



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 01:12 pm GMT

PDB ID : 5TAS  
EMDB ID: : EMD-8383  
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA 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 : 6.20 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](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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

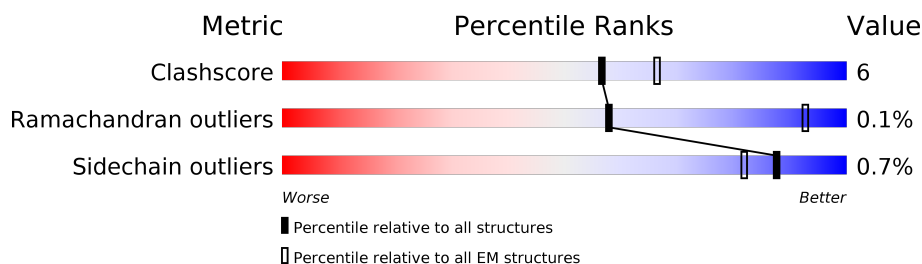
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.20 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  $\geq 3$ , 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	69% 31% .
1	F	108	70% 29% .
1	H	108	71% 28% .
1	J	108	72% 27% .
2	B	4416	82% 12% 5%
2	E	4416	82% 12% 5%
2	G	4416	82% 12% 5%
2	I	4416	83% 12% 5%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

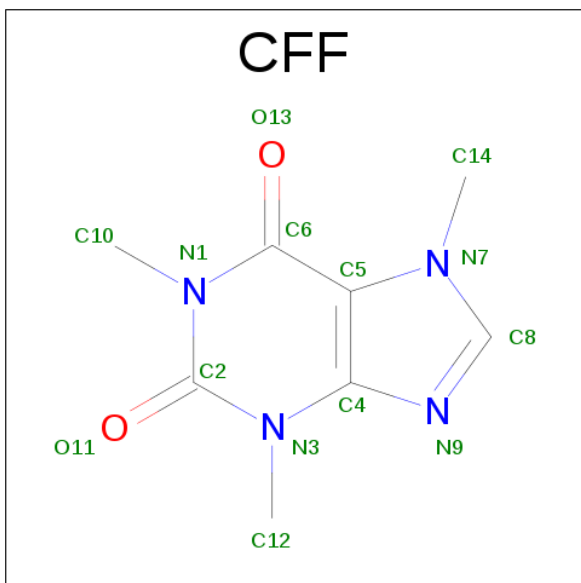
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula:  $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ ).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

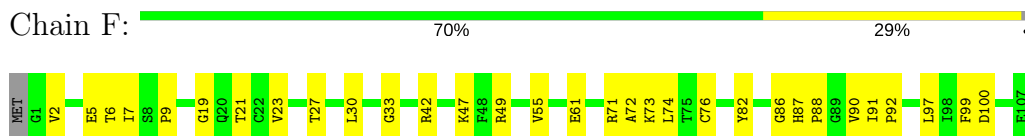
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

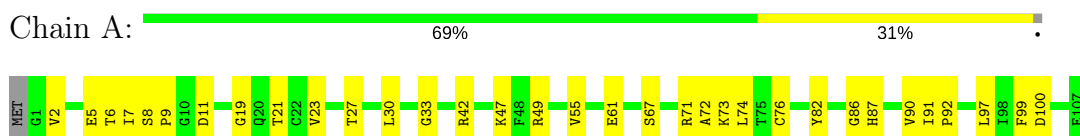
### 3 Residue-property plots

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

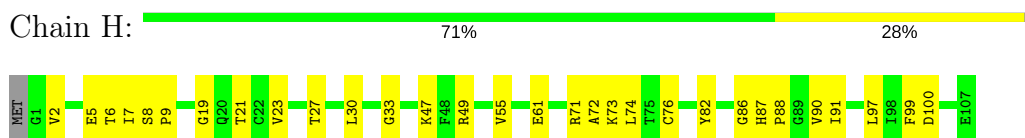
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



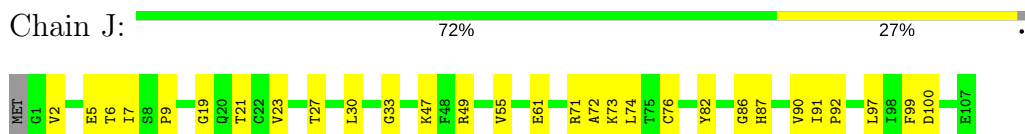
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



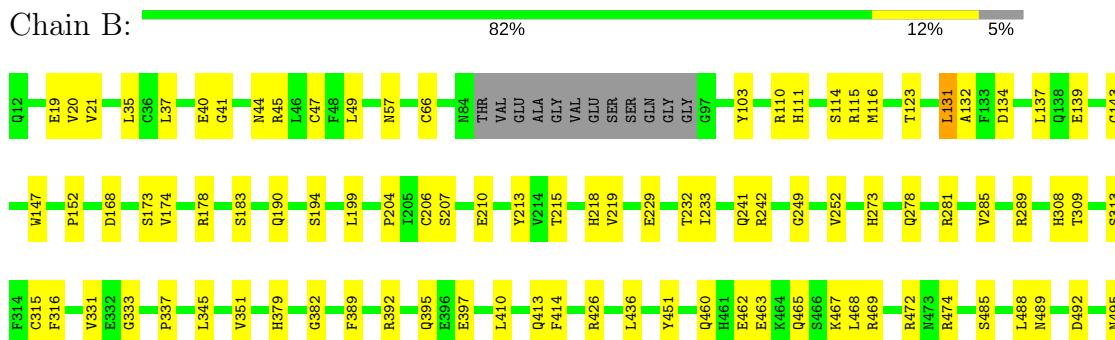
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



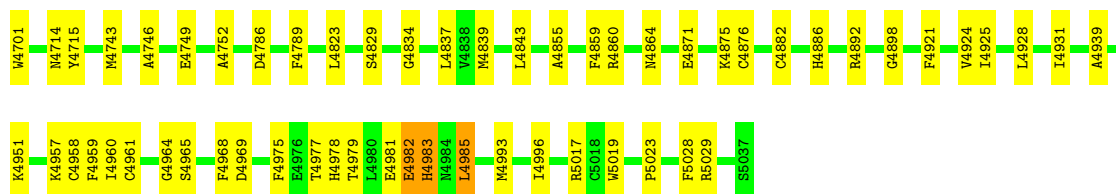
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

