



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 02:21 PM EDT

PDB ID : 5T9V
EMDB ID: : EMD-8376
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 Å(reported)

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

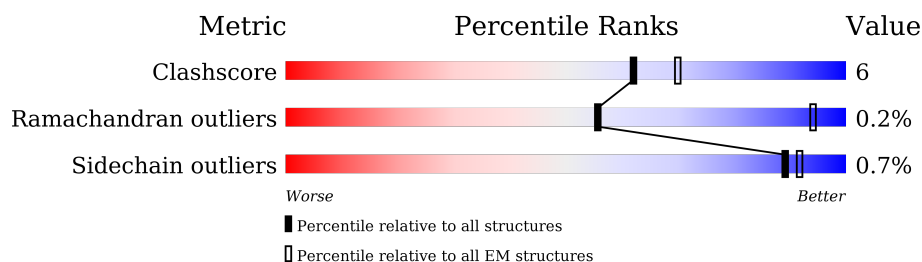
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	108	81% 18% .
1	F	108	81% 18% .
1	H	108	81% 18% .
1	J	108	81% 19% .
2	B	4416	83% 12% 5%
2	E	4416	83% 11% 5%
2	G	4416	83% 11% 5%
2	I	4416	83% 12% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

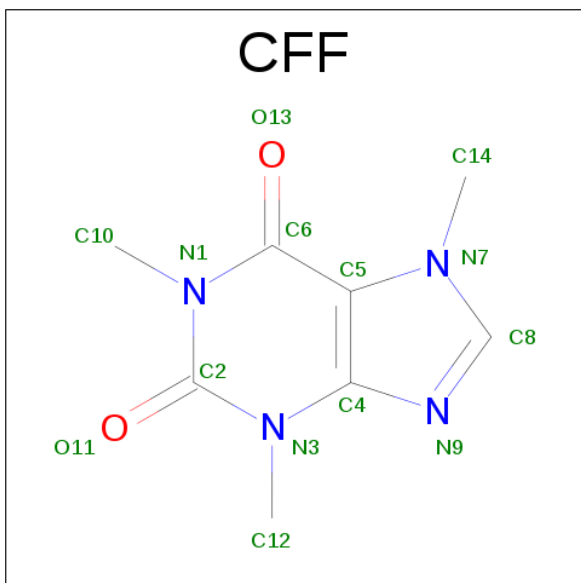
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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	G	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

- 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	G	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	

- 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	


- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

3 Residue-property plots


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

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

Chain F: 




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

Chain A: 




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

Chain H: 




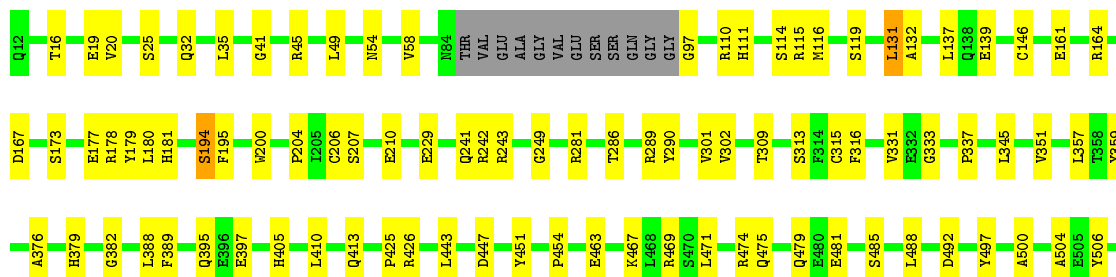
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

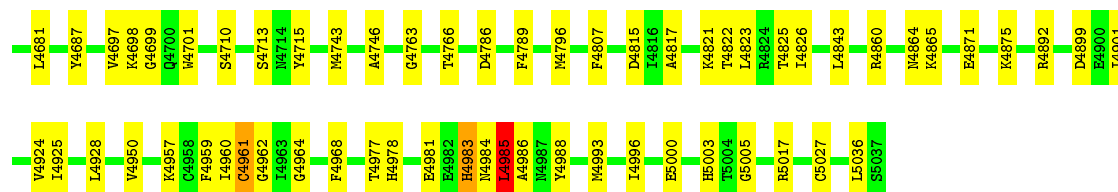


- Molecule 2: Ryanodine receptor 1

Chain B: 

