD12	1.98	0.45
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.49	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.51	0.45
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.49	0.45
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.99	0.45
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.97	0.45
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.49	0.45
2:E:2758:PHE:O	2:E:2762:THR:N	2.47	0.45
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.99	0.45
2:G:3806:ASN:HA	2:G:3890:LEU:HD13	1.98	0.45
2:I:2346:VAL:HG13	2:I:2349:ASN:H	1.82	0.45
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.49	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.28	0.45
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.49	0.45
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.49	0.45
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.45
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.51	0.45
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	3.04	0.45
2:E:662:TRP:H	2:E:748:LEU:HB3	1.82	0.45
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.98	0.45
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.98	0.45
2:G:662:TRP:H	2:G:748:LEU:HB3	1.82	0.45
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.49	0.45
2:I:1723:ALA:HB1	2:I:1775:HIS:HD2	1.80	0.45
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.45
2:B:2346:VAL:HG13	2:B:2349:ASN:H	1.82	0.45
2:E:2214:VAL:HG23	2:E:2215:LEU:HD12	1.99	0.45
2:E:2346:VAL:HG13	2:E:2349:ASN:H	1.82	0.45
2:E:792:LEU:HD22	2:E:799:GLU:H	1.80	0.45
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.99	0.45
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.50	0.45
2:I:2381:GLU:HA	2:I:2384:ILE:HD12	1.98	0.45
2:I:792:LEU:HD22	2:I:799:GLU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.50	0.45
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.52	0.45
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.98	0.45
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.99	0.45
2:E:3806:ASN:HA	2:E:3890:LEU:HD13	1.98	0.45
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.52	0.45
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.99	0.45
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.50	0.45
2:I:2214:VAL:HG23	2:I:2215:LEU:HD12	1.99	0.45
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.50	0.45
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.49	0.45
2:G:4982:GLU:HB3	2:G:4983:HIS:CD2	2.51	0.45
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.99	0.45
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	1.99	0.45
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.97	0.45
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	1.99	0.45
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.50	0.45
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.50	0.44
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.77	0.44
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	1.99	0.44
2:I:195:PHE:HB3	2:I:196:MET:HG2	1.98	0.44
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.99	0.44
2:I:718:GLY:HA3	2:I:737:LEU:HA	2.00	0.44
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.35	0.44
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.99	0.44
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.50	0.44
2:E:3927:GLN:O	2:E:3931:SER:N	2.47	0.44
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.99	0.44
2:E:875:ALA:HB1	2:E:921:ASN:HB3	1.99	0.44
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	2.00	0.44
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.81	0.44
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.82	0.44
2:I:1973:GLN:O	2:I:1977:TYR:N	2.49	0.44
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.44
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	2.00	0.44
2:B:718:GLY:HA3	2:B:737:LEU:HA	2.00	0.44