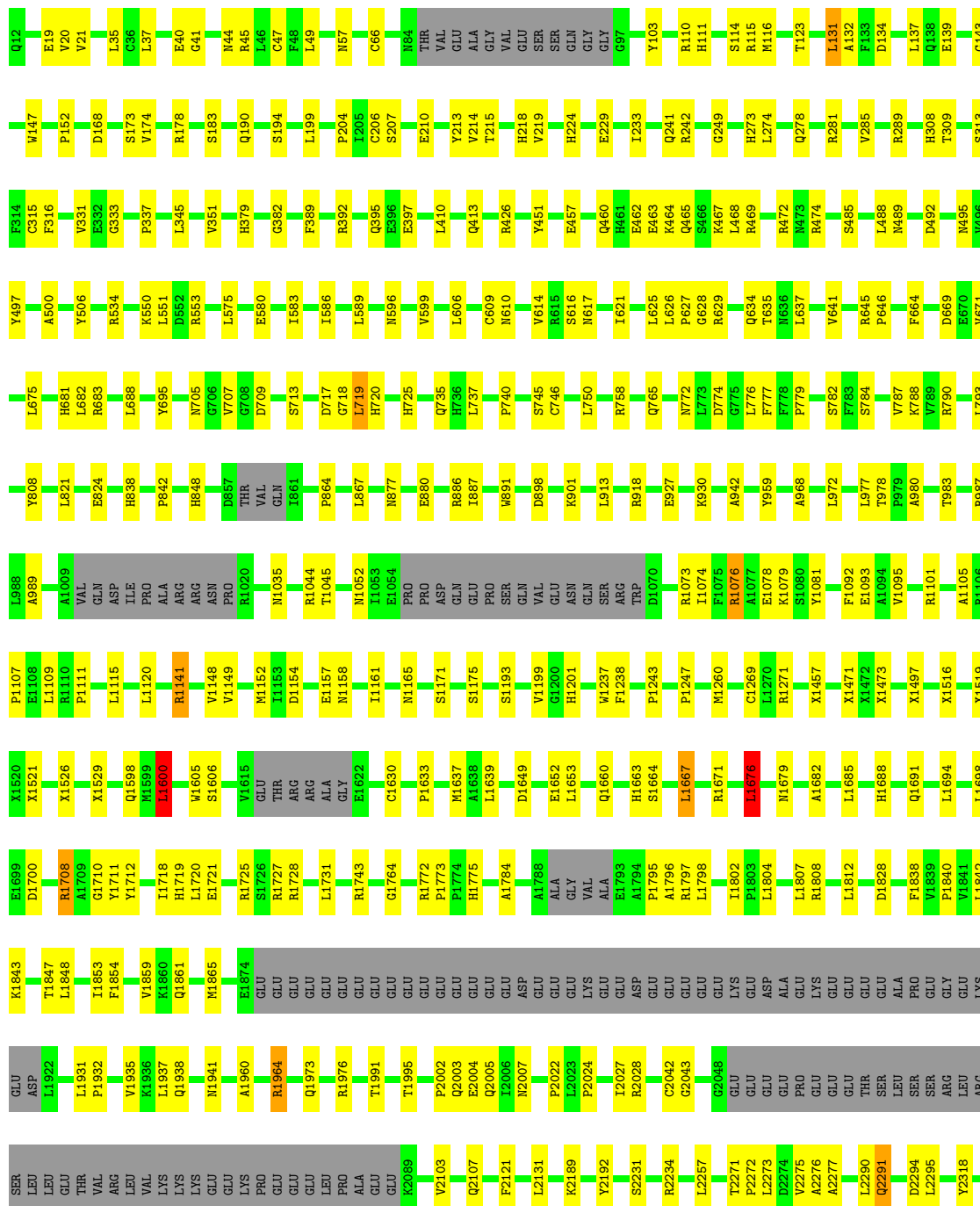




• Molecule 2: Ryanodine receptor 1


Chain I: 83% 12% 5%





C2326	G2327	K2770	W2775	P2793	E2803	R2806	W2807	K2810	K2814	L2823	E2830	GLU	ARG	ARG	THR	GLU	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	N2414	H2420	R2452	L2466	I2469	L2472	X2493	P2737	E2738	P2739	P2748	L2751	I2755	F2758	T2762	
L2930	Q3850	X3362	X3365	X3366	X3369	X3552	X3556	I3662	L3663	L3710	T3711	E3712	Y3725	T3905	Q3906	T3910	T3911	T3912	E3747	Q3767	L3770	H3771	T3772	L3780	Q3781	S3784	Q3946	G3947	K3948	R3949	N3950	M3955	Q3960	G3971	P3972	C3973	N3976	R3984	K4002	L4003	
S4008	L4013	L4019	L4031	N4034	E4056	K4060	M4064	L4068	R4085	T4104	G4105	P4106	N4120	E4126	N4130	R4131	E4152	P4155	R4180	T4181	E4182	I4190	Y4194	P4208	K4211	R4215	K4230	M4231	E4232	M4558	T4561	L4577									
Y4580	K4581	V4582	S4583	D4584	P4587	GLU	ASP	MET	GLU	GLU	SER	ALA	ALA	GLY	LEU	ALA	ALA	GLY	SER	GLY	GLY	GLY	TRP	GLY	SER	ALA	GLY	GLU	GLU	ASP	ASP	GLU	M4626	M4627	P4641	V4666	V4669	R4673	E4674	L4681	Y4687
V4697	K4698	G4699	W4700	W4701	N4714	Y4715	M4743	A4746	E4749	A4752	D4786	F4789	I4826	S4829	G4834	L4837	V4838	M4839	L4843	A4855	F4859	R4860	M4864	E4871	K4875	C4876	C4882	H4886	R4892	G4898	F4921	V4924	I4925	L4928							
I4931	A4939	K4957	C4958	F4959	I4960	C4961	G4964	S4965	F4968	D4969	F4975	E4976	T4977	L4978	T4979	E4980	E4981	E4982	H4983	L4984	L4985	M4993	I4996	R5017	C5018	W5019	P5023	F5028	L5036	S5037											

• Molecule 2: Ryanodine receptor 1

Chain E:  82% 12% 5%

R987	L988	A989	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ALA	ARG	ARG	ASN	PRO	R1020	N1035	R1044	T1045	M1052	E1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	R918	E927	K930	G940	P941	A942	Y959	A968	L972	L977	T978	P979	A980	T983
V671	L675	H681	L682	R683	L688	Y695	N705	G706	V707	G708	D709	S713	D717	G718	L719	H720	H725	Q735	H736	L737	P740	S745	C746	L750	R758	Q765	N772	L773	D774	G775	L776	F777	F778	P779	S782	F783	S784	V787	K788	R789	R790					
V496	Y497	A500	A504	E505	Y506	R534	K550	L551	B552	R553	L575	E580	I583	L589	N596	V599	L606	C609	N610	V614	R615	S616	N617	I621	L625	L626	P627	C628	Q634	T635	N636	L637	V641	R645	P646	F664	D669	E670								
F314	C315	F316	V331	E332	G333	P337	L345	V351	H379	G382	F389	R392	Q395	E396	E397	L410	Q413	F414	R426	L436	Y451	Q460	H461	E462	K464	Q465	S466	K467	L468	R469	R472	N473	R474	S485	R488	N489	F664	D492	N495							
W147	P152	D168	S173	V174	R178	S194	L199	P204	T205	C206	S207	E210	Y213	V214	T215	H218	V219	E229	T232	T233	Q241	R242	R243	G249	V252	H273	L274	Q278	R281	V285	R289	V301	H308	T309	S313											
Q12	E19	V20	V21	L35	C36	L37	E40	G41	M44	R45	L46	C47	F48	L49	N57	C66	N84	THR	VAL	GLU	GLY	ALA	GLY	VAL	GLU	SER	SER	GLN	GLY	GLY	C97	Y103	R110	H111	S114	R115	M116	T123	L131	A132	F133	D134	V137	Q138	E139	C142



Response	Percentage
Yes, I have used a mobile app to book a flight	82%
No, I have not used a mobile app to book a flight	12%
I am unsure	5%





V4924	E4232	V4666	E4232	Q3960
I4925	E4239	V4669	E4239	G3971
L4928	N4558	R4673	N4558	P3972
I4931	T4561	E4674	T4561	C3973
A4939	L4577	L4681	L4577	N3976
K4957	Y4580	Y4687	Y4580	K4002
C4958	K4581	V4697	K4581	L4003
F4959	K4582	K4698	K4582	S4008
I4960	S4583	G4699	S4583	L4013
C4961	D4584	Q4700	D4584	L4019
G4964	P4587	W4701	P4587	L4031
S4965	GLY	M4714	GLY	N4034
F4968	GLU	Y4715	GLU	E4056
D4969	ASP	M4743	ASP	K4060
F4975	NET	A4746	NET	M4064
E4976	GLU	A4746	GLU	L4068
T4977	GLY	E4749	GLY	R4085
H4978	SER	E4749	SER	T4104
T4979	ALA	A4752	ALA	G4105
L4980	ALA	A4752	ALA	P4106
E4981	GLY	K4821	GLY	M4120
F4982	ASP	T4822	ASP	E4126
H4983	LEU	L4823	LEU	N4130
A4984	ALA	L4823	ALA	R4131
L4985	ALA	S4829	ALA	E4152
M4993	GLY	G4834	GLY	R4180
I4996	SER	L4837	SER	E4182
Y5014	GLY	V4838	GLY	I4190
R5017	GLY	M4839	GLY	Y4194
C5018	TRP	A4855	TRP	P4208
W5019	GLY	F4859	GLY	K4211
P5023	SER	R4860	SER	R4215
F5028	ALA	N4864	ALA	K4230
S5037	GLU	E4871	GLU	E4233
	ALA	K4876	ALA	
	GLY	C4876	GLY	
	ASP	C4882	ASP	
	ASP	R4892	ASP	
	GLU	G4898	GLU	
	M4826	F4921	M4826	
	P4641		P4641	

## 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: CFF, ZN, ATP

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	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.29	0/25428	0.53	9/34534 (0.0%)
2	E	0.29	0/25428	0.53	9/34534 (0.0%)
2	G	0.29	0/25428	0.53	9/34534 (0.0%)
2	I	0.29	0/25428	0.53	9/34534 (0.0%)
All	All	0.29	0/105048	0.53	36/142628 (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	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.04	133.78	115.30
2	B	131	LEU	CA-CB-CG	8.02	133.75	115.30
2	I	131	LEU	CA-CB-CG	8.01	133.73	115.30
2	E	131	LEU	CA-CB-CG	8.00	133.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1600	LEU	CA-CB-CG	7.20	131.87	115.30
2	E	1600	LEU	CA-CB-CG	7.20	131.86	115.30
2	B	1600	LEU	CA-CB-CG	7.19	131.83	115.30
2	I	1600	LEU	CA-CB-CG	7.18	131.81	115.30
2	B	1676	LEU	CA-CB-CG	6.80	130.94	115.30
2	I	1676	LEU	CA-CB-CG	6.79	130.93	115.30
2	G	1676	LEU	CA-CB-CG	6.79	130.92	115.30
2	E	1676	LEU	CA-CB-CG	6.78	130.90	115.30
2	E	4985	LEU	CA-CB-CG	6.70	130.72	115.30
2	B	4985	LEU	CA-CB-CG	6.70	130.70	115.30
2	G	4985	LEU	CA-CB-CG	6.69	130.69	115.30
2	I	4985	LEU	CA-CB-CG	6.69	130.69	115.30
2	I	1667	LEU	CA-CB-CG	5.54	128.04	115.30
2	E	1667	LEU	CA-CB-CG	5.53	128.02	115.30
2	B	1667	LEU	CA-CB-CG	5.53	128.02	115.30
2	G	1667	LEU	CA-CB-CG	5.52	127.99	115.30
2	I	977	LEU	CA-CB-CG	5.52	127.99	115.30
2	B	977	LEU	CA-CB-CG	5.51	127.97	115.30
2	G	977	LEU	CA-CB-CG	5.50	127.95	115.30
2	E	977	LEU	CA-CB-CG	5.49	127.93	115.30
2	E	2290	LEU	CA-CB-CG	5.34	127.59	115.30
2	I	2290	LEU	CA-CB-CG	5.34	127.58	115.30
2	B	2290	LEU	CA-CB-CG	5.33	127.57	115.30
2	G	2290	LEU	CA-CB-CG	5.33	127.57	115.30
2	G	719	LEU	CA-CB-CG	5.32	127.54	115.30
2	E	719	LEU	CA-CB-CG	5.32	127.53	115.30
2	B	719	LEU	CA-CB-CG	5.30	127.50	115.30
2	I	719	LEU	CA-CB-CG	5.28	127.44	115.30
2	G	688	LEU	CA-CB-CG	5.10	127.04	115.30
2	B	688	LEU	CA-CB-CG	5.09	127.00	115.30
2	I	688	LEU	CA-CB-CG	5.09	127.00	115.30
2	E	688	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (44) 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	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	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	3971	GLY	Peptide
2	E	4666	VAL	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	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	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	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	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	21	0
1	F	818	0	824	20	0
1	H	818	0	824	18	0
1	J	818	0	824	18	0
2	B	29499	0	24746	316	0
2	E	29499	0	24746	322	0
2	G	29499	0	24746	319	0
2	I	29499	0	24746	317	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102368	1324	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 6.