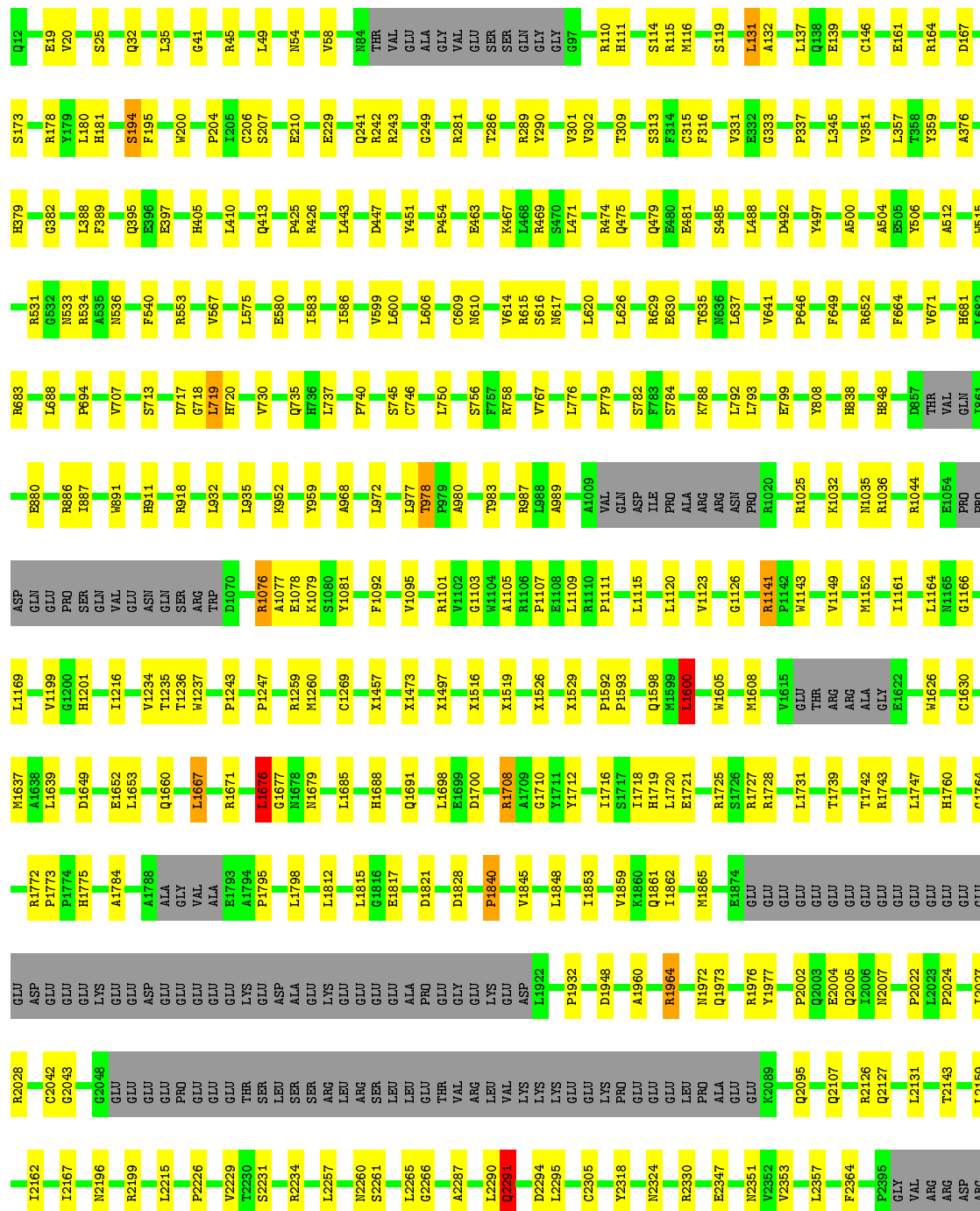


M4231	H9994	V3812	X2954	T2762	F2364	Q2107	N2007	GLU	T1742	ARG	M1152	M1035	GLN	H681	A512
E4232	H9998	X3361	X3362	K2770	F2395	R2126	P2022	GLU	R1743	ALA	I1161	R1044	I861	L582	W515
R4563	K4002	X3365	X3366	W2775	P2395	Q2127	P2024	GLU	L1747	E1622	L1164	T1045	N877	R683	A531
F4571	L4017	X3367	X3366	W2807	VAL	L2131	I2027	GLU	H1760	W1626	L1165	E1054	E830	L688	A532
F4575	E4032	X3368	X3366	W2807	ARG	L2159	I2028	GLU	G1764	C1630	G1166	PRO	R886	P894	W533
V4582	G4033	X3369	X3366	K2810	ASP	L2162	Q2029	ASP	R1772	M1637	L1169	PRO	I887	V707	A534
V4587	G4034	X3370	X3366	K2814	ARG	L2167	D2033	GLU	P1773	A1638	V1199	GLN	W891	S713	W536
P4587	N4034	X3371	X3366	K2814	ARG	L2167	C2042	GLU	H1774	L1639	G1200	PRO	L907	D717	F540
GLY	V4049	X3372	X3366	L2823	HIS	N2196	G2043	LYS	A1784	D1649	H1201	SER	H911	C718	R553
GLU	I4066	X3373	X3366	E2830	GLY	R2199	G2048	GLU	A1788	E1652	I1216	GLN	H911	L719	W567
ASP	E4075	X3374	X3366	GLU	GLY	R2199	GLU	ASP	A1788	L1653	V1234	VAL	R918	H720	L575
MET	E4075	X3375	X3366	GLU	GLY	R2199	GLU	ASP	A1788	L1657	T1235	ASN	R918	V730	L575
GLY	Q4078	X3376	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	GLN	R918	V730	L575
SER	V4081	X3377	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
ALA	V4081	X3378	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	R4085	X3379	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
ASP	L4088	X3380	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
LEU	L4088	X3381	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
ALA	T4104	X3382	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	G4105	X3383	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
ALA	P4106	X3384	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	P4106	X3385	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
SER	M4120	X3386	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	M4120	X3387	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	E4126	X3388	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
SER	M4130	X3389	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	M4130	X3390	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
TRP	I4139	X3391	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
SER	E4152	X3392	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
ALA	P4155	X3393	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	P4155	X3394	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLU	P4158	X3395	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
ALA	R4161	X3396	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
ASP	L4166	X3397	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
ASP	S4169	X3398	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLU	R4180	X3399	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	R4192	X3400	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	V4222	X3401	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
GLY	E4227	X3402	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
E4674	R4673	X3403	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3404	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3405	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3406	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3407	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3408	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3409	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3410	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3411	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3412	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3413	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3414	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3415	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3416	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3417	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3418	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3419	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3420	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3421	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3422	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3423	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
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		X3426	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3427	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3428	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3429	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3430	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3431	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3432	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3433	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3434	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3435	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3436	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3437	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3438	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3439	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3440	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3441	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3442	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3443	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3444	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3445	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3446	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3447	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3448	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3449	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3450	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
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		X3452	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3453	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3454	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3455	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3456	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3457	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575
		X3458	X3366	GLU	GLY	R2199	GLU	GLU	A1788	L1657	T1235	SER	R918	V730	L575




• Molecule 2: Ryanodine receptor 1

Chain G: 83% 11% 5%



ASP	LEU	I4088	L3890	I3674	GLU	ARG
ALA	GLY	T4104	L3891	I3680	LYS	ARG
ALA	GLY	I4816	N3896	A3680	LYS	GLU
GLY	ALA	G4105	N3897	G3681	THR	HIS
SER	SER	P4106	D3898	ARG	GLY	PHE
GLY	SER	N4120	F3899	E3712	LYS	GLY
GLY	GLY	E4126	Q3900	I3728	GLU	GLU
GLY	GLY	E4126	N3901	I3728	PRO	PRO
SER	SER	N4130	L3903	C3733	THR	GLU
GLY	THR	I4139	T3910	N3741	ALA	GLU
GLY	SER	E4152	T3911	GLY	GLN	N2414
ALA	ALA	P4155	I3915	ALA	THR	I2429
GLY	GLY	S3929	I3915	ALA	ASP	I2430
GLU	GLU	P4166	S3937	GLU	PRO	P2438
GLU	GLU	P4166	Y3937	E3747	ARG	
ASP	ASP	S4169	Q3946	E3759	GLY	R2452
GLU	GLU	R4180	Q3946	R3762	GLY	I2453
GLY	GLY	R4180	N3950	R3762	S2868	L2472
GLY	GLY	R4180	N3950	Q3766	R2869	
GLY	GLY	R4180	Q3960	Q3766	Q2872	L2479
GLY	GLY	R4180	E3967	T3772	X2487	
GLY	GLY	R4180	G3971	R3773	X2502	
GLY	GLY	R4180	L3980	Q3781	R2888	P2737
GLY	GLY	R4180	A3981	S3784	L2911	R2738
GLY	GLY	R4180	L3985	K3787	K2916	P2748
GLY	GLY	R4180	V3986	S3803	L2927	L2751
GLY	GLY	R4180	H3994	I3804	L2930	L2755
GLY	GLY	R4180	H3998	L3805	L2930	
GLY	GLY	R4180	H3998	N3809	X2950	F2758
GLY	GLY	R4180	K4002	V3812	X2954	T2762
GLY	GLY	R4180	L4017	K3815	X3361	K2770
GLY	GLY	R4180	E4032	F3816	X3362	W2775
GLY	GLY	R4180	G4033	L3817	X3365	W2807
GLY	GLY	R4180	N4034	Q3830	X3366	K2810
GLY	GLY	R4180	V4049	Q3833	X3552	K2814
GLY	GLY	R4180	V4049	L3842	X3556	I2823
GLY	GLY	R4180	L4066	F3847	N3651	
GLY	GLY	R4180	E4075	Q3850	K3658	E2830
GLY	GLY	R4180	Q4078	A3853	W3661	GLU
GLY	GLY	R4180	V4081	I3662	I3662	ARG
GLY	GLY	R4180	R4085	Q3889	I3663	THR

• Molecule 2: Ryanodine receptor 1

Chain I:  83% 12% 5%

E1054	I887	S713	R553	L388	Y179	Q12
W891	T892	D717	V567	F389	L180	T16
ASP	R902	L718	L575	Q395	S194	E19
GLU	H911	H720	E580	E396	F195	V20
SER	R918	V730	I583	H405	W200	S25
GLN	M924	Q735	I586	L410	P204	Q32
VAL	T928	H736	V599	Q413	C206	L35
ASN	L932	L737	L600	P425	S207	G41
GLN	L935	P740	L606	R426	E210	R45
SER	L952	S745	L609	L443	E229	L49
ARG	K952	C746	N610	D447	Q241	L69
TRP	Y959	L750	V614	Y451	R242	N54
D1070	A968	S756	R615	P454	R243	V58
R1076	S1080	F757	S616	E463	G249	R64
A1077	Y1081	R758	N617	E467	R281	THR
E1078	F1092	V767	L620	T286	V301	VAL
K1079	V1095	L776	L626	R289	V302	GLU
S1080	R1101	P779	P627	Y290	T309	ALA
Y1081	V1102	S782	G628	S470	S313	GLY
F1092	G1103	F783	R629	L471	F314	GLY
V1095	A1104	S784	E630	R474	C315	R110
R1101	E1105	K788	Q634	Q475	F316	H111
V1102	P1107	L792	T635	Q479	V331	S114
G1103	A1106	L793	N636	E481	E332	R115
A1105	E1108	E799	V641	S485	G332	M116
P1107	L1109	Y808	P646	L488	Y497	L131
E1108	P1111	H838	R652	Y497	P337	A132
L1110	L1115	H848	F664	A500	L345	L137
P1111	L1120	D857	V671	E504	V351	Q138
L1115	L1123	THR	E505	Y506	E139	E139
L1120	G1126	VAL	H681	R531	L357	R164
V1123	R1141	GLN	L682	G532	T358	R164
G1126	P1142	R683	R683	N533	Y359	D167
R1141	W1143	E876	L688	R534	A376	S173
W1143	V1149	N877	P694	A535	H379	E177
V1149	M1152	E880	E880	N536	C320	R178
M1152	I1161	R886	W707	F540		
I1161						