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.99	0.44
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.99	0.44
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.35	0.44
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.81	0.44
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ARG:N	2:B:167:ASP:OD2	2.47	0.44
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.50	0.44
1:F:55:VAL:HA	2:E:1784:ALA:HA	2.00	0.44
2:E:4959:PHE:CG	2:E:4959:PHE:O	2.71	0.44
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.83	0.44
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.52	0.44
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.80	0.44
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.99	0.44
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.44
2:B:4344:UNK:N	2:G:4909:TYR:OH	2.50	0.44
2:G:4959:PHE:CG	2:G:4959:PHE:O	2.71	0.44
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.50	0.44
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	2.00	0.44
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.82	0.44
2:G:3941:ASP:OD1	2:G:3941:ASP:N	2.50	0.44
2:G:4886:HIS:O	2:G:4890:GLY:N	2.50	0.44
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.00	0.44
2:I:4959:PHE:CG	2:I:4959:PHE:O	2.71	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.53	0.44
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	2.00	0.44
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	1.99	0.44
2:I:2902:HIS:HB3	2:I:2905:LEU:HG	2.00	0.44
2:I:875:ALA:HB1	2:I:921:ASN:HB3	1.99	0.44
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.51	0.44
2:B:875:ALA:HB1	2:B:921:ASN:HB3	1.99	0.44
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	1.99	0.44
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.98	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.49	0.44
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.50	0.44
2:G:875:ALA:HB1	2:G:921:ASN:HB3	1.99	0.44
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.43	0.44
2:B:134:ASP:OD1	2:B:134:ASP:N	2.50	0.44
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.50	0.44
2:B:662:TRP:H	2:B:748:LEU:HB3	1.82	0.44
2:B:811:CYS:HB3	2:B:815:VAL:HG11	2.00	0.44
2:G:2902:HIS:HB3	2:G:2905:LEU:HG	2.00	0.44
2:I:2868:SER:O	2:I:2872:GLN:N	2.39	0.44
2:I:451:TYR:O	2:I:474:ARG:NH1	2.43	0.44
2:B:4909:TYR:OH	2:G:4344:UNK:N	2.51	0.43
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.71	0.43
2:E:2902:HIS:HB3	2:E:2905:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:HIS:HD2	2:G:114:SER:H	1.65	0.43
2:G:4181:ILE:HG23	2:G:4193:ILE:HB	2.00	0.43
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.51	0.43
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.83	0.43
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.99	0.43
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.51	0.43
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.00	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.84	0.43
2:E:4713:SER:HA	2:E:4718:LYS:HE2	2.00	0.43
2:E:811:CYS:HB3	2:E:815:VAL:HG11	2.00	0.43
2:G:195:PHE:HB3	2:G:196:MET:HG2	1.98	0.43
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.00	0.43
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.29	0.43
2:G:3365:UNK:O	2:G:3369:UNK:N	2.52	0.43
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.00	0.43
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.39	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.82	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.53	0.43
2:E:1973:GLN:O	2:E:1977:TYR:N	2.49	0.43
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.77	0.43
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.00	0.43
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.50	0.43
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.29	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	1.99	0.43