All (1324) 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:4230:LYS:HD2	2:G:4959:PHE:CE2	1.25	1.69
2:E:4230:LYS:HD2	2:E:4959:PHE:CE2	1.25	1.64
2:I:4230:LYS:HD2	2:I:4959:PHE:CE2	1.25	1.60
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.25	1.58
2:B:4230:LYS:HD2	2:B:4959:PHE:CZ	1.55	1.42
2:E:4230:LYS:HD2	2:E:4959:PHE:CZ	1.55	1.42
2:E:4230:LYS:CD	2:E:4959:PHE:CZ	2.04	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4230:LYS:CD	2:B:4959:PHE:CZ	2.04	1.41
2:I:4230:LYS:HD2	2:I:4959:PHE:CZ	1.55	1.40
2:G:4230:LYS:HD2	2:G:4959:PHE:CZ	1.55	1.40
2:I:4230:LYS:CD	2:I:4959:PHE:CZ	2.04	1.40
2:G:4230:LYS:CD	2:G:4959:PHE:CZ	2.04	1.39
2:I:4230:LYS:CD	2:I:4959:PHE:CE2	2.15	1.29
2:B:4230:LYS:CD	2:B:4959:PHE:CE2	2.15	1.27
2:E:4230:LYS:CD	2:E:4959:PHE:CE2	2.15	1.25
2:G:4230:LYS:CD	2:G:4959:PHE:CE2	2.15	1.20
2:I:4230:LYS:HD3	2:I:4959:PHE:CZ	1.76	1.19
2:G:4230:LYS:HD3	2:G:4959:PHE:CZ	1.76	1.13
2:B:4230:LYS:HD3	2:B:4959:PHE:HZ	1.07	1.12
2:E:4230:LYS:HD3	2:E:4959:PHE:CZ	1.76	1.12
2:B:4230:LYS:HD3	2:B:4959:PHE:CZ	1.76	1.09
2:E:4230:LYS:HD3	2:E:4959:PHE:HZ	1.07	1.09
2:I:4230:LYS:HD3	2:I:4959:PHE:HZ	1.07	1.07
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.37	1.06
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.37	1.06
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.37	1.06
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.37	1.06
2:G:4230:LYS:HD3	2:G:4959:PHE:HZ	1.07	1.04
2:I:4230:LYS:HD2	2:I:4959:PHE:HE2	1.25	0.96
2:B:4230:LYS:HD2	2:B:4959:PHE:HE2	1.26	0.96
2:E:4230:LYS:HD2	2:E:4959:PHE:HE2	1.26	0.92
2:G:4230:LYS:HD2	2:G:4959:PHE:HE2	1.26	0.90
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.51	0.75
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.51	0.75
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.51	0.74
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.51	0.73
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.89	0.70
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.57	0.69
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.57	0.69
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.57	0.69
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.89	0.69
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.57	0.68
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.89	0.68
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.91	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.66
2:E:4957:LYS:CG	2:E:4964:GLY:HA2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.65
2:I:4957:LYS:CG	2:I:4964:GLY:HA2	2.22	0.64
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.79	0.64
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.79	0.64
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.64
2:B:4983:HIS:H	2:B:4983:HIS:CD2	2.16	0.64
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.64
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.79	0.63
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.64	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.16	0.63
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.81	0.63
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.79	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.80	0.63
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.16	0.63
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.81	0.62
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.64	0.62
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.81	0.62
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.81	0.62
2:B:4957:LYS:CG	2:B:4964:GLY:HA2	2.22	0.62
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.64	0.62
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.64	0.62
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.62
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.33	0.62
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.62
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.33	0.62
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.62
2:E:313:SER:HB3	2:E:351:VAL:HB	1.82	0.61
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.16	0.61
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.82	0.61
2:B:313:SER:HB3	2:B:351:VAL:HB	1.82	0.61
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.81	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.81	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.33	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.33	0.61
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.34	0.61
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.34	0.61
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.82	0.61
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.33	0.61
2:B:111:HIS:HD2	2:B:114:SER:H	1.49	0.61
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.34	0.61
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.33	0.61
2:G:313:SER:HB3	2:G:351:VAL:HB	1.82	0.61
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.34	0.61
2:E:111:HIS:HD2	2:E:114:SER:H	1.49	0.60
2:G:111:HIS:HD2	2:G:114:SER:H	1.49	0.60
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.82	0.60
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.83	0.60
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.60
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.34	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.84	0.60
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.83	0.60
2:I:313:SER:HB3	2:I:351:VAL:HB	1.83	0.60
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.33	0.60
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.34	0.60
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.84	0.60
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.83	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.83	0.60
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.84	0.60
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.84	0.60
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.82	0.60
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.60
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.83	0.60
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.85	0.59
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.84	0.59
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.82	0.59
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.84	0.59
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.84	0.59
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.83	0.59
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.84	0.59
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.84	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.84	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.84	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.84	0.59
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.84	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.33	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.36	0.58
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.36	0.58
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.33	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.58
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.37	0.58
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.58
1:H:6:THR:HA	1:H:72:ALA:HA	1.85	0.58
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.86	0.58
2:E:331:VAL:HG12	2:E:333:GLY:H	1.68	0.58
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.36	0.58
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.36	0.58
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.85	0.58
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.36	0.58
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.36	0.58
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.37	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.85	0.58
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.85	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.36	0.58
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.85	0.58
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.36	0.58
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.37	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.68	0.58
1:A:6:THR:HA	1:A:72:ALA:HA	1.85	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.85	0.57
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.69	0.57
2:G:4957:LYS:CG	2:G:4964:GLY:HA2	2.22	0.57
2:I:331:VAL:HG12	2:I:333:GLY:H	1.68	0.57
2:B:331:VAL:HG12	2:B:333:GLY:H	1.68	0.57
2:E:4898:GLY:O	2:G:4892:ARG:NH2	2.37	0.57
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.86	0.57
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.87	0.57
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.85	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
1:J:6:THR:HA	1:J:72:ALA:HA	1.85	0.57
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.87	0.57
1:F:6:THR:HA	1:F:72:ALA:HA	1.85	0.57
1:H:87:HIS:H	1:H:91:ILE:HB	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.57
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.69	0.57
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.86	0.57
1:F:87:HIS:H	1:F:91:ILE:HB	1.69	0.57
2:I:4829:SER:HB2	2:I:4939:ALA:HB1	1.86	0.57
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.37	0.57
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.70	0.57
2:B:4960:ILE:HG22	2:B:4960:ILE:O	2.05	0.57
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.57
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.85	0.57
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.70	0.57
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	1.87	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.57
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.87	0.57
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.57
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.70	0.57
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.85	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.86	0.57
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.70	0.57
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	1.87	0.57
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.70	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.57
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.86	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.70	0.57
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	1.87	0.57
2:E:4829:SER:HB2	2:E:4939:ALA:HB1	1.86	0.57
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.57
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.56
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.38	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.56
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.86	0.56
2:G:4829:SER:HB2	2:G:4939:ALA:HB1	1.86	0.56
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.86	0.56
2:E:4960:ILE:HG22	2:E:4960:ILE:O	2.05	0.56
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.86	0.56
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.88	0.56
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.69	0.56
2:I:4957:LYS:HG2	2:I:4964:GLY:CA	2.25	0.56
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.73	0.56
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.87	0.56
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.69	0.56
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.87	0.56
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.86	0.56
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.87	0.56
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.86	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.86	0.56
1:A:87:HIS:H	1:A:91:ILE:HB	1.69	0.56
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.85	0.56
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.38	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.56
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.38	0.56
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.70	0.56
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.34	0.56
2:I:4960:ILE:HG22	2:I:4960:ILE:O	2.05	0.56
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.39	0.56
2:B:4829:SER:HB2	2:B:4939:ALA:HB1	1.86	0.56
2:G:4957:LYS:HG2	2:G:4964:GLY:CA	2.25	0.56
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	1.87	0.56
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.56
2:E:4230:LYS:CD	2:E:4959:PHE:HE2	1.94	0.55
2:G:4230:LYS:CD	2:G:4959:PHE:HE2	1.94	0.55
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.70	0.55
1:J:87:HIS:H	1:J:91:ILE:HB	1.69	0.55
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.39	0.55
2:G:4960:ILE:O	2:G:4960:ILE:HG22	2.05	0.55
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.39	0.55
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.86	0.55
2:G:4230:LYS:CG	2:G:4959:PHE:CE2	2.88	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.38	0.55
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.34	0.55
2:B:4957:LYS:HG2	2:B:4964:GLY:CA	2.25	0.55
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.55
2:G:4230:LYS:CG	2:G:4959:PHE:HE2	2.19	0.55
2:G:41:GLY:O	2:G:45:ARG:NH1	2.40	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4230:LYS:CG	2:B:4959:PHE:HE2	2.19	0.55
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.40	0.55
2:I:4230:LYS:CG	2:I:4959:PHE:HE2	2.19	0.55
2:B:41:GLY:O	2:B:45:ARG:NH1	2.40	0.55
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.40	0.55
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.89	0.55
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.39	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.89	0.54
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.40	0.54
2:I:41:GLY:O	2:I:45:ARG:NH1	2.40	0.54
2:E:4190:ILE:HD13	2:E:5028:PHE:H	1.73	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.80	0.54
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.54
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.40	0.54
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.89	0.54
2:E:4230:LYS:CG	2:E:4959:PHE:HE2	2.19	0.54