L1164	M1637	H1760	P2024	R2126	F2364	K2810	X3552	K3815	K4002	F4575	Q4700	G4964
M1165	A1638	G1764	I2027	Q2127	P2395	K2814	X3556	M3816	L4017	V4582	W4701	F4968
G1166	L1639	R1772	R2028	L2131	GLY	L2823	N3651	L3817	E4032	Y4715	Y4715	T4977
L1169	H1640	P1773	Q2029	T2143	ARG	E2830	K3658	Q3830	G4033	M4743	M4743	H4978
V1199	P1642	H1775	D2033	L2159	ASP	GLU	K3658	Q3833	N4034	P4587	A4746	E4981
H1200	D1649	A1784	F2034	I2162	ASP	THR	W3661	L3842	V4049	GLY	G4763	E4982
H1201	E1652	L1653	L2038	I2167	ARG	LYS	I3662	F3847	L4066	ASP	T4766	H4983
I1216	L1653	A1788	C2042	L2196	GLU	LYS	L3663	Q3850	E4075	MET	D4786	A4985
V1234	Q1660	ALA	G2043	M2196	PHE	LYS	I3674	A3853	Q4078	ALA	F4789	A4986
T1235	Q1667	GLY	G2048	R2199	GLY	LYS	L3677	Q3889	V4081	ALA	M4796	K4987
T1236	L1667	VAL	G2048	R2199	GLU	THR	A3680	L3890	L4085	ASP	F4807	Y4988
W1237	R1671	ALA	G2048	L2215	PRO	ARG	G3681	L3891	R4085	LEU	F4807	M4993
P1243	P1676	GLY	G2048	P2226	GLU	ILE	L3698	L3891	I4088	ALA	D4815	I4996
P1247	M1679	L1798	G2048	V2229	GLU	SER	E3712	N3896	T4104	GLY	I4816	K4997
R1259	L1685	L1812	G2048	S2231	THR	GLN	I3728	D3898	G4105	GLY	A4917	D4999
M1260	H1688	L1815	G2048	R2234	LEU	THR	C3733	Q3900	P4106	GLY	T4822	E5000
C1269	Q1691	G1816	G2048	L2257	SER	ASP	N3741	N3901	N4120	GLY	R4823	G5005
X1457	X1497	E1817	G2048	S2261	ARG	ASP	GLY	L3903	E4126	GLY	R4824	Q5006
X1516	L1698	D1821	G2048	I2260	LEU	ARG	ALA	L3903	E4126	TRP	I4826	E5007
X1519	E1693	D1700	G2048	S2261	SER	GLY	GLU	T3910	M4130	GLY	L4843	R5017
X1526	R1708	R1840	G2048	G2266	LEU	S2868	GLU	I3915	I4139	ALA	R4860	C5027
X1529	G1710	Y1711	G2048	A2287	THR	R2869	E3747	S3929	E4152	GLY	N4864	L5036
P1593	Y1712	V1845	G2048	L2290	ARG	Q2872	E3759	Y3937	P4155	ALA	K4865	S5037
Q1598	I1716	L1848	G2048	Q2291	LEU	N2884	R3762	Q3946	P4158	GLY	E4871	
M1599	S1717	I1853	G2048	D2294	VAL	R2888	Q3766	N3950	R4159	GLY	K4875	
L1600	H1719	V1859	G2048	L2295	LYS	L2911	H3771	Q3960	R4161	ASP	R4892	
W1605	L1720	K1860	G2048	C2305	GLU	L2916	T3772	E3967	L4166	ASP	D4899	
M1608	E1721	Q1861	G2048	R2330	GLU	K2916	R3773	G3971	S4169	GLY	E4900	
V1615	R1725	M1865	G2048	E2347	PRQ	X2950	G3774	A3981	R4180	M4639	I4901	
GLU	S1728	E1874	G2048	R2330	GLU	X2950	Q3781	L3980	R4192	E4640	V4924	
THR	R1728	GLU	G2048	E2347	LEU	X2950	S3784	A3981	E4227	P4641	I4925	
ARG	L1731	GLU	G2048	E2347	PRQ	X2950	K3787	R3984	A4228	I4658	L4928	
ALA	T1739	GLU	G2048	E2347	PRQ	X2950	S3803	L3985	E4674	E4674	K4957	
GLY	T1742	GLU	G2048	E2347	PRQ	X2950	I3804	V3986	M4231	C4958	F4959	
E1622	R1743	GLU	G2048	E2347	PRQ	X2950	L3805	H3994	E4232	Y4687	I4960	
W1626	L1747	GLU	G2048	E2347	PRQ	X2950	N3809	H3998	R4563	V4697	C4961	
C1630	L1747	GLU	G2048	E2347	PRQ	X2950	V3812	H3998	F4571	K4698	G4962	
			G2048	E2347	PRQ	X2950				G4699	I4963	

• Molecule 2: Ryanodine receptor 1

Chain E: 83% 11% 5%

Q12	R110	S114	L131	L137	R164	D167	S173	E177	Y178	L180
E19	H111	R115	A132	Q138	L139	L143	L149	R178		
V20		M116		E139						
S25										
Q32										
L35										
G41										
R45										
L49										
N54										
V58										
N84										
THR										
VAL										
GLU										
ALA										
GLY										
VAL										
GLU										
SER										
SER										
GLN										
GLY										
GLY										
G97										