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.01	0.43
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.00	0.43
2:E:1152:MET:HB2	2:E:1161:ILE:HB	2.00	0.43
2:E:3992:PHE:O	2:E:3996:PHE:N	2.43	0.43
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.50	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.53	0.43
2:G:718:GLY:HA3	2:G:737:LEU:HA	2.00	0.43
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.53	0.43
2:I:662:TRP:H	2:I:748:LEU:HB3	1.82	0.43
2:B:938:HIS:N	2:B:1054:GLU:O	2.52	0.43
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.52	0.43
2:G:134:ASP:OD1	2:G:134:ASP:N	2.50	0.43
2:G:811:CYS:HB3	2:G:815:VAL:HG11	2.00	0.43
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.43
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.00	0.43
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.82	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.84	0.43
2:E:111:HIS:HD2	2:E:114:SER:H	1.66	0.43
2:E:718:GLY:HA3	2:E:737:LEU:HA	2.00	0.43
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.52	0.43
2:I:4181:ILE:HG23	2:I:4193:ILE:HB	2.00	0.43
2:B:794:GLY:H	2:B:798:GLY:HA3	1.84	0.43
2:E:134:ASP:OD1	2:E:134:ASP:N	2.50	0.43
2:E:3761:GLN:NE2	2:E:4750:ILE:O	2.50	0.43
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.51	0.43
2:G:180:LEU:O	2:G:200:TRP:NE1	2.43	0.43
2:G:4713:SER:HA	2:G:4718:LYS:HE2	2.00	0.43
2:I:811:CYS:HB3	2:I:815:VAL:HG11	2.00	0.43
2:B:1973:GLN:O	2:B:1977:TYR:N	2.49	0.43
2:E:4984:ASN:C	2:E:4986:ALA:H	2.22	0.43
2:E:794:GLY:H	2:E:798:GLY:HA3	1.84	0.43
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.00	0.43
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.52	0.43
2:I:4984:ASN:C	2:I:4986:ALA:H	2.22	0.43
2:B:111:HIS:HD2	2:B:114:SER:H	1.65	0.43
2:B:1152:MET:HB2	2:B:1161:ILE:HB	2.00	0.43
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.43
2:B:4713:SER:HA	2:B:4718:LYS:HE2	2.00	0.43
2:E:938:HIS:N	2:E:1054:GLU:O	2.52	0.43
2:E:4181:ILE:HG23	2:E:4193:ILE:HB	2.00	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.43
2:G:3927:GLN:O	2:G:3931:SER:N	2.47	0.43
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.84	0.43
2:G:4984:ASN:C	2:G:4986:ALA:H	2.22	0.43
2:I:111:HIS:HD2	2:I:114:SER:H	1.65	0.43
2:I:134:ASP:OD1	2:I:134:ASP:N	2.50	0.43
2:I:4713:SER:HA	2:I:4718:LYS:HE2	2.00	0.43
2:B:1936:LYS:O	2:B:1940:CYS:N	2.48	0.43
2:B:2170:MET:HG3	2:B:2214:VAL:HG12	2.01	0.43
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.28	0.43
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.43
2:E:4909:TYR:OH	2:I:4344:UNK:N	2.52	0.43
2:G:1101:ARG:HG2	2:G:1125:ASN:HA	2.01	0.43
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.72	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.42
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.83	0.42
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:G:1152:MET:HB2	2:G:1161:ILE:HB	2.00	0.42
2:G:2438:PRO:HG2	2:G:2454:ARG:HB2	2.01	0.42
2:I:1152:MET:HB2	2:I:1161:ILE:HB	2.00	0.42
2:I:4181:ILE:HG13	2:I:4988:TYR:CE1	2.54	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.50	0.42
2:B:4181:ILE:HG13	2:B:4988:TYR:CE1	2.54	0.42
2:E:1739:THR:H	2:E:1742:THR:HB	1.85	0.42
2:E:4886:HIS:O	2:E:4890:GLY:N	2.50	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.46	0.42
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.49	0.42
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.46	0.42
2:I:2170:MET:HG3	2:I:2214:VAL:HG12	2.01	0.42
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.84	0.42
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.01	0.42
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.93	0.42
2:B:1739:THR:H	2:B:1742:THR:HB	1.85	0.42
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	2.02	0.42
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	2.02	0.42
2:E:2170:MET:HG3	2:E:2214:VAL:HG12	2.01	0.42
2:E:4250:GLN:O	2:E:4553:ASN:ND2	2.53	0.42