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.40	0.54
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.89	0.54
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.90	0.54
2:E:41:GLY:O	2:E:45:ARG:NH1	2.40	0.54
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.89	0.54
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.54
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.89	0.54
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.89	0.54
2:B:1727:ARG:HH12	2:B:1772:ARG:HB3	1.73	0.54
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.90	0.54
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.40	0.54
2:B:4190:ILE:HD13	2:B:5028:PHE:H	1.73	0.54
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.40	0.54
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.90	0.54
2:B:609:CYS:SG	2:B:610:ASN:N	2.80	0.54
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.90	0.54
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.90	0.54
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.76	0.54
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.90	0.53
2:E:451:TYR:O	2:E:474:ARG:NH1	2.41	0.53
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.76	0.53
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.39	0.53
2:G:4190:ILE:HD13	2:G:5028:PHE:H	1.73	0.53
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.76	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.90	0.53
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.89	0.53
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.90	0.53
2:E:1727:ARG:HH12	2:E:1772:ARG:HB3	1.73	0.53
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.34	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.91	0.53
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.89	0.53
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.39	0.53
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.89	0.53
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.40	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.91	0.53
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.90	0.53
2:I:4190:ILE:HD13	2:I:5028:PHE:H	1.73	0.53
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.89	0.53
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.74	0.53
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.89	0.53
2:B:168:ASP:HB3	2:B:199:LEU:HD22	1.91	0.53
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.74	0.53
2:G:315:CYS:SG	2:G:316:PHE:N	2.82	0.53
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.90	0.53
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.90	0.53
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.90	0.53
2:B:315:CYS:SG	2:B:316:PHE:N	2.82	0.53
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.89	0.53
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.89	0.53
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.74	0.53
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.34	0.53
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.74	0.53
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.74	0.53
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.91	0.53
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.91	0.53
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.74	0.53
2:E:241:GLN:O	2:E:289:ARG:NH1	2.42	0.53
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.90	0.53
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.53
2:G:451:TYR:O	2:G:474:ARG:NH1	2.41	0.53
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.90	0.53
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.76	0.53
2:I:1727:ARG:HH12	2:I:1772:ARG:HB3	1.73	0.53
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.91	0.53
2:I:315:CYS:SG	2:I:316:PHE:N	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.91	0.53
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.90	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.53
2:I:451:TYR:O	2:I:474:ARG:NH1	2.41	0.53
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.91	0.52
2:E:315:CYS:SG	2:E:316:PHE:N	2.82	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.52
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.90	0.52
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.89	0.52
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.90	0.52
2:G:1727:ARG:HH12	2:G:1772:ARG:HB3	1.73	0.52
2:I:168:ASP:HB3	2:I:199:LEU:HD22	1.91	0.52
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.91	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.52
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.89	0.52
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.91	0.52
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.91	0.52
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.90	0.52
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.74	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.52
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.91	0.52
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.90	0.52
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.90	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.90	0.52
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.90	0.52
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.92	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.52
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.92	0.52
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.91	0.52
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.92	0.52
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.89	0.52
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.90	0.52
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.91	0.52
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.92	0.52
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.91	0.52
2:G:168:ASP:HB3	2:G:199:LEU:HD22	1.91	0.52
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.91	0.52
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.92	0.52
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.91	0.52
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.91	0.52
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.92	0.52
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.52
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.92	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.90	0.52
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.92	0.52
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.74	0.52
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.92	0.52
2:E:168:ASP:HB3	2:E:199:LEU:HD22	1.91	0.51
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.92	0.51
2:E:4230:LYS:CG	2:E:4959:PHE:CE2	2.88	0.51
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.93	0.51
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.43	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.44	0.51
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.91	0.51
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.92	0.51
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.93	0.51
2:I:132:ALA:HA	2:I:194:SER:HB2	1.93	0.51
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.91	0.51
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.93	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.93	0.51
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.91	0.51
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.51
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.44	0.51
2:B:451:TYR:O	2:B:474:ARG:NH1	2.41	0.51
2:B:4230:LYS:CG	2:B:4959:PHE:CE2	2.88	0.51
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.91	0.51
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.92	0.51
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.92	0.51
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.91	0.51
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.76	0.51
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.51
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.44	0.51
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.93	0.51
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.44	0.51
2:I:4230:LYS:CG	2:I:4959:PHE:CE2	2.88	0.51
2:I:4958:CYS:SG	2:I:4961:CYS:N	2.84	0.51
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.91	0.51
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.91	0.51
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.44	0.51
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.84	0.51
2:G:682:LEU:HD13	2:G:787:VAL:HG11	1.92	0.51
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.92	0.51
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.51
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.84	0.51
2:B:4958:CYS:SG	2:B:4961:CYS:N	2.84	0.51
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.76	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.51
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.44	0.51
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.84	0.51
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.91	0.51
2:B:4182:GLU:OE1	2:B:4983:HIS:NE2	2.44	0.51
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.92	0.51
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.92	0.51
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.93	0.51
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.51
2:I:682:LEU:HD13	2:I:787:VAL:HG11	1.92	0.51
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.92	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.93	0.51
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.84	0.51
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.76	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.51
2:I:241:GLN:O	2:I:289:ARG:NH1	2.42	0.51
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.92	0.51
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.51
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.44	0.50
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.92	0.50
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.93	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.50
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.93	0.50
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.93	0.50
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.76	0.50
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.44	0.50
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.50
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.93	0.50
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.50
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.93	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.50
2:I:2347:GLU:O	2:I:2351:ASN:N	2.40	0.50
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.94	0.50
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.50
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.93	0.50
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.94	0.50
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.94	0.50
2:I:485:SER:O	2:I:489:ASN:N	2.40	0.50
2:B:132:ALA:HA	2:B:194:SER:HB2	1.93	0.50
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.93	0.50
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.94	0.50
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.29	0.50
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.29	0.50
2:G:485:SER:O	2:G:489:ASN:N	2.40	0.50
2:G:4958:CYS:SG	2:G:4961:CYS:N	2.84	0.50
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.93	0.50
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.94	0.50
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.93	0.50
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.94	0.50
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.92	0.50
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.29	0.50
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.76	0.50
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.94	0.50
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.94	0.50
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.94	0.50
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.93	0.50
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.93	0.50
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.50
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.94	0.50
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.41	0.50
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.76	0.50
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.93	0.50
2:E:1269:CYS:HA	2:E:1473:UNK:HA	1.93	0.50
2:E:218:HIS:HB3	2:E:392:ARG:HD3	1.94	0.50
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.94	0.50
2:G:173:SER:HB3	2:G:178:ARG:H	1.77	0.50
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.93	0.50
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.94	0.50
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.41	0.50
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.94	0.50
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.94	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.45	0.50
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.29	0.50
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.93	0.50
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.93	0.50
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.50
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.93	0.50
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.93	0.50
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.45	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.94	0.49
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.94	0.49
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.45	0.49
2:E:4958:CYS:SG	2:E:4961:CYS:N	2.84	0.49
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.76	0.49
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.94	0.49
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.39	0.49
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.93	0.49
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.49