N3901	I3902	L3903	T3910	T3911	I3915	S3929	Y3937	Q3946	N3950	Q3960	E3967	R3984	L3985	W3986	H3994	H3998	K4002	L4017	E4032	G4033	N4034	V4049	L4066	E4075	Q4078	V4081	R4085	I4088	T4104	G4105	P4106												
SER	GLN	THR	ALA	GLN	THR	ASP	GLY	GLY	S2868	R2869	Q2872	N2884	R2888	L2911	Y2916	S2927	I3804	L3805	N3809	V3812	K3815	W3816	L3817	Q3830	Q3833	L3842	F3847	Q3850	A3853	Q3889	L3891	N3896	N3897	D3898	F3899	Q3900							
M2414	L2429	L2430	P2438	R2452	L2453	V2467	L2470	S2471	L2472	L2479	X2487	X2502	P2737	R2738	P2739	P2748	L2751	I2755	P2758	T2762	K2770	W2775	W2807	K2810	K2814	L2823	E2830	GLU	GLU	THR	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE					
T2230	S2231	R2234	L2257	N2260	S2261	L2265	G2266	A2287	L2290	Q2291	D2294	L2295	C2305	R2738	Y2318	N2324	R2330	E2347	N2351	V2352	V2353	L2357	L2358	R2359	F2364	P2395	GLY	VAL	ARG	ASP	ARG	ARG	GLU	THR	GLY	THR	ARG	GLU					
GLU	THR	SER	LEU	SER	ARG	LEU	LEU	GLU	THR	VAL	ARG	VAL	LYS	LYS	GLU	PRO	GLU	GLU	LEU	ALA	GLU	GLU	PRO	ALA	L2107	R2126	Q2127	L2131	L2159	I2162	L2167	N2196	R2199	L2215	P2226	V2229							
T2230	S2231	R2234	L2257	N2260	S2261	L2265	G2266	A2287	L2290	Q2291	D2294	L2295	C2305	R2738	Y2318	N2324	R2330	E2347	N2351	V2352	V2353	L2357	L2358	R2359	F2364	P2395	GLY	VAL	ARG	ASP	ARG	ARG	GLU	THR	GLY	THR	ARG	GLU					
ALA	GLU	LYS	GLU	GLU	GLU	GLU	GLU	GLU	ASP	L1922	P1932	D1948	A1960	Q1861	R1964	N1972	Q1973	Y1977	Q2002	E2004	Q2005	I2006	N2007	P2022	L2023	P2024	I2027	R2028	Q2029	D2033	F2034	L2038	C2042	G2043	G2048	GLU	GLU	GLU	PRO	GLU			
E1793	A1794	P1795	L1798	L1812	L1815	D1828	P1840	V1845	L1848	L1853	V1859	K1860	Q1861	L1862	M1865	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	LYS	GLU	GLU	GLU	ASP				
L1667	R1671	L1676	M1679	L1685	H1688	Q1691	L1698	D1700	R1708	A1709	G1710	Y1711	Y1712	L1718	H1719	E1721	R1725	S1726	R1727	R1728	L1731	T1739	T1742	R1743	L1747	H1760	G1764	R1772	P1773	H1775	A1784	A1788	ALA	GLY	VAL	ALA							
T1235	T1236	W1237	P1243	P1247	R1259	M1260	G1269	X1457	X1473	X1497	X1516	X1519	X1526	X1529	P1593	Q1598	M1599	L1603	W1605	M1608	V1615	GLU	THR	ARG	ARG	ALA	GLY	W1626	G1630	M1637	A1638	L1639	D1649	E1652	L1653	Q1660							
GLN	SER	ARG	TRP	D1070	R1076	A1077	E1078	K1079	S1080	Y1081	F1092	V1095	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	P1111	L1115	L1120	V1123	G1126	R1141	P1142	W1143	V1149	M1152	I1161	L1164	M1165	G1166	L1169	V1199	G1200	H1201	I1216	V1234		
W891	R911	R918	L932	L935	K952	Y959	A968	L972	L977	T978	P979	A980	A989	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	R1025	L792	L793	V641	P646	F649	R652	F664	PRO	THR	ASP	GLN	GLU	GLN	VAL	GLU	ASN		
V707	S713	D717	Q718	L719	H720	L575	E580	Q735	H736	L737	P740	S745	C746	L750	S756	F757	R758	V614	R615	S616	N617	L620	L626	R629	F783	E630	W635	R636	L637	V641	P646	F649	R652	F664	PRO	THR	ASP	GLN	GLU	GLN	VAL	GLU	ASN
G382	I388	F389	Q395	E396	E397	H405	L410	Q413	P425	R426	L443	D447	Y451	N610	L606	C609	N610	V614	R615	S616	N617	L620	L626	R629	F783	E630	W635	R636	L637	V641	P646	F649	R652	F664	PRO	THR	ASP	GLN	GLU	GLN	VAL	GLU	ASN