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.72	0.42
2:E:4181:ILE:HG13	2:E:4988:TYR:CE1	2.54	0.42
2:E:893:TYR:HD1	2:E:907:LEU:HB2	1.85	0.42
2:G:2170:MET:HG3	2:G:2214:VAL:HG12	2.01	0.42
2:G:649:PHE:HB3	2:G:776:LEU:HD13	2.00	0.42
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	2.02	0.42
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	2.02	0.42
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.72	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.42
2:B:893:TYR:HD1	2:B:907:LEU:HB2	1.85	0.42
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.85	0.42
2:E:145:ALA:HA	2:E:175:SER:HB3	2.01	0.42
2:E:180:LEU:O	2:E:200:TRP:NE1	2.43	0.42
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.42
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.85	0.42
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.42
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.42
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1739:THR:H	2:I:1742:THR:HB	1.85	0.42
2:I:145:ALA:HA	2:I:175:SER:HB3	2.01	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.50	0.42
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.84	0.42
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.42	0.42
2:I:652:ARG:HD2	2:I:750:LEU:HB3	2.02	0.42
2:I:758:ARG:HH22	2:I:805:PRO:HD3	1.84	0.42
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.72	0.42
2:B:4984:ASN:C	2:B:4986:ALA:H	2.22	0.42
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.42
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.93	0.42
2:E:2438:PRO:HG2	2:E:2454:ARG:HB2	2.01	0.42
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.02	0.42
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	1.99	0.42
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.53	0.42
2:G:1739:THR:H	2:G:1742:THR:HB	1.85	0.42
2:G:794:GLY:H	2:G:798:GLY:HA3	1.84	0.42
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.02	0.42
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.53	0.42
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.02	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.42
2:I:708:GLY:HA3	2:I:722:TRP:HB3	2.01	0.42
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.00	0.42
1:J:30:LEU:HB3	1:J:33:GLY:HA3	2.01	0.42
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.52	0.42
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.01	0.42
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.39	0.42
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	2.02	0.42
1:F:30:LEU:HB3	1:F:33:GLY:HA3	2.01	0.42
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	2.02	0.42
2:G:793:LEU:HD12	2:G:797:HIS:H	1.85	0.42
2:I:2432:LEU:O	2:I:2436:CYS:N	2.52	0.42
2:I:794:GLY:H	2:I:798:GLY:HA3	1.84	0.42
2:B:1101:ARG:HG2	2:B:1125:ASN:HA	2.01	0.42
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.02	0.42
2:B:3927:GLN:O	2:B:3931:SER:N	2.47	0.42
2:B:4181:ILE:HG23	2:B:4193:ILE:HB	2.00	0.42
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.41	0.42
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.53	0.42
2:E:621:ILE:O	2:E:625:LEU:N	2.49	0.42
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.00	0.42
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	2.02	0.42
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.42
2:G:621:ILE:O	2:G:625:LEU:N	2.49	0.42
2:I:2438:PRO:HG2	2:I:2454:ARG:HB2	2.01	0.42
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.85	0.42
1:A:30:LEU:HB3	1:A:33:GLY:HA3	2.01	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.02	0.42
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.02	0.42
2:B:2432:LEU:O	2:B:2436:CYS:N	2.52	0.42
2:B:652:ARG:HD2	2:B:750:LEU:HB3	2.02	0.42
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.46	0.42
2:E:2432:LEU:O	2:E:2436:CYS:N	2.52	0.42
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.02	0.42