2:G:241:GLN:O	2:G:289:ARG:NH1	2.42	0.49
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.46	0.49
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.94	0.49
2:I:3922:TYR:O	2:I:3926:LEU:N	2.44	0.49
2:B:173:SER:HB3	2:B:178:ARG:H	1.77	0.49
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.95	0.49
2:B:218:HIS:HB3	2:B:392:ARG:HD3	1.94	0.49
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.94	0.49
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.39	0.49
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.78	0.49
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.94	0.49
2:G:1660:GLN:O	2:G:1664:SER:N	2.45	0.49
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.49
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.45	0.49
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.94	0.49
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.94	0.49
1:A:27:THR:HB	1:A:100:ASP:HB3	1.93	0.49
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.94	0.49
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.94	0.49
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.42	0.49
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.94	0.49
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.95	0.49
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.49
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1269:CYS:HA	2:G:1473:UNK:HA	1.93	0.49
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.49
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.94	0.49
2:B:241:GLN:O	2:B:289:ARG:NH1	2.42	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.49
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.49
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.49
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.49
2:G:4975:PHE:O	2:G:4979:THR:HG23	2.12	0.49
2:I:1148:VAL:HB	2:I:1165:ASN:HA	1.94	0.49
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.93	0.49
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.49
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.46	0.49
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.49
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.94	0.49
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.49
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.46	0.49
2:E:3840:SER:O	2:E:3922:TYR:OH	2.31	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.44	0.49
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.49
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.94	0.49
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.94	0.49
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.95	0.49
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.44	0.49
2:B:4928:LEU:HD23	2:B:4931:ILE:HD12	1.95	0.49
2:I:4892:ARG:NH2	2:G:4898:GLY:O	2.46	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.46	0.49
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.39	0.49
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.95	0.49
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.94	0.49
2:I:880:GLU:OE1	2:I:968:ALA:N	2.44	0.49
2:I:978:THR:HB	2:I:980:ALA:H	1.78	0.49
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.93	0.49
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.46	0.49
2:E:1991:THR:O	2:E:1995:THR:OG1	2.31	0.49
2:E:2347:GLU:O	2:E:2351:ASN:N	2.40	0.49
2:E:485:SER:O	2:E:489:ASN:N	2.40	0.49
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.49
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.95	0.49
2:G:1991:THR:O	2:G:1995:THR:OG1	2.31	0.49
2:G:4056:GLU:O	2:G:4060:LYS:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.95	0.49
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.46	0.49
2:I:4928:LEU:HD23	2:I:4931:ILE:HD12	1.95	0.49
2:B:978:THR:HB	2:B:980:ALA:H	1.78	0.49
2:E:3922:TYR:O	2:E:3926:LEU:N	2.44	0.49
2:E:4182:GLU:OE1	2:E:4983:HIS:NE2	2.44	0.49
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.42	0.49
2:E:4928:LEU:HD23	2:E:4931:ILE:HD12	1.95	0.49
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.94	0.49
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.95	0.49
2:G:4928:LEU:HD23	2:G:4931:ILE:HD12	1.95	0.49
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.94	0.49
2:I:709:ASP:HA	2:I:725:HIS:H	1.78	0.49
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.94	0.49
2:B:4975:PHE:O	2:B:4979:THR:HG23	2.12	0.48
2:E:1660:GLN:O	2:E:1664:SER:N	2.45	0.48
2:G:1148:VAL:HB	2:G:1165:ASN:HA	1.95	0.48
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.46	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.78	0.48
2:I:173:SER:HB3	2:I:178:ARG:H	1.77	0.48
2:I:4056:GLU:O	2:I:4060:LYS:N	2.43	0.48
2:B:1148:VAL:HB	2:B:1165:ASN:HA	1.94	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.48
2:B:709:ASP:HA	2:B:725:HIS:H	1.78	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.44	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.47	0.48
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.94	0.48
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.48
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.94	0.48
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.45	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.94	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.95	0.48
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.78	0.48
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.95	0.48
2:I:3840:SER:O	2:I:3922:TYR:OH	2.31	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.46	0.48
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.46	0.48
2:B:645:ARG:N	2:B:824:GLU:O	2.45	0.48
2:E:1148:VAL:HB	2:E:1165:ASN:HA	1.95	0.48
2:E:4056:GLU:O	2:E:4060:LYS:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3840:SER:O	2:G:3922:TYR:OH	2.31	0.48
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.94	0.48
2:E:173:SER:HB3	2:E:178:ARG:H	1.77	0.48
2:E:278:GLN:N	2:E:315:CYS:SG	2.87	0.48
2:E:4921:PHE:HA	2:E:4925:ILE:HD13	1.95	0.48
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.95	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:G:4182:GLU:OE1	2:G:4983:HIS:NE2	2.44	0.48
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.48
2:I:4975:PHE:O	2:I:4979:THR:HG23	2.12	0.48
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.46	0.48
2:G:3767:GLN:HA	2:G:3770:LEU:HB2	1.95	0.48
2:G:218:HIS:HB3	2:G:392:ARG:HD3	1.94	0.48
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.95	0.48
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.78	0.48
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.95	0.48
2:G:2347:GLU:O	2:G:2351:ASN:N	2.40	0.48
2:G:626:LEU:HG	2:G:628:GLY:H	1.79	0.48
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.93	0.48
2:I:626:LEU:HG	2:I:628:GLY:H	1.79	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.48
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.95	0.48
2:E:4975:PHE:O	2:E:4979:THR:HG23	2.12	0.48
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.48
2:G:4215:ARG:NH2	3:G:5101:ATP:O1A	2.47	0.48
2:I:4182:GLU:OE1	2:I:4983:HIS:NE2	2.44	0.48
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.41	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.47	0.48
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.46	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.94	0.48
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.46	0.48
2:G:709:ASP:HA	2:G:725:HIS:H	1.79	0.48
2:I:218:HIS:HB3	2:I:392:ARG:HD3	1.94	0.48
2:I:4230:LYS:CD	2:I:4959:PHE:HE2	1.94	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
2:B:1991:THR:O	2:B:1995:THR:OG1	2.31	0.48
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.95	0.48
2:G:645:ARG:N	2:G:824:GLU:O	2.45	0.48
2:B:1660:GLN:O	2:B:1664:SER:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3767:GLN:HA	2:B:3770:LEU:HB2	1.95	0.48
2:E:709:ASP:HA	2:E:725:HIS:H	1.79	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.46	0.48
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.78	0.48
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.32	0.48
2:G:278:GLN:N	2:G:315:CYS:SG	2.87	0.48
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.95	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.31	0.48
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.32	0.47
2:B:278:GLN:N	2:B:315:CYS:SG	2.87	0.47
2:B:4921:PHE:HA	2:B:4925:ILE:HD13	1.95	0.47
2:E:1171:SER:OG	2:E:1175:SER:N	2.45	0.47
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.79	0.47
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.46	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.47
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.95	0.47
2:I:4921:PHE:HA	2:I:4925:ILE:HD13	1.95	0.47
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.96	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.47
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.48	0.47
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.97	0.47
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.47
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.96	0.47
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.94	0.47
2:B:3840:SER:O	2:B:3922:TYR:OH	2.31	0.47
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.46	0.47
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.96	0.47
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.94	0.47
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.32	0.47
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.97	0.47
2:B:4056:GLU:O	2:B:4060:LYS:N	2.43	0.47
2:I:2880:GLU:O	2:I:2884:ASN:N	2.47	0.47
1:A:82:TYR:O	1:A:86:GLY:N	2.48	0.47
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.97	0.47
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	1.96	0.47
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.47	0.47
1:H:82:TYR:O	1:H:86:GLY:N	2.48	0.47
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.97	0.47
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.32	0.47
2:E:309:THR:O	2:E:313:SER:OG	2.33	0.47
2:E:4957:LYS:HG2	2:E:4964:GLY:CA	2.25	0.47
2:E:978:THR:HB	2:E:980:ALA:H	1.78	0.47
2:G:1663:HIS:O	2:G:1667:LEU:N	2.47	0.47
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.48	0.47
2:E:3767:GLN:HA	2:E:3770:LEU:HB2	1.96	0.47
2:I:3767:GLN:HA	2:I:3770:LEU:HB2	1.95	0.47
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.96	0.47
2:B:4215:ARG:NH2	3:B:5101:ATP:O1A	2.47	0.47
2:E:626:LEU:HG	2:E:628:GLY:H	1.79	0.47
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.48	0.47
2:I:645:ARG:N	2:I:824:GLU:O	2.45	0.47
2:B:2880:GLU:O	2:B:2884:ASN:N	2.47	0.47
2:B:626:LEU:HG	2:B:628:GLY:H	1.79	0.47
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.47	0.47
2:G:309:THR:O	2:G:313:SER:OG	2.33	0.47
2:G:4921:PHE:HA	2:G:4925:ILE:HD13	1.95	0.47
2:G:880:GLU:OE1	2:G:968:ALA:N	2.44	0.47
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.96	0.47
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.96	0.47
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.96	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.50	0.47
2:G:842:PRO:HD3	2:G:1073:ARG:HG3	1.97	0.47
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	1.96	0.47
2:I:1663:HIS:O	2:I:1667:LEU:N	2.47	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.44	0.47
1:J:82:TYR:O	1:J:86:GLY:N	2.48	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.41	0.46
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.97	0.46
1:F:82:TYR:O	1:F:86:GLY:N	2.48	0.46
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	1.96	0.46
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.96	0.46
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.97	0.46
2:B:309:THR:O	2:B:313:SER:OG	2.33	0.46
2:E:645:ARG:N	2:E:824:GLU:O	2.45	0.46
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.97	0.46
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.46
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.96	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:880:GLU:OE1	2:E:968:ALA:N	2.44	0.46
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.96	0.46
2:G:913:LEU:O	2:G:918:ARG:NH2	2.49	0.46
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.49	0.46
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.80	0.46
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.96	0.46
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.96	0.46
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.80	0.46
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.96	0.46
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.49	0.46
2:E:842:PRO:HD3	2:E:1073:ARG:HG3	1.97	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.50	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.41	0.46
2:E:4215:ARG:NH2	3:E:5101:ATP:O1A	2.47	0.46
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.81	0.46
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.98	0.46
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.97	0.46
2:B:1101:ARG:HE	2:B:1115:LEU:HB3	1.81	0.46
2:B:488:LEU:O	2:B:492:ASP:N	2.47	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.96	0.46
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.98	0.46
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.97	0.46
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.46
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.46
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.81	0.46
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.96	0.46
2:G:2880:GLU:O	2:G:2884:ASN:N	2.47	0.46
2:I:278:GLN:N	2:I:315:CYS:SG	2.87	0.46
2:B:913:LEU:O	2:B:918:ARG:NH2	2.49	0.46
2:E:913:LEU:O	2:E:918:ARG:NH2	2.49	0.46
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.50	0.46
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.46
2:E:488:LEU:O	2:E:492:ASP:N	2.47	0.45
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.97	0.45
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.50	0.45
2:E:1663:HIS:O	2:E:1667:LEU:N	2.47	0.45
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.98	0.45
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.81	0.45
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.45