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, CA, 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	0.30	0/25428	0.54	10/34534 (0.0%)
2	E	0.30	0/25428	0.54	10/34534 (0.0%)
2	G	0.30	0/25428	0.54	10/34534 (0.0%)
2	I	0.30	0/25428	0.54	10/34534 (0.0%)
All	All	0.30	0/105048	0.54	40/142628 (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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	7.69	132.98	115.30
2	B	131	LEU	CA-CB-CG	7.67	132.95	115.30
2	E	131	LEU	CA-CB-CG	7.67	132.93	115.30
2	G	131	LEU	CA-CB-CG	7.65	132.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4985	LEU	CA-CB-CG	6.48	130.20	115.30
2	B	4985	LEU	CA-CB-CG	6.47	130.19	115.30
2	G	4985	LEU	CA-CB-CG	6.46	130.16	115.30
2	E	4985	LEU	CA-CB-CG	6.46	130.16	115.30
2	I	1676	LEU	CA-CB-CG	6.45	130.14	115.30
2	B	1676	LEU	CA-CB-CG	6.45	130.14	115.30
2	E	1676	LEU	CA-CB-CG	6.45	130.12	115.30
2	G	1676	LEU	CA-CB-CG	6.44	130.12	115.30
2	G	1600	LEU	CA-CB-CG	6.37	129.95	115.30
2	B	1600	LEU	CA-CB-CG	6.37	129.94	115.30
2	I	1600	LEU	CA-CB-CG	6.37	129.94	115.30
2	E	1600	LEU	CA-CB-CG	6.35	129.91	115.30
2	G	4901	ILE	CG1-CB-CG2	-6.05	98.08	111.40
2	B	4901	ILE	CG1-CB-CG2	-6.05	98.08	111.40
2	I	4901	ILE	CG1-CB-CG2	-6.05	98.09	111.40
2	E	4901	ILE	CG1-CB-CG2	-6.05	98.10	111.40
2	G	977	LEU	CA-CB-CG	5.51	127.97	115.30
2	E	977	LEU	CA-CB-CG	5.50	127.95	115.30
2	B	977	LEU	CA-CB-CG	5.50	127.94	115.30
2	I	977	LEU	CA-CB-CG	5.49	127.93	115.30
2	G	719	LEU	CA-CB-CG	5.26	127.40	115.30
2	I	719	LEU	CA-CB-CG	5.25	127.39	115.30
2	B	719	LEU	CA-CB-CG	5.25	127.38	115.30
2	E	719	LEU	CA-CB-CG	5.24	127.35	115.30
2	I	4639	MET	C-N-CA	5.15	134.57	121.70
2	B	4639	MET	C-N-CA	5.15	134.57	121.70
2	E	4639	MET	C-N-CA	5.15	134.57	121.70
2	G	4639	MET	C-N-CA	5.13	134.52	121.70
2	G	1667	LEU	CA-CB-CG	5.09	127.01	115.30
2	B	1667	LEU	CA-CB-CG	5.08	126.99	115.30
2	E	1667	LEU	CA-CB-CG	5.08	126.98	115.30
2	I	688	LEU	CA-CB-CG	5.07	126.97	115.30
2	I	1667	LEU	CA-CB-CG	5.07	126.96	115.30
2	E	688	LEU	CA-CB-CG	5.06	126.94	115.30
2	B	688	LEU	CA-CB-CG	5.06	126.93	115.30
2	G	688	LEU	CA-CB-CG	5.05	126.93	115.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	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	1840	PRO	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	15	0
2	B	29499	0	24748	311	0
2	E	29499	0	24748	298	0
2	G	29499	0	24748	300	0
2	I	29499	0	24748	305	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102376	1234	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 (1234) 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:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.64	0.86
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.64	0.86
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.64	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.64	0.85
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.81	0.78
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.82	0.78
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	2.02	0.78
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.83	0.77
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	2.02	0.77
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.82	0.77
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	2.02	0.77
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	2.02	0.76
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.51	0.75
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.51	0.75
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.75
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.72	0.72
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.72	0.71
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.73	0.71
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.72	0.71
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.73	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.76	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.68
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.76	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.76	0.67
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.28	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.43	0.66
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.60	0.66
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.28	0.66
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.60	0.66
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.28	0.65
2:B:379:HIS:HD2	2:B:382:GLY:H	1.43	0.65
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.79	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.43	0.65
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.79	0.65
2:B:4983:HIS:H	2:B:4983:HIS:CD2	2.16	0.64
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.16	0.64
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.61	0.64
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.16	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.43	0.63
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	1.80	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.81	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.81	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.81	0.63
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.60	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.16	0.62
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.82	0.62
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.33	0.62
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.82	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.62
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.62
2:E:132:ALA:HA	2:E:194:SER:HB2	1.82	0.62
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.81	0.62
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62
2:G:626:LEU:HD23	2:G:630:GLU:H	1.65	0.61
2:I:626:LEU:HD23	2:I:630:GLU:H	1.65	0.61
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.61
2:E:626:LEU:HD23	2:E:630:GLU:H	1.65	0.61
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.82	0.61
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.61
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.82	0.61
2:B:132:ALA:HA	2:B:194:SER:HB2	1.82	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.61
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.81	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ALA:HA	2:I:194:SER:HB2	1.82	0.61
2:E:111:HIS:HD2	2:E:114:SER:H	1.48	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.61
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.82	0.61
2:B:626:LEU:HD23	2:B:630:GLU:H	1.65	0.61
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.82	0.61
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.61
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.33	0.61
2:G:111:HIS:HD2	2:G:114:SER:H	1.48	0.61
2:I:4978:HIS:CE1	2:I:5027:CYS:SG	2.94	0.61
2:B:4978:HIS:CE1	2:B:5027:CYS:SG	2.94	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.61
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.34	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.34	0.61
2:E:4978:HIS:CE1	2:E:5027:CYS:SG	2.94	0.60
2:G:132:ALA:HA	2:G:194:SER:HB2	1.82	0.60
2:G:4978:HIS:CE1	2:G:5027:CYS:SG	2.94	0.60
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.83	0.60
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.82	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
2:B:111:HIS:HD2	2:B:114:SER:H	1.48	0.60
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.82	0.60
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.60
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.83	0.60
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.66	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.60
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.60
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.34	0.60
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.60
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.60
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.60
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.67	0.60
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.67	0.60
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.83	0.60
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.67	0.60
2:I:359:TYR:HA	2:I:376:ALA:HA	1.84	0.60
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.67	0.59
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.59
2:B:359:TYR:HA	2:B:376:ALA:HA	1.84	0.59
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.84	0.59
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.85	0.59
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	1.85	0.59
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.85	0.59
2:G:359:TYR:HA	2:G:376:ALA:HA	1.84	0.59
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.84	0.59
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.33	0.59
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.33	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.59
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.85	0.59
2:B:4957:LYS:HG2	2:B:4964:GLY:CA	2.33	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.84	0.59
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.59
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.84	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.84	0.58
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.58
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.68	0.58
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.58
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.67	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.84	0.58
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.85	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.58
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.67	0.58
2:E:4977:THR:HG23	2:E:4981:GLU:HG3	1.85	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.58
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.67	0.58
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.85	0.58
2:E:4957:LYS:HG2	2:E:4964:GLY:CA	2.33	0.58
2:G:4977:THR:HG23	2:G:4981:GLU:HG3	1.85	0.58
2:I:313:SER:HB3	2:I:351:VAL:HB	1.86	0.58
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.85	0.58
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.85	0.58
2:B:4977:THR:HG23	2:B:4981:GLU:HG3	1.85	0.58
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.86	0.58
2:E:313:SER:HB3	2:E:351:VAL:HB	1.86	0.58
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.84	0.58
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.85	0.58
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.85	0.58
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.86	0.58
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.67	0.57
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.68	0.57
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.85	0.57
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.86	0.57
2:G:313:SER:HB3	2:G:351:VAL:HB	1.86	0.57
2:G:4957:LYS:HG2	2:G:4964:GLY:CA	2.33	0.57
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.86	0.57
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.86	0.57
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.85	0.57
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.70	0.57
2:I:4957:LYS:HG2	2:I:4964:GLY:CA	2.33	0.57
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.87	0.57
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.86	0.57
2:G:173:SER:HB3	2:G:178:ARG:H	1.70	0.57
2:I:4977:THR:HG23	2:I:4981:GLU:HG3	1.85	0.57
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.86	0.57
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.86	0.57
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.86	0.57
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.86	0.57
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.70	0.57
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.86	0.57
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.86	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.57
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.87	0.57
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.86	0.57
2:I:173:SER:HB3	2:I:178:ARG:H	1.70	0.57
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.86	0.57
2:B:313:SER:HB3	2:B:351:VAL:HB	1.86	0.57
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.86	0.57
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.57
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.68	0.57
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.86	0.57
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.85	0.57
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4978:HIS:HE1	2:B:5027:CYS:SG	2.28	0.57
2:E:173:SER:HB3	2:E:178:ARG:H	1.70	0.57
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.87	0.57
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.87	0.56
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.70	0.56
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.86	0.56
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.86	0.56
2:E:4978:HIS:HE1	2:E:5027:CYS:SG	2.28	0.56
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.87	0.56
2:G:4843:LEU:HD12	2:I:4823:LEU:HD23	1.86	0.56
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.68	0.56
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.86	0.56
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.86	0.56
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.86	0.56
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.87	0.56
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.79	0.56
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.79	0.56
2:B:173:SER:HB3	2:B:178:ARG:H	1.70	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.56
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.87	0.56
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.79	0.56
2:B:241:GLN:O	2:B:289:ARG:NH1	2.37	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.86	0.56
2:G:4978:HIS:HE1	2:G:5027:CYS:SG	2.28	0.56
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.71	0.56
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.38	0.56