2:E:793:LEU:HD12	2:E:797:HIS:H	1.85	0.42
2:E:758:ARG:HH22	2:E:805:PRO:HD3	1.85	0.42
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.00	0.42
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.02	0.42
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.35	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.02	0.42
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.42	0.42
2:G:3992:PHE:O	2:G:3996:PHE:N	2.43	0.42
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.01	0.42
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.02	0.42
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.42
2:B:145:ALA:HA	2:B:175:SER:HB3	2.01	0.42
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.53	0.42
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.02	0.42
2:G:451:TYR:O	2:G:474:ARG:NH1	2.43	0.42
2:G:914:PRO:O	2:G:918:ARG:N	2.52	0.42
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.38	0.42
2:I:4250:GLN:O	2:I:4553:ASN:ND2	2.53	0.42
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.73	0.42
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	2.02	0.42
2:B:758:ARG:HH22	2:B:805:PRO:HD3	1.84	0.42
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.93	0.42
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.02	0.42
2:G:2128:TYR:HB3	2:G:3669:PHE:HB3	2.02	0.42
2:G:4250:GLN:O	2:G:4553:ASN:ND2	2.53	0.42
2:G:893:TYR:HD1	2:G:907:LEU:HB2	1.85	0.42
2:I:614:VAL:HA	2:I:2169:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.03	0.41
2:B:4250:GLN:O	2:B:4553:ASN:ND2	2.53	0.41
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.85	0.41
2:G:758:ARG:HH22	2:G:805:PRO:HD3	1.84	0.41
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	2.02	0.41
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.85	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.02	0.41
2:B:2384:ILE:O	2:B:2388:GLU:N	2.53	0.41
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.85	0.41
2:G:652:ARG:HD2	2:G:750:LEU:HB3	2.02	0.41
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.86	0.41
2:I:2384:ILE:O	2:I:2388:GLU:N	2.53	0.41
2:I:621:ILE:O	2:I:625:LEU:N	2.49	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.41
2:B:3556:UNK:O	2:B:3560:UNK:N	2.54	0.41
2:E:1101:ARG:HG2	2:E:1125:ASN:HA	2.01	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.02	0.41
1:F:21:THR:HA	1:F:49:ARG:HA	2.03	0.41
2:G:157:ARG:HH21	2:G:164:ARG:HD2	1.86	0.41
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.02	0.41
2:G:2384:ILE:O	2:G:2388:GLU:N	2.53	0.41
2:G:4719:PHE:HD1	2:G:4722:ARG:HD3	1.85	0.41
2:G:4181:ILE:HG13	2:G:4988:TYR:CE1	2.54	0.41
2:G:708:GLY:HA3	2:G:722:TRP:HB3	2.01	0.41
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.03	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.38	0.41
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.00	0.41
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.02	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.03	0.41
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.35	0.41
2:B:708:GLY:HA3	2:B:722:TRP:HB3	2.01	0.41
2:B:793:LEU:HD12	2:B:797:HIS:H	1.85	0.41
2:E:2384:ILE:O	2:E:2388:GLU:N	2.53	0.41
2:G:145:ALA:HA	2:G:175:SER:HB3	2.01	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.02	0.41
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	2.02	0.41
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.35	0.41
2:I:3556:UNK:O	2:I:3560:UNK:N	2.54	0.41
2:I:3941:ASP:N	2:I:3941:ASP:OD1	2.50	0.41
2:B:2777:TYR:HD1	2:B:2791:LEU:HB2	1.86	0.41
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4886:HIS:O	2:B:4890:GLY:N	2.50	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.85	0.41
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.02	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.02	0.41
2:E:614:VAL:HA	2:E:2169:GLN:HB3	2.02	0.41
2:E:708:GLY:HA3	2:E:722:TRP:HB3	2.01	0.41