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.49	0.45
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.45
2:B:842:PRO:HD3	2:B:1073:ARG:HG3	1.97	0.45
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.81	0.45
2:B:3922:TYR:O	2:B:3926:LEU:N	2.44	0.45
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.97	0.45
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.99	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.45
2:I:842:PRO:HD3	2:I:1073:ARG:HG3	1.97	0.45
2:I:309:THR:O	2:I:313:SER:OG	2.33	0.45
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.50	0.45
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.45
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.45
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.98	0.45
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.81	0.45
2:I:913:LEU:O	2:I:918:ARG:NH2	2.49	0.45
2:B:2347:GLU:O	2:B:2351:ASN:N	2.40	0.45
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.82	0.45
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.81	0.45
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.99	0.45
2:E:621:ILE:O	2:E:625:LEU:N	2.47	0.45
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.81	0.45
2:G:1101:ARG:HE	2:G:1115:LEU:HB3	1.81	0.45
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.45
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.49	0.45
2:G:488:LEU:O	2:G:492:ASP:N	2.47	0.45
2:G:776:LEU:HG	2:G:848:HIS:HA	1.98	0.45
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.45
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.49	0.45
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.99	0.45
2:G:4558:ASN:HB2	2:G:4561:THR:HB	1.99	0.45
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.98	0.45
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.98	0.45
1:H:21:THR:HA	1:H:49:ARG:HA	1.99	0.45
2:I:776:LEU:HG	2:I:848:HIS:HA	1.98	0.45
1:A:19:GLY:HA2	1:A:49:ARG:HH21	1.81	0.45
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.82	0.45
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.98	0.45
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.99	0.45
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.99	0.45
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.81	0.45
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1660:GLN:O	2:I:1664:SER:N	2.45	0.45
2:I:793:LEU:HD22	2:I:821:LEU:HD13	1.99	0.45
1:A:21:THR:HA	1:A:49:ARG:HA	1.99	0.45
2:G:621:ILE:O	2:G:625:LEU:N	2.47	0.45
2:I:1154:ASP:O	2:I:1158:ASN:N	2.50	0.45
2:I:1843:LYS:HB2	2:I:1938:GLN:HE22	1.82	0.45
2:E:1101:ARG:HE	2:E:1115:LEU:HB3	1.81	0.45
2:E:1843:LYS:HB2	2:E:1938:GLN:HE22	1.82	0.45
2:E:2880:GLU:O	2:E:2884:ASN:N	2.47	0.45
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.81	0.45
2:G:1154:ASP:O	2:G:1158:ASN:N	2.50	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.99	0.45
1:H:19:GLY:HA2	1:H:49:ARG:HH21	1.81	0.45
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.82	0.45
2:I:4558:ASN:HB2	2:I:4561:THR:HB	1.99	0.45
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.50	0.44
2:B:776:LEU:HG	2:B:848:HIS:HA	1.98	0.44
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.44
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.98	0.44
2:E:776:LEU:HG	2:E:848:HIS:HA	1.98	0.44
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.46	0.44
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.81	0.44
2:G:4855:ALA:HA	2:G:4859:PHE:HB2	1.99	0.44
2:I:1101:ARG:HE	2:I:1115:LEU:HB3	1.81	0.44
2:I:614:VAL:HG22	2:I:616:SER:H	1.82	0.44
1:A:11:ASP:OD1	1:A:67:SER:OG	2.27	0.44
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.98	0.44
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.44
2:E:468:LEU:HB3	2:E:472:ARG:HH12	1.82	0.44
2:G:1171:SER:OG	2:G:1175:SER:N	2.45	0.44
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.44
2:G:3922:TYR:O	2:G:3926:LEU:N	2.44	0.44
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.99	0.44
2:G:614:VAL:HG22	2:G:616:SER:H	1.82	0.44
1:H:30:LEU:HD23	1:H:33:GLY:HA3	1.99	0.44
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.81	0.44
1:J:21:THR:HA	1:J:49:ARG:HA	1.99	0.44
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.99	0.44
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.83	0.44
2:E:4924:VAL:HG23	2:E:4925:ILE:HD12	2.00	0.44
2:E:614:VAL:HG22	2:E:616:SER:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.50	0.44
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.99	0.44
2:G:395:GLN:HG3	2:G:397:GLU:H	1.82	0.44
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.99	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:B:1171:SER:OG	2:B:1175:SER:N	2.45	0.44
2:B:4697:VAL:O	2:B:4701:TRP:N	2.51	0.44
2:B:614:VAL:HG22	2:B:616:SER:H	1.82	0.44
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.99	0.44
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.98	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.51	0.44
2:E:460:GLN:HG2	2:E:462:GLU:H	1.83	0.44
2:E:793:LEU:HD22	2:E:821:LEU:HD13	1.99	0.44
2:G:1843:LYS:HB2	2:G:1938:GLN:HE22	1.82	0.44
2:G:2758:PHE:O	2:G:2762:THR:N	2.44	0.44
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.82	0.44
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.98	0.44
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.81	0.44
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.99	0.44
2:B:1973:GLN:O	2:B:1977:TYR:N	2.45	0.44
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.00	0.44
2:B:793:LEU:HD22	2:B:821:LEU:HD13	1.99	0.44
2:B:880:GLU:OE1	2:B:968:ALA:N	2.44	0.44
2:E:2810:LYS:O	2:E:2814:LYS:N	2.45	0.44
2:E:3362:UNK:O	2:E:3366:UNK:N	2.51	0.44
2:G:3362:UNK:O	2:G:3366:UNK:N	2.51	0.44
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.51	0.44
2:G:460:GLN:HG2	2:G:462:GLU:H	1.83	0.44
2:G:4924:VAL:HG23	2:G:4925:ILE:HD12	2.00	0.44
2:I:3362:UNK:O	2:I:3366:UNK:N	2.51	0.44
2:I:460:GLN:HG2	2:I:462:GLU:H	1.83	0.44
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.98	0.44
1:J:19:GLY:HA2	1:J:49:ARG:HH21	1.81	0.44
2:B:1154:ASP:O	2:B:1158:ASN:N	2.50	0.44
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.83	0.44
2:E:1457:UNK:N	2:E:1497:UNK:O	2.51	0.44
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.82	0.44
2:E:395:GLN:HG3	2:E:397:GLU:H	1.82	0.44
2:E:4843:LEU:HD12	2:G:4823:LEU:HD23	1.99	0.44
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.82	0.44
1:F:30:LEU:HD23	1:F:33:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.99	0.44
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.44
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.83	0.44
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.82	0.44
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.83	0.44
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.99	0.44
2:B:460:GLN:HG2	2:B:462:GLU:H	1.83	0.44
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.99	0.44
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.00	0.44
1:F:19:GLY:HA2	1:F:49:ARG:HH21	1.81	0.44
2:G:468:LEU:HB3	2:G:472:ARG:HH12	1.82	0.44
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.42	0.44
2:I:621:ILE:O	2:I:625:LEU:N	2.47	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.91	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.44
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.46	0.44
2:B:3842:LEU:O	2:B:3929:SER:OG	2.36	0.44
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.44
1:F:21:THR:HA	1:F:49:ARG:HA	1.99	0.44
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.83	0.44
2:G:793:LEU:HD22	2:G:821:LEU:HD13	1.99	0.44
2:I:1457:UNK:N	2:I:1497:UNK:O	2.51	0.44
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.00	0.44
2:I:4924:VAL:HG23	2:I:4925:ILE:HD12	2.00	0.44
2:B:1843:LYS:HB2	2:B:1938:GLN:HE22	1.82	0.44
2:B:395:GLN:HG3	2:B:397:GLU:H	1.82	0.44
2:B:468:LEU:HB3	2:B:472:ARG:HH12	1.82	0.44
2:E:206:CYS:SG	2:E:207:SER:N	2.91	0.44
2:I:395:GLN:HG3	2:I:397:GLU:H	1.82	0.44
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.44
2:B:116:MET:HB2	2:B:137:LEU:HD12	2.00	0.43
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.81	0.43
2:E:3905:THR:HA	2:E:3912:THR:HG23	2.00	0.43
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.81	0.43
2:G:3905:THR:HA	2:G:3912:THR:HG23	2.00	0.43
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.99	0.43
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.51	0.43
2:I:4855:ALA:HA	2:I:4859:PHE:HB2	1.99	0.43
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.99	0.43
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.83	0.43
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2868:SER:O	2:B:2872:GLN:N	2.45	0.43
2:B:4924:VAL:HG23	2:B:4925:ILE:HD12	2.00	0.43
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.41	0.43
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.52	0.43
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.99	0.43
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.84	0.43
2:G:3842:LEU:O	2:G:3929:SER:OG	2.36	0.43
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	2.00	0.43
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.01	0.43
2:I:468:LEU:HB3	2:I:472:ARG:HH12	1.82	0.43
2:I:4215:ARG:NH2	3:I:5101:ATP:O1A	2.47	0.43
1:A:30:LEU:HD23	1:A:33:GLY:HA3	1.99	0.43
2:B:210:GLU:HG3	2:B:337:PRO:HG3	2.00	0.43
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.51	0.43
2:E:116:MET:HB2	2:E:137:LEU:HD12	2.00	0.43
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.99	0.43
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.00	0.43
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.00	0.43
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.99	0.43
2:B:3362:UNK:O	2:B:3366:UNK:N	2.51	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.83	0.43
2:B:4855:ALA:HA	2:B:4859:PHE:HB2	1.99	0.43
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.84	0.43
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.00	0.43
2:E:3842:LEU:O	2:E:3929:SER:OG	2.36	0.43
2:G:1973:GLN:O	2:G:1977:TYR:N	2.45	0.43
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	2.00	0.43
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.83	0.43
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.51	0.43
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.00	0.43
1:J:30:LEU:HD23	1:J:33:GLY:HA3	1.99	0.43
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.00	0.43
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	2.00	0.43
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.00	0.43
2:B:4558:ASN:HB2	2:B:4561:THR:HB	1.99	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:G:1937:LEU:O	2:G:1941:ASN:ND2	2.52	0.43
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.82	0.43
2:G:4834:GLY:HA2	2:G:4837:LEU:HD12	2.00	0.43
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.52	0.43
2:I:1865:MET:SD	2:I:1865:MET:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:210:GLU:HG3	2:I:337:PRO:HG3	2.00	0.43
2:I:3842:LEU:O	2:I:3929:SER:OG	2.36	0.43
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.83	0.43
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.99	0.43
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.00	0.43
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.84	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.83	0.43
2:E:4697:VAL:O	2:E:4701:TRP:N	2.51	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.91	0.43
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.00	0.43
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.84	0.43
2:I:183:SER:N	2:I:190:GLN:O	2.51	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	2.00	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.99	0.43
2:B:1937:LEU:O	2:B:1941:ASN:ND2	2.52	0.43
2:B:4977:THR:HG22	2:B:4981:GLU:HB2	2.01	0.43
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.52	0.43
2:E:4558:ASN:HB2	2:E:4561:THR:HB	1.99	0.43
1:F:7:ILE:N	1:F:71:ARG:O	2.46	0.43
2:I:2103:VAL:O	2:I:2107:GLN:N	2.47	0.43
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.84	0.43
2:B:1457:UNK:N	2:B:1497:UNK:O	2.51	0.43
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.52	0.43
2:E:1154:ASP:O	2:E:1158:ASN:N	2.50	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.83	0.43
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	2.00	0.43
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.01	0.43
2:E:4834:GLY:HA2	2:E:4837:LEU:HD12	2.00	0.43
2:E:4882:CYS:HG	2:E:4886:HIS:CD2	2.37	0.43
2:E:4977:THR:HG22	2:E:4981:GLU:HB2	2.01	0.43
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.83	0.43
2:G:1238:PHE:O	2:G:1606:SER:N	2.50	0.43
2:G:1457:UNK:N	2:G:1497:UNK:O	2.51	0.43
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.00	0.43
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.51	0.43
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.34	0.43
2:G:4875:LYS:HB3	2:G:4882:CYS:HA	2.01	0.43
2:B:1865:MET:SD	2:B:1865:MET:N	2.92	0.43
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:SER:O	2:B:489:ASN:N	2.40	0.43
2:E:1154:ASP:HB3	2:E:1157:GLU:HB3	2.01	0.43
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.00	0.43
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.01	0.43
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.00	0.43
2:G:1865:MET:N	2:G:1865:MET:SD	2.92	0.43
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.43
2:I:1937:LEU:O	2:I:1941:ASN:ND2	2.52	0.43
2:I:4977:THR:HG22	2:I:4981:GLU:HB2	2.01	0.43
2:B:1154:ASP:HB3	2:B:1157:GLU:HB3	2.01	0.43
2:B:1663:HIS:O	2:B:1667:LEU:N	2.47	0.43
2:B:21:VAL:HG12	2:B:66:CYS:HA	2.01	0.43
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.84	0.43
2:E:3365:UNK:O	2:E:3369:UNK:N	2.52	0.43
2:E:3902:TYR:O	2:E:3906:GLN:NE2	2.52	0.43
2:G:101:LEU:HB3	2:G:150:MET:HE1	2.01	0.43
2:G:3880:PHE:O	2:G:3884:LEU:N	2.52	0.43
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.91	0.43
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.46	0.43
2:I:4834:GLY:HA2	2:I:4837:LEU:HD12	2.00	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.52	0.42
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.84	0.42
2:E:1238:PHE:O	2:E:1606:SER:N	2.50	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.42