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.86	0.56
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.38	0.56
2:I:4978:HIS:HE1	2:I:5027:CYS:SG	2.28	0.56
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.87	0.56
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.38	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.39	0.56
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.71	0.56
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.79	0.56
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.71	0.56
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.71	0.56
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.38	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.39	0.56
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.56
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.88	0.56
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.88	0.56
2:G:241:GLN:O	2:G:289:ARG:NH1	2.37	0.56
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.88	0.56
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.39	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.71	0.56
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.71	0.56
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.88	0.56
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.56
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.56
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.88	0.55
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.71	0.55
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.70	0.55
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.87	0.55
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.88	0.55
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.88	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.39	0.55
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.72	0.55
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.87	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.88	0.55
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.88	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.71	0.55
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.72	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.88	0.55
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.40	0.55
2:E:241:GLN:O	2:E:289:ARG:NH1	2.37	0.54
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.41	0.54
2:G:395:GLN:HG3	2:G:397:GLU:H	1.72	0.54
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.40	0.54
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.40	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.73	0.54
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.41	0.54
2:E:1032:LYS:O	2:E:1036:ARG:N	2.40	0.54
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.41	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.54
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.90	0.54
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.90	0.54
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.72	0.54
2:I:241:GLN:O	2:I:289:ARG:NH1	2.37	0.54
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.56	0.54
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.90	0.54
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.90	0.54
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.39	0.54
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.41	0.54
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.41	0.53
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.90	0.53
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.53
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.91	0.53
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.72	0.53
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.41	0.53
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.90	0.53
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.90	0.53
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.90	0.53
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.90	0.53
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.90	0.53
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.90	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.42	0.53
2:E:243:ARG:NH1	2:E:301:VAL:O	2.38	0.53
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.56	0.53
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.90	0.53
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.90	0.53
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.91	0.53
2:B:395:GLN:HG3	2:B:397:GLU:H	1.73	0.53
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.41	0.53
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.91	0.53
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.91	0.53
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.91	0.53
2:I:395:GLN:HG3	2:I:397:GLU:H	1.73	0.53
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.90	0.53
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.90	0.53
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.42	0.53
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.41	0.53
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.41	0.53
2:E:606:LEU:O	2:E:617:ASN:ND2	2.42	0.53
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.41	0.53
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.74	0.53
2:I:180:LEU:O	2:I:200:TRP:NE1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:SER:O	2:B:32:GLN:NE2	2.42	0.53
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.90	0.53
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.42	0.53
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.74	0.53
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.42	0.53
2:E:4231:MET:CE	2:E:4960:ILE:HA	2.39	0.53
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.41	0.53
2:G:606:LEU:O	2:G:617:ASN:ND2	2.42	0.53
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.42	0.53
2:I:606:LEU:O	2:I:617:ASN:ND2	2.42	0.53
2:B:4231:MET:CE	2:B:4960:ILE:HA	2.39	0.52
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.73	0.52
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.90	0.52
2:G:180:LEU:O	2:G:200:TRP:NE1	2.37	0.52
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.52
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.73	0.52
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.41	0.52
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.56	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.52
2:I:4231:MET:CE	2:I:4960:ILE:HA	2.39	0.52
2:B:606:LEU:O	2:B:617:ASN:ND2	2.42	0.52
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.74	0.52
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.73	0.52
2:G:25:SER:O	2:G:32:GLN:NE2	2.42	0.52
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.90	0.52
2:G:243:ARG:NH1	2:G:301:VAL:O	2.38	0.52
2:G:776:LEU:HG	2:G:848:HIS:HA	1.92	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:180:LEU:O	2:B:200:TRP:NE1	2.37	0.52
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.91	0.52
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.52
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.92	0.52
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.92	0.52
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.91	0.52
2:I:25:SER:O	2:I:32:GLN:NE2	2.42	0.52
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.73	0.52
1:J:21:THR:HA	1:J:49:ARG:HA	1.92	0.52
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.42	0.52
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.52
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.91	0.52
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:793:LEU:HD11	2:G:1626:TRP:HE1	1.75	0.52
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.90	0.52
2:I:793:LEU:HD11	2:I:1626:TRP:HE1	1.75	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.92	0.52
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.41	0.52
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.91	0.52
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.73	0.52
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.91	0.52
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.92	0.52
2:E:25:SER:O	2:E:32:GLN:NE2	2.42	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.41	0.52
2:I:243:ARG:NH1	2:I:301:VAL:O	2.38	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.92	0.52
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.52
2:B:1032:LYS:O	2:B:1036:ARG:N	2.40	0.52
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.42	0.52
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.43	0.52
2:G:4231:MET:CE	2:G:4960:ILE:HA	2.39	0.52
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.92	0.52
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.74	0.51
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.43	0.51
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.92	0.51
2:E:776:LEU:HG	2:E:848:HIS:HA	1.92	0.51
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.92	0.51
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.92	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.92	0.51
2:I:4983:HIS:HD2	2:I:4983:HIS:H	1.56	0.51
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.91	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.91	0.51
2:E:2479:LEU:O	2:E:2487:UNK:N	2.44	0.51
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.91	0.51
1:H:21:THR:HA	1:H:49:ARG:HA	1.92	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:880:GLU:OE1	2:I:968:ALA:N	2.43	0.51
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.91	0.51
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.90	0.51
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.43	0.51
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.43	0.51
2:E:793:LEU:HD11	2:E:1626:TRP:HE1	1.75	0.51
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.51
2:E:331:VAL:HG12	2:E:333:GLY:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1032:LYS:O	2:G:1036:ARG:N	2.40	0.51
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.43	0.51
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.74	0.51
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.92	0.51
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.42	0.51
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.43	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.51
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.44	0.51
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.76	0.51
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.43	0.51
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.92	0.51
1:F:21:THR:HA	1:F:49:ARG:HA	1.92	0.51
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.42	0.51
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.92	0.51
2:G:331:VAL:HG12	2:G:333:GLY:H	1.76	0.51
2:I:1032:LYS:O	2:I:1036:ARG:N	2.40	0.51
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.92	0.51
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.44	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.76	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.76	0.51
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.51
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.51
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.44	0.51
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.44	0.51
2:E:1865:MET:SD	2:E:1865:MET:N	2.84	0.51
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.93	0.51
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.51
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.93	0.51
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.93	0.51
2:G:1865:MET:SD	2:G:1865:MET:N	2.84	0.51
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.92	0.51
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.43	0.51
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.51
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.93	0.51
2:B:793:LEU:HD11	2:B:1626:TRP:HE1	1.75	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.93	0.51
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.51
2:G:911:HIS:O	2:G:918:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1865:MET:SD	2:B:1865:MET:N	2.84	0.51
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.51
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.43	0.51
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.92	0.51
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.44	0.50
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.93	0.50
2:B:4983:HIS:HB2	2:B:4988:TYR:HE2	1.77	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.91	0.50
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.93	0.50
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.91	0.50
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.92	0.50
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.94	0.50
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.93	0.50
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.93	0.50
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.50
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.94	0.50
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.44	0.50
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.50
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.94	0.50
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.44	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.50
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.93	0.50
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.93	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.45	0.50
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.44	0.50
2:I:2159:LEU:HA	2:I:2162:ILE:HD12	1.94	0.50
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.94	0.50
2:I:4983:HIS:HB2	2:I:4988:TYR:HE2	1.77	0.50
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.93	0.50
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.93	0.50
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.44	0.50
2:E:206:CYS:SG	2:E:207:SER:N	2.84	0.50
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.92	0.50
2:I:1865:MET:SD	2:I:1865:MET:N	2.84	0.50
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.94	0.50