1:H:30:LEU:HB3	1:H:33:GLY:HA3	2.01	0.41
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.49	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.02	0.41
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.41
2:B:2438:PRO:HG2	2:B:2454:ARG:HB2	2.01	0.41
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.41
2:B:4156:HIS:CE1	2:B:5036:LEU:HD11	2.56	0.41
2:E:3556:UNK:O	2:E:3560:UNK:N	2.54	0.41
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	2.02	0.41
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.41
1:F:21:THR:N	1:F:107:GLU:OE1	2.43	0.41
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	2.02	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.41
2:G:614:VAL:HA	2:G:2169:GLN:HB3	2.02	0.41
2:I:1101:ARG:HG2	2:I:1125:ASN:HA	2.01	0.41
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.93	0.41
2:I:157:ARG:HH21	2:I:164:ARG:HD2	1.86	0.41
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.85	0.41
2:I:793:LEU:HD12	2:I:797:HIS:H	1.85	0.41
2:I:893:TYR:HD1	2:I:907:LEU:HB2	1.85	0.41
2:B:1931:LEU:HD13	2:B:1935:VAL:HG11	2.03	0.41
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.85	0.41
2:B:3761:GLN:NE2	2:B:4750:ILE:O	2.50	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.03	0.41
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	2.02	0.41
2:I:3761:GLN:NE2	2:I:4750:ILE:O	2.50	0.41
1:A:21:THR:N	1:A:107:GLU:OE1	2.43	0.41
2:B:2128:TYR:HB3	2:B:3669:PHE:HB3	2.02	0.41
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.03	0.41
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.54	0.41
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.41
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.36	0.41
2:E:652:ARG:HD2	2:E:750:LEU:HB3	2.02	0.41
2:G:938:HIS:N	2:G:1054:GLU:O	2.52	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4156:HIS:CE1	2:I:5036:LEU:HD11	2.56	0.41
1:J:21:THR:HA	1:J:49:ARG:HA	2.03	0.41
2:B:180:LEU:O	2:B:200:TRP:NE1	2.43	0.41
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.03	0.41
2:B:4056:GLU:HG2	2:B:4166:LEU:HD23	2.03	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.38	0.41
2:E:4719:PHE:HD1	2:E:4722:ARG:HD3	1.85	0.41
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.41	0.41
1:F:26:TYR:N	1:F:39:SER:OG	2.48	0.41
2:G:2777:TYR:HD1	2:G:2791:LEU:HB2	1.86	0.41
2:G:3556:UNK:O	2:G:3560:UNK:N	2.54	0.41
2:G:953:THR:HB	2:G:969:PRO:HD2	2.03	0.41
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.73	0.41
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.02	0.41
2:I:278:GLN:N	2:I:315:CYS:SG	2.91	0.41
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.02	0.41
1:A:21:THR:HA	1:A:49:ARG:HA	2.03	0.41
2:B:157:ARG:HH21	2:B:164:ARG:HD2	1.86	0.41
2:B:4558:ASN:N	2:B:4558:ASN:OD1	2.53	0.41
2:G:236:ALA:HA	2:G:242:ARG:HD2	2.03	0.41
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.85	0.41
2:I:2777:TYR:HD1	2:I:2791:LEU:HB2	1.86	0.41
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.54	0.41
2:B:4148:THR:HG21	2:B:4178:LEU:HD21	2.03	0.41
2:B:4719:PHE:HD1	2:B:4722:ARG:HD3	1.85	0.41
2:E:1931:LEU:HD13	2:E:1935:VAL:HG11	2.03	0.41
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.41
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.03	0.41
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.85	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.93	0.41
2:G:2432:LEU:O	2:G:2436:CYS:N	2.52	0.41
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	2.02	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.41
2:I:2128:TYR:HB3	2:I:3669:PHE:HB3	2.02	0.41
2:I:4719:PHE:HD1	2:I:4722:ARG:HD3	1.85	0.41
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.86	0.41
2:B:2674:UNK:O	2:B:2676:UNK:N	2.55	0.40
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.02	0.40
2:E:206:CYS:SG	2:E:207:SER:N	2.94	0.40
2:E:278:GLN:N	2:E:315:CYS:SG	2.91	0.40
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:953:THR:HB	2:E:969:PRO:HD2	2.03	0.40