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.46	0.42
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	2.00	0.42
2:G:4064:MET:O	2:G:4068:LEU:N	2.52	0.42
2:I:116:MET:HB2	2:I:137:LEU:HD12	2.00	0.42
2:I:2868:SER:O	2:I:2872:GLN:N	2.45	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.52	0.42
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.84	0.42
2:B:1659:LEU:O	2:B:1663:HIS:N	2.49	0.42
2:B:183:SER:N	2:B:190:GLN:O	2.51	0.42
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.84	0.42
2:B:3880:PHE:O	2:B:3884:LEU:N	2.52	0.42
2:B:3902:TYR:O	2:B:3906:GLN:NE2	2.52	0.42
2:B:3905:THR:HA	2:B:3912:THR:HG23	2.00	0.42
2:E:1937:LEU:O	2:E:1941:ASN:ND2	2.52	0.42
2:E:210:GLU:HG3	2:E:337:PRO:HG3	2.00	0.42
2:E:21:VAL:HG12	2:E:66:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.54	0.42
2:E:4875:LYS:HB3	2:E:4882:CYS:HA	2.01	0.42
2:E:606:LEU:O	2:E:617:ASN:ND2	2.52	0.42
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.02	0.42
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.83	0.42
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.41	0.42
2:G:4977:THR:HG22	2:G:4981:GLU:HB2	2.01	0.42
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.52	0.42
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	2.00	0.42
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.42
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.53	0.42
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.01	0.42
2:B:4834:GLY:HA2	2:B:4837:LEU:HD12	2.00	0.42
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.53	0.42
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.84	0.42
2:G:21:VAL:HG12	2:G:66:CYS:HA	2.01	0.42
2:G:3902:TYR:O	2:G:3906:GLN:NE2	2.52	0.42
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.84	0.42
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.89	0.42
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.52	0.42
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.54	0.42
2:I:3880:PHE:O	2:I:3884:LEU:N	2.52	0.42
2:I:3905:THR:HA	2:I:3912:THR:HG23	2.00	0.42
2:I:606:LEU:O	2:I:617:ASN:ND2	2.52	0.42
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	2.00	0.42
2:B:606:LEU:O	2:B:617:ASN:ND2	2.52	0.42
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.38	0.42
1:F:7:ILE:HG22	1:F:9:PRO:HD2	2.01	0.42
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.02	0.42
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.36	0.42
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.01	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.52	0.42
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.85	0.42
2:I:21:VAL:HG12	2:I:66:CYS:HA	2.01	0.42
2:I:4697:VAL:O	2:I:4701:TRP:N	2.51	0.42
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.52	0.42
2:B:233:ILE:HD12	2:B:242:ARG:HB3	2.01	0.42
2:E:1973:GLN:O	2:E:1977:TYR:N	2.45	0.42
2:E:2132:GLY:O	2:E:2136:ARG:N	2.53	0.42
2:G:116:MET:HB2	2:G:137:LEU:HD12	2.00	0.42
2:G:183:SER:N	2:G:190:GLN:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:210:GLU:HG3	2:G:337:PRO:HG3	2.00	0.42
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.52	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.54	0.42
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.84	0.42
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.53	0.42
2:B:37:LEU:HD11	2:B:47:CYS:HB3	2.01	0.42
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.85	0.42
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.00	0.42
2:E:1865:MET:SD	2:E:1865:MET:N	2.92	0.42
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.85	0.42
2:E:4855:ALA:HA	2:E:4859:PHE:HB2	1.99	0.42
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.52	0.42
2:G:3552:UNK:O	2:G:3556:UNK:N	2.52	0.42
1:H:55:VAL:HA	2:G:1784:ALA:HA	2.02	0.42
2:I:3902:TYR:O	2:I:3906:GLN:NE2	2.52	0.42
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.84	0.42
2:I:488:LEU:O	2:I:492:ASP:N	2.48	0.42
1:A:7:ILE:HG22	1:A:9:PRO:HD2	2.01	0.42
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.84	0.42
2:E:3880:PHE:O	2:E:3884:LEU:N	2.52	0.42
2:E:4064:MET:O	2:E:4068:LEU:N	2.52	0.42
2:G:37:LEU:HD11	2:G:47:CYS:HB3	2.01	0.42
2:I:1154:ASP:HB3	2:I:1157:GLU:HB3	2.01	0.42
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.02	0.42
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.02	0.42
2:I:4064:MET:O	2:I:4068:LEU:N	2.52	0.42
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.46	0.42
2:E:37:LEU:HD11	2:E:47:CYS:HB3	2.01	0.42
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.34	0.42
2:G:1154:ASP:HB3	2:G:1157:GLU:HB3	2.01	0.42
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.85	0.42
2:G:215:THR:H	2:G:218:HIS:CE1	2.38	0.42
2:G:224:HIS:N	2:G:229:GLU:O	2.44	0.42
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.02	0.42
2:G:606:LEU:O	2:G:617:ASN:ND2	2.52	0.42
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.83	0.42
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.54	0.42
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.51	0.42
2:E:1105:ALA:N	2:E:1189:LEU:O	2.53	0.42
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.52	0.42
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.51	0.42
2:G:1074:ILE:HA	2:G:1193:SER:HA	2.02	0.42
2:G:233:ILE:HD12	2:G:242:ARG:HB3	2.01	0.42
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	2.01	0.42
1:H:7:ILE:HG22	1:H:9:PRO:HD2	2.01	0.42
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.38	0.42
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	2.02	0.42
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.02	0.42
2:E:4965:SER:O	2:E:4969:ASP:N	2.53	0.42
2:E:4993:MET:HA	2:E:4996:ILE:HD12	2.02	0.42
2:E:940:GLY:O	2:E:1052:ASN:N	2.52	0.42
2:G:2103:VAL:O	2:G:2107:GLN:N	2.47	0.42
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.52	0.42
2:I:37:LEU:HD11	2:I:47:CYS:HB3	2.01	0.42
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.85	0.42
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.02	0.41
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.52	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.41
2:B:927:GLU:HA	2:B:930:LYS:HB2	2.02	0.41
2:E:1074:ILE:HA	2:E:1193:SER:HA	2.02	0.41
2:E:2143:THR:H	2:E:3651:ASN:HD21	1.68	0.41
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.41
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.35	0.41
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.53	0.41
2:I:224:HIS:N	2:I:229:GLU:O	2.44	0.41
2:E:1659:LEU:O	2:E:1663:HIS:N	2.49	0.41
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.42	0.41
2:I:4965:SER:O	2:I:4969:ASP:N	2.53	0.41
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.02	0.41
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.02	0.41
2:B:4993:MET:HA	2:B:4996:ILE:HD12	2.02	0.41
2:E:3552:UNK:O	2:E:3556:UNK:N	2.52	0.41
2:G:1105:ALA:N	2:G:1189:LEU:O	2.53	0.41
2:G:983:THR:O	2:G:987:ARG:N	2.51	0.41
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.52	0.41
2:B:1074:ILE:HA	2:B:1193:SER:HA	2.02	0.41
2:B:4965:SER:O	2:B:4969:ASP:N	2.53	0.41
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.35	0.41
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.85	0.41
2:E:215:THR:H	2:E:218:HIS:CE1	2.38	0.41
2:E:233:ILE:HD12	2:E:242:ARG:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:927:GLU:HA	2:E:930:LYS:HB2	2.02	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.51	0.41
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.35	0.41
2:I:215:THR:H	2:I:218:HIS:CE1	2.38	0.41
2:I:233:ILE:HD12	2:I:242:ARG:HB3	2.01	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.52	0.41
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.86	0.41
2:I:983:THR:O	2:I:987:ARG:N	2.51	0.41
1:A:7:ILE:N	1:A:71:ARG:O	2.46	0.41
2:B:4951:LYS:HB3	2:B:4951:LYS:HE2	1.94	0.41
1:A:8:SER:H	2:B:736:HIS:HB3	1.85	0.41
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.86	0.41
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	2.02	0.41
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.86	0.41
2:G:485:SER:HA	2:G:488:LEU:HB2	2.03	0.41
2:G:4983:HIS:CE1	2:G:5023:PRO:HG2	2.56	0.41
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.02	0.41
2:B:4064:MET:O	2:B:4068:LEU:N	2.52	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.52	0.41
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.03	0.41
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.02	0.41
2:E:414:PHE:HE1	2:E:436:LEU:HB3	1.86	0.41
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	2.02	0.41
2:E:4983:HIS:CE1	2:E:5023:PRO:HG2	2.56	0.41
2:G:4993:MET:HA	2:G:4996:ILE:HD12	2.01	0.41
2:I:4826:ILE:O	2:I:4829:SER:OG	2.35	0.41
2:I:4993:MET:HA	2:I:4996:ILE:HD12	2.02	0.41
2:B:1238:PHE:O	2:B:1606:SER:N	2.50	0.41
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.56	0.41
2:E:485:SER:HA	2:E:488:LEU:HB2	2.03	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.54	0.41
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	2.02	0.41
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.41
2:G:4965:SER:O	2:G:4969:ASP:N	2.53	0.41
1:H:8:SER:H	2:G:736:HIS:HB3	1.84	0.41
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.85	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.56	0.41
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.03	0.41
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.01	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	2.02	0.41
2:B:621:ILE:O	2:B:625:LEU:N	2.47	0.41
2:I:134:ASP:OD1	2:I:134:ASP:N	2.54	0.41
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.41	0.41
2:I:4983:HIS:CE1	2:I:5023:PRO:HG2	2.56	0.41
1:J:7:ILE:HG22	1:J:9:PRO:HD2	2.01	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:215:THR:H	2:B:218:HIS:CE1	2.38	0.41
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.03	0.41
2:B:4875:LYS:HB3	2:B:4882:CYS:HA	2.01	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:4951:LYS:HB3	2:E:4951:LYS:HE2	1.94	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:G:2143:THR:H	2:G:3651:ASN:HD21	1.68	0.41
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.02	0.41
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.02	0.41
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.36	0.41
2:I:457:GLU:OE1	2:I:464:LYS:NZ	2.50	0.41
2:I:485:SER:HA	2:I:488:LEU:HB2	2.03	0.41
1:J:7:ILE:N	1:J:71:ARG:O	2.46	0.41
2:B:2132:GLY:O	2:B:2136:ARG:N	2.53	0.41
2:B:232:THR:HB	2:B:252:VAL:HG11	2.03	0.41
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.03	0.41
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.41
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.02	0.41
2:E:243:ARG:NH1	2:E:301:VAL:O	2.42	0.41
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.03	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	2.02	0.41
2:I:2810:LYS:O	2:I:2814:LYS:N	2.45	0.41
2:I:4875:LYS:HB3	2:I:4882:CYS:HA	2.01	0.41
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.36	0.41
2:B:1270:LEU:N	2:B:1472:UNK:O	2.54	0.41
2:B:4882:CYS:HG	2:B:4886:HIS:CD2	2.39	0.41
2:B:4983:HIS:CE1	2:B:5023:PRO:HG2	2.56	0.41
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	2.02	0.41
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.89	0.41
2:G:1965:TYR:OH	2:G:2027:ILE:O	2.33	0.41
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.56	0.41
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.03	0.41
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.46	0.40
2:E:1270:LEU:N	2:E:1472:UNK:O	2.54	0.40
2:E:232:THR:HB	2:E:252:VAL:HG11	2.03	0.40
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.03	0.40
2:E:983:THR:O	2:E:987:ARG:N	2.51	0.40
2:G:1092:PHE:N	2:G:1149:VAL:O	2.39	0.40
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.38	0.40
2:G:1659:LEU:O	2:G:1663:HIS:N	2.49	0.40
2:G:4821:LYS:HE2	2:G:4821:LYS:HB3	1.97	0.40
2:I:1238:PHE:O	2:I:1606:SER:N	2.50	0.40
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.02	0.40
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.40
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	2.02	0.40
2:B:495:ASN:HD21	2:B:550:LYS:HE3	1.87	0.40
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.87	0.40
2:E:134:ASP:OD1	2:E:134:ASP:N	2.54	0.40
2:E:4787:ASN:O	2:E:4791:TYR:N	2.49	0.40
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.86	0.40
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.85	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.97	0.40
2:E:4968:PHE:HE1	2:E:5029:ARG:HD3	1.86	0.40
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.02	0.40
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.56	0.40
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.86	0.40
2:G:495:ASN:HD21	2:G:550:LYS:HE3	1.87	0.40
2:G:927:GLU:HA	2:G:930:LYS:HB2	2.02	0.40
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.87	0.40
2:I:4882:CYS:HG	2:I:4886:HIS:CD2	2.39	0.40
2:I:927:GLU:HA	2:I:930:LYS:HB2	2.02	0.40
2:B:1130:GLN:HG2	2:B:1138:PRO:HA	2.04	0.40
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.86	0.40
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.56	0.40
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.03	0.40
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.03	0.40
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.03	0.40
2:G:243:ARG:NH1	2:G:301:VAL:O	2.42	0.40
2:I:1074:ILE:HA	2:I:1193:SER:HA	2.02	0.40
2:B:1090:PHE:HD2	2:B:1202:LEU:HD11	1.87	0.40
2:B:2143:THR:H	2:B:3651:ASN:HD21	1.68	0.40
2:B:4968:PHE:HE1	2:B:5029:ARG:HD3	1.86	0.40
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:495:ASN:HD21	2:E:550:LYS:HE3	1.87	0.40
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.52	0.40
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.27	0.40
2:I:1804:LEU:O	2:I:1808:ARG:N	2.53	0.40
2:I:495:ASN:HD21	2:I:550:LYS:HE3	1.87	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%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	302 (9%)	4 (0%)	55	88
2	E	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	55	88
2	G	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	55	88
2	I	3235/4416 (73%)	2928 (90%)	303 (9%)	4 (0%)	55	88
All	All	13360/18096 (74%)	12101 (91%)	1243 (9%)	16 (0%)	58	88