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.76	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.93	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.92	0.50
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.50
2:B:2159:LEU:HA	2:B:2162:ILE:HD12	1.94	0.50
2:B:290:TYR:O	2:B:302:VAL:N	2.45	0.50
2:B:331:VAL:HG12	2:B:333:GLY:H	1.76	0.50
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.44	0.50
2:I:2479:LEU:O	2:I:2487:UNK:N	2.44	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:E:4983:HIS:HB2	2:E:4988:TYR:HE2	1.77	0.50
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.94	0.50
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.47	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.44	0.50
2:G:2479:LEU:O	2:G:2487:UNK:N	2.44	0.50
1:H:82:TYR:O	1:H:86:GLY:N	2.44	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.93	0.50
2:B:2479:LEU:O	2:B:2487:UNK:N	2.44	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.49
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.49
2:G:206:CYS:SG	2:G:207:SER:N	2.84	0.49
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.45	0.49
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.45	0.49
2:B:978:THR:HB	2:B:980:ALA:H	1.78	0.49
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.93	0.49
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.76	0.49
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.49
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.94	0.49
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.94	0.49
2:G:880:GLU:OE1	2:G:968:ALA:N	2.43	0.49
2:I:978:THR:HB	2:I:980:ALA:H	1.78	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.94	0.49
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.94	0.49
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.47	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.44	0.49
2:E:290:TYR:O	2:E:302:VAL:N	2.45	0.49
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.45	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.46	0.49
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:290:TYR:O	2:I:302:VAL:N	2.45	0.49
2:I:331:VAL:HG12	2:I:333:GLY:H	1.76	0.49
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.94	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.49
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.47	0.49
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.49
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.46	0.49
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.49
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.76	0.49
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.41	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.93	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.95	0.49
2:B:206:CYS:SG	2:B:207:SER:N	2.84	0.49
2:E:2159:LEU:HA	2:E:2162:ILE:HD12	1.94	0.49
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.49
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.44	0.49
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.49
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.49
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.39	0.49
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.78	0.49
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.93	0.49
2:E:978:THR:HB	2:E:980:ALA:H	1.78	0.49
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.94	0.49
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.95	0.49
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.49
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.94	0.49
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.46	0.49
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.47	0.49
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.93	0.49
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.78	0.49
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.93	0.49
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.95	0.49
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.93	0.49
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.76	0.49
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.81	0.49
2:G:290:TYR:O	2:G:302:VAL:N	2.45	0.49
2:G:4983:HIS:HB2	2:G:4988:TYR:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.39	0.49
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.95	0.49
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.94	0.49
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.95	0.49
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.95	0.49
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.95	0.49
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.95	0.49
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.39	0.48
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.95	0.48
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.48
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.48
2:E:41:GLY:O	2:E:45:ARG:NH1	2.47	0.48
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.96	0.48
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.95	0.48
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.93	0.48
2:E:880:GLU:OE1	2:E:968:ALA:N	2.43	0.48
2:G:2159:LEU:HA	2:G:2162:ILE:HD12	1.94	0.48
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.95	0.48
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.95	0.48
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.48
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.45	0.48
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.78	0.48
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.95	0.48
2:E:180:LEU:O	2:E:200:TRP:NE1	2.37	0.48
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.78	0.48
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.95	0.48
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.48
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.96	0.48
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.46	0.48
2:B:41:GLY:O	2:B:45:ARG:NH1	2.47	0.48
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.95	0.48
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.44	0.48
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.42	0.48
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.48
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.95	0.48
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.48
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.96	0.48
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:978:THR:HB	2:G:980:ALA:H	1.77	0.48
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.95	0.48
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.48
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.82	0.48
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.95	0.48
2:I:41:GLY:O	2:I:45:ARG:NH1	2.47	0.48
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.95	0.48
2:I:206:CYS:SG	2:I:207:SER:N	2.84	0.48
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.94	0.48
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.82	0.48
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.42	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.48
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.46	0.48
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.95	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:I:164:ARG:N	2:I:167:ASP:OD2	2.43	0.48
2:I:4817:ALA:HA	2:I:4823:LEU:HD22	1.96	0.48
2:G:41:GLY:O	2:G:45:ARG:NH1	2.47	0.48
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.96	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.47
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.95	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.46	0.47
2:E:4817:ALA:HA	2:E:4823:LEU:HD22	1.96	0.47
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.47
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.96	0.47
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.47
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.47	0.47
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.82	0.47
2:B:54:ASN:O	2:B:58:VAL:N	2.44	0.47
2:E:1516:UNK:N	2:E:1529:UNK:O	2.48	0.47
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.47	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.95	0.47
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.39	0.47
2:G:4817:ALA:HA	2:G:4823:LEU:HD22	1.96	0.47
2:I:500:ALA:HB1	2:I:504:ALA:HB2	1.96	0.47
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.97	0.47
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.79	0.47
2:G:500:ALA:HB1	2:G:504:ALA:HB2	1.97	0.47
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.48	0.47
2:B:4066:LEU:HD12	2:B:4169:SER:HB2	1.96	0.47
2:G:1516:UNK:N	2:G:1529:UNK:O	2.48	0.47
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.38	0.47
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.73	0.47
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.47
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.96	0.47
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.97	0.47
2:B:4817:ALA:HA	2:B:4823:LEU:HD22	1.96	0.47
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.97	0.47
2:E:500:ALA:HB1	2:E:504:ALA:HB2	1.97	0.47
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.97	0.47
2:B:1516:UNK:N	2:B:1529:UNK:O	2.48	0.47
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.47	0.47
2:B:500:ALA:HB1	2:B:504:ALA:HB2	1.96	0.47
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.97	0.47
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.97	0.47
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.81	0.47
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.47
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.81	0.47
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.47
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.73	0.47
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.96	0.47
2:E:3994:HIS:O	2:E:3998:HIS:ND1	2.39	0.47
2:E:4066:LEU:HD12	2:E:4169:SER:HB2	1.97	0.47
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.95	0.47
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.97	0.47
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.97	0.47
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.97	0.47
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.80	0.47
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.97	0.47
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.13	0.47
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.47
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.97	0.47
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.80	0.47
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.47
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	1.97	0.47
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.73	0.47
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.97	0.47
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.47	0.47
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.13	0.47
2:I:2353:VAL:O	2:I:2357:LEU:N	2.48	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:B:614:VAL:HG22	2:B:616:SER:H	1.80	0.47
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.96	0.47
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	1.97	0.47
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.96	0.47
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.97	0.47
2:I:2347:GLU:O	2:I:2351:ASN:N	2.48	0.47
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.97	0.47
2:B:3994:HIS:O	2:B:3998:HIS:ND1	2.39	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.46	0.46
2:B:4823:LEU:HA	2:B:4826:ILE:HD12	1.97	0.46
2:E:4823:LEU:HA	2:E:4826:ILE:HD12	1.97	0.46
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.48	0.46
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.97	0.46
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.98	0.46
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.80	0.46
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.46
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.48	0.46
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.48	0.46
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.46
2:B:2347:GLU:O	2:B:2351:ASN:N	2.48	0.46
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.97	0.46
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.82	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.46
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.46	0.46
2:I:614:VAL:HG22	2:I:616:SER:H	1.80	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.95	0.46
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.46
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.46
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.46	0.46
2:G:2353:VAL:O	2:G:2357:LEU:N	2.48	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.46
2:I:4066:LEU:HD12	2:I:4169:SER:HB2	1.96	0.46
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.48	0.46
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.46
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.46
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.51	0.46
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.49	0.46
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	1.97	0.46
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.49	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.38	0.46
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.49	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.97	0.46
2:E:2868:SER:O	2:E:2872:GLN:N	2.49	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.49	0.46
2:G:1077:ALA:HB1	2:G:1234:VAL:HG11	1.98	0.46
2:G:2868:SER:O	2:G:2872:GLN:N	2.49	0.46
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.46
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.49	0.46
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.97	0.46
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.48	0.46
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.81	0.46
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.49	0.46
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.51	0.46
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.81	0.46
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.49	0.46