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.96	0.40
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.85	0.40
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.02	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.94	0.40
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.03	0.40
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	2.02	0.40
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	2.02	0.40
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.49	0.40
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.03	0.40
2:B:953:THR:HB	2:B:969:PRO:HD2	2.03	0.40
2:E:1171:SER:OG	2:E:1175:SER:N	2.44	0.40
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.02	0.40
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.35	0.40
2:E:4148:THR:HG21	2:E:4178:LEU:HD21	2.03	0.40
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.40
2:G:404:ILE:HD13	2:G:481:GLU:HG3	2.03	0.40
2:G:4156:HIS:CE1	2:G:5036:LEU:HD11	2.56	0.40
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.85	0.40
2:I:1931:LEU:HD13	2:I:1935:VAL:HG11	2.03	0.40
2:I:1936:LYS:O	2:I:1940:CYS:N	2.48	0.40
2:I:232:THR:OG1	2:I:233:ILE:N	2.55	0.40
2:I:4886:HIS:O	2:I:4890:GLY:N	2.50	0.40
1:J:7:ILE:HD13	1:J:71:ARG:HG2	2.04	0.40
1:A:7:ILE:HD13	1:A:71:ARG:HG2	2.04	0.40
2:B:1078:GLU:HB2	2:B:1235:THR:HG22	2.04	0.40
2:B:463:GLU:O	2:B:466:SER:OG	2.30	0.40
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.85	0.40
2:E:3663:LEU:H	2:E:3663:LEU:HG	1.77	0.40
2:E:404:ILE:HD13	2:E:481:GLU:HG3	2.03	0.40
2:E:4056:GLU:HG2	2:E:4166:LEU:HD23	2.03	0.40
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.03	0.40
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.03	0.40
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.54	0.40
2:I:485:SER:O	2:I:489:ASN:N	2.44	0.40
2:I:914:PRO:O	2:I:918:ARG:N	2.52	0.40
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.86	0.40
2:B:206:CYS:SG	2:B:207:SER:N	2.94	0.40
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	2.02	0.40
2:E:2777:TYR:HD1	2:E:2791:LEU:HB2	1.86	0.40
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:914:PRO:O	2:E:918:ARG:N	2.52	0.40
2:G:206:CYS:SG	2:G:207:SER:N	2.94	0.40
2:G:2674:UNK:O	2:G:2676:UNK:N	2.55	0.40
2:G:463:GLU:O	2:G:466:SER:OG	2.30	0.40
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.86	0.40
2:I:236:ALA:HA	2:I:242:ARG:HD2	2.03	0.40
2:I:4148:THR:HG21	2:I:4178:LEU:HD21	2.03	0.40
2:B:4060:LYS:NZ	2:B:4107:GLU:OE2	2.41	0.40
2:B:4821:LYS:HB3	2:B:4821:LYS:HE2	1.94	0.40
2:E:157:ARG:HH21	2:E:164:ARG:HD2	1.86	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.37	0.40
2:E:236:ALA:HA	2:E:242:ARG:HD2	2.03	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.55	0.40
2:I:953:THR:HB	2:I:969:PRO:HD2	2.03	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%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	51	85
2	E	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	51	85
2	G	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	51	85
2	I	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	51	85
All	All	13360/18096 (74%)	11956 (90%)	1376 (10%)	28 (0%)	54	85

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	I	1708	ARG
2	I	1932	PRO
2	G	1708	ARG
2	G	1932	PRO
2	B	4641	PRO
2	B	4982	GLU
2	B	4985	LEU
2	E	4641	PRO
2	E	4982	GLU
2	E	4985	LEU
2	I	4641	PRO
2	I	4982	GLU
2	I	4985	LEU
2	G	4641	PRO
2	G	4982	GLU
2	G	4985	LEU
2	B	1840	PRO
2	B	2292	GLU
2	E	1840	PRO
2	E	2292	GLU
2	I	1840	PRO
2	I	2292	GLU
2	G	1840	PRO
2	G	2292	GLU

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	2476 (99%)	17 (1%)	87	93
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	87	93

All (68) 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	3762	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4959	PHE
2	B	4983	HIS