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	1840	PRO

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Mol	Chain	Res	Type
2	B	1932	PRO
2	I	1840	PRO
2	I	1932	PRO
2	E	1840	PRO
2	E	1932	PRO
2	G	1840	PRO
2	G	1932	PRO
2	B	4641	PRO
2	I	4641	PRO
2	E	4641	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%)	2475 (99%)	18 (1%)	87	93
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	87	93
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	87	93
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	87	93
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	87	93

All (72) 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

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Mol	Chain	Res	Type
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4839	MET
2	B	4982	GLU
2	B	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	3663	LEU
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4839	MET
2	I	4982	GLU
2	I	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	3663	LEU
2	E	3787	LYS

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Mol	Chain	Res	Type
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4839	MET
2	E	4982	GLU
2	E	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	3663	LEU
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4839	MET
2	G	4982	GLU
2	G	4983	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	71	GLN
2	B	111	HIS
2	B	113	HIS

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Mol	Chain	Res	Type
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	413	GLN
2	B	765	GLN
2	B	949	ASN
2	B	1598	GLN
2	B	1660	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1702	HIS
2	B	1719	HIS
2	B	1775	HIS
2	B	1941	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	3647	HIS
2	B	3809	ASN
2	B	3830	GLN
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	3994	HIS
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4833	ASN
2	B	5003	HIS
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	413	GLN

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Mol	Chain	Res	Type
2	I	765	GLN
2	I	949	ASN
2	I	1598	GLN
2	I	1660	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1941	ASN
2	I	2005	GLN
2	I	2127	GLN
2	I	3647	HIS
2	I	3809	ASN
2	I	3830	GLN
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	3994	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4833	ASN
2	I	5003	HIS
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	413	GLN
2	E	765	GLN
2	E	949	ASN
2	E	1220	GLN
2	E	1598	GLN
2	E	1660	GLN

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Mol	Chain	Res	Type
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1941	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	3647	HIS
2	E	3809	ASN
2	E	3830	GLN
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	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4833	ASN
2	E	5003	HIS
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	413	GLN
2	G	765	GLN
2	G	949	ASN
2	G	1598	GLN
2	G	1660	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS

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Mol	Chain	Res	Type
2	G	1941	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	3647	HIS
2	G	3809	ASN
2	G	3830	GLN
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	3994	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4833	ASN
2	G	5003	HIS

### 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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	B	5101	-	27,33,33	0.92	1 (3%)	25,52,52	1.65	2 (8%)
4	CFF	B	5102	-	7,15,15	1.83	2 (28%)	8,23,23	1.30	1 (12%)
3	ATP	E	5101	-	27,33,33	0.92	1 (3%)	25,52,52	1.64	2 (8%)
4	CFF	E	5102	-	7,15,15	1.82	2 (28%)	8,23,23	1.30	1 (12%)
3	ATP	G	5101	-	27,33,33	0.93	1 (3%)	25,52,52	1.65	2 (8%)
4	CFF	G	5102	-	7,15,15	1.83	2 (28%)	8,23,23	1.30	1 (12%)
3	ATP	I	5101	-	27,33,33	0.93	1 (3%)	25,52,52	1.66	2 (8%)
4	CFF	I	5102	-	7,15,15	1.82	2 (28%)	8,23,23	1.30	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	CFF	C6-N1	-3.79	1.32	1.38
4	E	5102	CFF	C6-N1	-3.79	1.32	1.38
4	G	5102	CFF	C6-N1	-3.78	1.32	1.38
4	I	5102	CFF	C6-N1	-3.75	1.32	1.38
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24
4	B	5102	CFF	O13-C6	-2.29	1.18	1.24
4	I	5102	CFF	O13-C6	-2.26	1.18	1.24
4	E	5102	CFF	O13-C6	-2.26	1.18	1.24
3	B	5101	ATP	C5-C4	3.02	1.47	1.40
3	E	5101	ATP	C5-C4	3.02	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-C4	3.02	1.47	1.40
3	G	5101	ATP	C5-C4	3.04	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	N3-C2-N1	-6.11	123.54	128.86
3	G	5101	ATP	N3-C2-N1	-6.06	123.58	128.86
3	B	5101	ATP	N3-C2-N1	-6.06	123.58	128.86
3	E	5101	ATP	N3-C2-N1	-6.02	123.61	128.86
3	I	5101	ATP	C4-C5-N7	-2.98	106.53	109.41
3	B	5101	ATP	C4-C5-N7	-2.98	106.53	109.41
3	G	5101	ATP	C4-C5-N7	-2.96	106.55	109.41
3	E	5101	ATP	C4-C5-N7	-2.92	106.58	109.41
4	B	5102	CFF	C14-N7-C8	-2.86	111.86	125.45
4	G	5102	CFF	C14-N7-C8	-2.86	111.87	125.45
4	I	5102	CFF	C14-N7-C8	-2.86	111.87	125.45
4	E	5102	CFF	C14-N7-C8	-2.85	111.89	125.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
4	B	5102	CFF	1	0
3	E	5101	ATP	2	0
4	E	5102	CFF	1	0
3	G	5101	ATP	2	0
4	G	5102	CFF	1	0
3	I	5101	ATP	2	0
4	I	5102	CFF	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.19
1	I	4345:UNK	C	4540:PHE	N	73.19
1	E	4345:UNK	C	4540:PHE	N	73.19
1	G	4345:UNK	C	4540:PHE	N	73.19
1	B	3613:UNK	C	3639:THR	N	44.63
1	I	3613:UNK	C	3639:THR	N	44.63
1	E	3613:UNK	C	3639:THR	N	44.63
1	G	3613:UNK	C	3639:THR	N	44.63
1	B	4253:GLU	C	4320:UNK	N	27.52
1	I	4253:GLU	C	4320:UNK	N	27.52
1	G	4253:GLU	C	4320:UNK	N	27.52
1	E	4253:GLU	C	4320:UNK	N	27.51
1	B	3163:UNK	C	3170:UNK	N	16.25
1	I	3163:UNK	C	3170:UNK	N	16.25
1	E	3163:UNK	C	3170:UNK	N	16.25
1	G	3163:UNK	C	3170:UNK	N	16.25
1	B	3063:UNK	C	3134:UNK	N	14.93
1	I	3063:UNK	C	3134:UNK	N	14.93
1	E	3063:UNK	C	3134:UNK	N	14.93
1	G	3063:UNK	C	3134:UNK	N	14.93
1	B	3468:UNK	C	3511:UNK	N	14.63
1	I	3468:UNK	C	3511:UNK	N	14.63
1	E	3468:UNK	C	3511:UNK	N	14.63
1	G	3468:UNK	C	3511:UNK	N	14.63
1	B	2703:UNK	C	2734:ASN	N	14.10
1	I	2703:UNK	C	2734:ASN	N	14.10
1	E	2703:UNK	C	2734:ASN	N	14.10
1	G	2703:UNK	C	2734:ASN	N	14.10
1	B	3236:UNK	C	3241:UNK	N	13.44
1	I	3236:UNK	C	3241:UNK	N	13.44
1	E	3236:UNK	C	3241:UNK	N	13.44
1	G	3236:UNK	C	3241:UNK	N	13.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2976:UNK	C	2995:UNK	N	12.48
1	I	2976:UNK	C	2995:UNK	N	12.48
1	E	2976:UNK	C	2995:UNK	N	12.48
1	G	2976:UNK	C	2995:UNK	N	12.48
1	B	1564:UNK	C	1573:MET	N	12.21
1	I	1564:UNK	C	1573:MET	N	12.21
1	E	1564:UNK	C	1573:MET	N	12.21
1	G	1564:UNK	C	1573:MET	N	12.21
1	B	3254:UNK	C	3261:UNK	N	8.37
1	I	3254:UNK	C	3261:UNK	N	8.37
1	E	3254:UNK	C	3261:UNK	N	8.37
1	G	3254:UNK	C	3261:UNK	N	8.37
1	B	1297:UNK	C	1430:UNK	N	5.79
1	I	1297:UNK	C	1430:UNK	N	5.79
1	E	1297:UNK	C	1430:UNK	N	5.79
1	G	1297:UNK	C	1430:UNK	N	5.79
1	B	2479:LEU	C	2487:UNK	N	3.60
1	I	2479:LEU	C	2487:UNK	N	3.60
1	E	2479:LEU	C	2487:UNK	N	3.60
1	G	2479:LEU	C	2487:UNK	N	3.60
1	B	2939:ARG	C	2942:UNK	N	3.57
1	I	2939:ARG	C	2942:UNK	N	3.57
1	E	2939:ARG	C	2942:UNK	N	3.57
1	G	2939:ARG	C	2942:UNK	N	3.57