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	3762	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN

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Mol	Chain	Res	Type
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4959	PHE
2	E	4983	HIS
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	3762	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4959	PHE
2	I	4983	HIS
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	3762	ARG
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4959	PHE
2	G	4983	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	520	ASN
2	B	765	GLN
2	B	1158	ASN
2	B	1678	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1952	GLN
2	B	2005	GLN
2	B	2127	GLN
2	B	3767	GLN
2	B	3809	ASN
2	B	3896	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4553	ASN
2	B	4978	HIS
2	B	4987	ASN
2	E	57	ASN
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	520	ASN
2	E	765	GLN
2	E	1158	ASN
2	E	1678	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1952	GLN
2	E	2005	GLN
2	E	2127	GLN

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Mol	Chain	Res	Type
2	E	3767	GLN
2	E	3809	ASN
2	E	3896	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4553	ASN
2	E	4978	HIS
2	E	4987	ASN
2	I	57	ASN
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	479	GLN
2	I	520	ASN
2	I	765	GLN
2	I	1158	ASN
2	I	1678	ASN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1952	GLN
2	I	2005	GLN
2	I	2127	GLN
2	I	3767	GLN
2	I	3809	ASN
2	I	3896	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4553	ASN
2	I	4978	HIS
2	I	4987	ASN
2	G	57	ASN
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	520	ASN

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Mol	Chain	Res	Type
2	G	765	GLN
2	G	1158	ASN
2	G	1678	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1952	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	3767	GLN
2	G	3809	ASN
2	G	3896	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4553	ASN
2	G	4978	HIS
2	G	4987	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	74.04
1	E	4345:UNK	C	4540:PHE	N	74.04
1	I	4345:UNK	C	4540:PHE	N	74.04
1	G	4345:UNK	C	4540:PHE	N	74.04
1	B	3613:UNK	C	3639:THR	N	46.14
1	E	3613:UNK	C	3639:THR	N	46.14
1	I	3613:UNK	C	3639:THR	N	46.14
1	G	3613:UNK	C	3639:THR	N	46.14
1	B	4253:GLU	C	4320:UNK	N	27.75
1	E	4253:GLU	C	4320:UNK	N	27.75
1	I	4253:GLU	C	4320:UNK	N	27.75
1	G	4253:GLU	C	4320:UNK	N	27.75
1	B	3163:UNK	C	3170:UNK	N	15.37
1	E	3163:UNK	C	3170:UNK	N	15.37
1	I	3163:UNK	C	3170:UNK	N	15.37
1	G	3163:UNK	C	3170:UNK	N	15.37
1	B	3468:UNK	C	3511:UNK	N	14.99
1	E	3468:UNK	C	3511:UNK	N	14.99
1	I	3468:UNK	C	3511:UNK	N	14.99
1	G	3468:UNK	C	3511:UNK	N	14.99
1	B	3063:UNK	C	3134:UNK	N	14.98

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3063:UNK	C	3134:UNK	N	14.98
1	I	3063:UNK	C	3134:UNK	N	14.98
1	G	3063:UNK	C	3134:UNK	N	14.98
1	B	2703:UNK	C	2734:ASN	N	14.84
1	E	2703:UNK	C	2734:ASN	N	14.84
1	I	2703:UNK	C	2734:ASN	N	14.84
1	G	2703:UNK	C	2734:ASN	N	14.84
1	B	3236:UNK	C	3241:UNK	N	13.23
1	E	3236:UNK	C	3241:UNK	N	13.23
1	I	3236:UNK	C	3241:UNK	N	13.23
1	G	3236:UNK	C	3241:UNK	N	13.23
1	B	2976:UNK	C	2995:UNK	N	12.15
1	E	2976:UNK	C	2995:UNK	N	12.15
1	I	2976:UNK	C	2995:UNK	N	12.15
1	G	2976:UNK	C	2995:UNK	N	12.15
1	B	1564:UNK	C	1573:MET	N	11.93
1	E	1564:UNK	C	1573:MET	N	11.93
1	I	1564:UNK	C	1573:MET	N	11.93
1	G	1564:UNK	C	1573:MET	N	11.93
1	B	3254:UNK	C	3261:UNK	N	7.98
1	E	3254:UNK	C	3261:UNK	N	7.98
1	I	3254:UNK	C	3261:UNK	N	7.98
1	G	3254:UNK	C	3261:UNK	N	7.98
1	B	1297:UNK	C	1430:UNK	N	5.84
1	E	1297:UNK	C	1430:UNK	N	5.84
1	I	1297:UNK	C	1430:UNK	N	5.84
1	G	1297:UNK	C	1430:UNK	N	5.84
1	B	2479:LEU	C	2487:UNK	N	3.80
1	E	2479:LEU	C	2487:UNK	N	3.80
1	I	2479:LEU	C	2487:UNK	N	3.80
1	G	2479:LEU	C	2487:UNK	N	3.80
1	B	2939:ARG	C	2942:UNK	N	3.24
1	E	2939:ARG	C	2942:UNK	N	3.24
1	I	2939:ARG	C	2942:UNK	N	3.24
1	G	2939:ARG	C	2942:UNK	N	3.24