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.81	0.46
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.98	0.46
2:G:4066:LEU:HD12	2:G:4169:SER:HB2	1.96	0.46
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.51	0.46
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.98	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.46
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.46
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.46	0.46
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.98	0.46
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.73	0.46
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.51	0.46
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.98	0.46
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.98	0.46
2:G:54:ASN:O	2:G:58:VAL:N	2.44	0.46
2:I:1077:ALA:HB1	2:I:1234:VAL:HG11	1.98	0.46
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46
2:B:911:HIS:O	2:B:918:ARG:NH2	2.44	0.46
2:G:3361:UNK:O	2:G:3365:UNK:N	2.49	0.46
2:I:2868:SER:O	2:I:2872:GLN:N	2.49	0.46
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.38	0.46
2:B:1077:ALA:HB1	2:B:1234:VAL:HG11	1.98	0.45
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.48	0.45
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.98	0.45
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.98	0.45
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.98	0.45
2:E:614:VAL:HG22	2:E:616:SER:H	1.80	0.45
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.97	0.45
2:G:471:LEU:O	2:G:475:GLN:N	2.47	0.45
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.99	0.45
2:I:3361:UNK:O	2:I:3365:UNK:N	2.49	0.45
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.45
2:E:2353:VAL:O	2:E:2357:LEU:N	2.48	0.45
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.98	0.45
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.96	0.45
2:B:2353:VAL:O	2:B:2357:LEU:N	2.48	0.45
2:B:2950:UNK:O	2:B:2954:UNK:N	2.50	0.45
2:B:3361:UNK:O	2:B:3365:UNK:N	2.49	0.45
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.33	0.45
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.81	0.45
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.80	0.45
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.99	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45
2:G:2347:GLU:O	2:G:2351:ASN:N	2.48	0.45
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.49	0.45
2:G:4571:PHE:O	2:G:4575:PHE:N	2.46	0.45
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.41	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.45
2:I:4823:LEU:HA	2:I:4826:ILE:HD12	1.97	0.45
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.97	0.45
2:E:1077:ALA:HB1	2:E:1234:VAL:HG11	1.98	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.48	0.45
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.98	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.49	0.45
2:I:911:HIS:O	2:I:918:ARG:NH2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.81	0.45
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.45
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.97	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.99	0.45
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.35	0.45
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.35	0.45
2:G:4823:LEU:HA	2:G:4826:ILE:HD12	1.97	0.45
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.98	0.45
2:G:614:VAL:HG22	2:G:616:SER:H	1.80	0.45
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.45
2:I:4822:THR:O	2:I:4825:THR:OG1	2.31	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1973:GLN:O	2:B:1977:TYR:N	2.49	0.45
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	1.99	0.45
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.98	0.45
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.13	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.45
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.97	0.45
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.48	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.49	0.45
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.45
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.99	0.45
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.97	0.45
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.99	0.45
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	1.99	0.45
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.82	0.45
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.45
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.99	0.45
2:E:3361:UNK:O	2:E:3365:UNK:N	2.49	0.45
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.97	0.45
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.45
2:G:4959:PHE:CG	2:G:4959:PHE:O	2.70	0.45
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.45
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.43	0.45
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.99	0.45
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.82	0.45
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.99	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.45
2:E:471:LEU:O	2:E:475:GLN:N	2.47	0.45
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.98	0.45
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.81	0.45
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.35	0.45
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.34	0.45
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.82	0.45
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.99	0.44
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.98	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.70	0.44
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.82	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.44
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.70	0.44
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	1.99	0.44
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.82	0.44
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.49	0.44
2:I:54:ASN:O	2:I:58:VAL:N	2.44	0.44
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.98	0.44
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.43	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.82	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.82	0.44
2:I:451:TYR:O	2:I:474:ARG:NH1	2.49	0.44
2:I:4571:PHE:O	2:I:4575:PHE:N	2.46	0.44
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.98	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.98	0.44
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.44
1:A:7:ILE:N	1:A:71:ARG:O	2.47	0.44
2:B:1247:PRO:HA	2:B:1598:GLN:HA	2.00	0.44
2:B:4231:MET:HE1	2:B:4960:ILE:HA	2.00	0.44
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	1.99	0.44
2:E:357:LEU:HD12	2:E:388:LEU:HD11	2.00	0.44
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.82	0.44
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.53	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.41	0.44
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.44
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.35	0.44
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.42	0.44
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	2.00	0.44
2:E:4959:PHE:CG	2:E:4959:PHE:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.44
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	1.99	0.44
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.53	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.00	0.44
2:G:756:SER:HB3	2:G:767:VAL:HG22	2.00	0.44
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.88	0.44
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.13	0.44
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.00	0.44
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.44
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.39	0.44
2:G:485:SER:HA	2:G:488:LEU:HB2	1.99	0.44
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.98	0.44
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	1.99	0.44
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.83	0.44
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.44
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.88	0.44
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.44
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.00	0.44
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.00	0.44
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.00	0.44
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.51	0.44
2:E:756:SER:HB3	2:E:767:VAL:HG22	2.00	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.49	0.44
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.99	0.44
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.41	0.44
2:I:485:SER:HA	2:I:488:LEU:HB2	1.99	0.44
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.44
2:G:4231:MET:HE1	2:G:4960:ILE:HA	2.00	0.44
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.44
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.81	0.44
2:I:4959:PHE:CG	2:I:4959:PHE:O	2.70	0.44
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.00	0.44
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	2.00	0.44
2:E:1973:GLN:O	2:E:1977:TYR:N	2.49	0.44
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.53	0.44
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.00	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.51	0.44
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.44
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.99	0.44
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.51	0.44
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.53	0.43
2:E:286:THR:HA	2:E:405:HIS:HB2	2.00	0.43
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.39	0.43
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.82	0.43
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.42	0.43
2:G:488:LEU:O	2:G:492:ASP:N	2.48	0.43
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.99	0.43
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.83	0.43
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.70	0.43
2:E:485:SER:HA	2:E:488:LEU:HB2	1.99	0.43
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.99	0.43
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.82	0.43
2:I:357:LEU:HD12	2:I:388:LEU:HD11	2.00	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.82	0.43
2:I:4959:PHE:CD1	2:I:4959:PHE:O	2.70	0.43
2:I:756:SER:HB3	2:I:767:VAL:HG22	2.00	0.43
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.48	0.43
2:B:451:TYR:O	2:B:474:ARG:NH1	2.49	0.43
2:E:425:PRO:HA	2:E:506:TYR:HD1	1.83	0.43
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.43
2:E:5000:GLU:HA	2:E:5003:HIS:CD2	2.53	0.43
2:I:2257:LEU:O	2:I:2261:SER:N	2.51	0.43
2:I:475:GLN:NE2	2:I:531:ARG:O	2.42	0.43
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.34	0.43
2:E:2257:LEU:O	2:E:2261:SER:N	2.51	0.43
2:E:488:LEU:O	2:E:492:ASP:N	2.48	0.43
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.00	0.43
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	2.01	0.43
2:G:357:LEU:HD12	2:G:388:LEU:HD11	2.00	0.43
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	2.00	0.43
2:G:4822:THR:O	2:G:4825:THR:OG1	2.31	0.43
2:G:5000:GLU:HA	2:G:5003:HIS:CD2	2.53	0.43
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.54	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.43
2:I:876:GLU:O	2:I:880:GLU:N	2.50	0.43
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.84	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.51	0.43
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.82	0.43
2:B:5000:GLU:HA	2:B:5003:HIS:CD2	2.53	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:E:4822:THR:O	2:E:4825:THR:OG1	2.31	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.54	0.43
2:G:286:THR:HA	2:G:405:HIS:HB2	2.00	0.43
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	2.01	0.43
2:G:2004:GLU:HA	2:G:2007:ASN:HB2	1.99	0.43
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	2.00	0.43
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.81	0.43
2:I:5000:GLU:HA	2:I:5003:HIS:CD2	2.53	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.43
2:B:425:PRO:HA	2:B:506:TYR:HD1	1.83	0.43
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.43
2:G:161:GLU:HA	2:I:3984:ARG:HH22	1.83	0.43
2:I:1247:PRO:HA	2:I:1598:GLN:HA	2.00	0.43
2:I:1973:GLN:O	2:I:1977:TYR:N	2.49	0.43
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.33	0.43
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.54	0.43
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.01	0.43
2:B:3771:HIS:O	2:B:3774:GLY:N	2.48	0.43
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.43
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.01	0.43
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.48	0.43
2:B:4158:PRO:HA	2:B:4161:ARG:HB2	2.00	0.43
2:B:485:SER:HA	2:B:488:LEU:HB2	1.99	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.43
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.46	0.43
2:G:181:HIS:CE1	2:G:195:PHE:HB2	2.54	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	2.01	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.54	0.43
2:E:181:HIS:CE1	2:E:195:PHE:HB2	2.54	0.43
2:G:2107:GLN:NE2	2:G:3680:ALA:O	2.52	0.43
2:G:425:PRO:HA	2:G:506:TYR:HD1	1.83	0.43
1:J:23:VAL:H	1:J:105:ASN:HB3	1.84	0.43
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.88	0.43
2:B:286:THR:HA	2:B:405:HIS:HB2	2.00	0.42
2:B:2107:GLN:NE2	2:B:3680:ALA:O	2.52	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.48	0.42
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.33	0.42
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.01	0.42
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.01	0.42
2:I:2107:GLN:NE2	2:I:3680:ALA:O	2.52	0.42
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	2.00	0.42
2:I:425:PRO:HA	2:I:506:TYR:HD1	1.83	0.42
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.84	0.42
2:B:1817:GLU:O	2:B:1821:ASP:N	2.49	0.42
2:B:181:HIS:CE1	2:B:195:PHE:HB2	2.54	0.42
2:B:4658:ILE:HD11	2:B:4796:MET:HG3	2.01	0.42
2:B:488:LEU:O	2:B:492:ASP:N	2.48	0.42
2:B:756:SER:HB3	2:B:767:VAL:HG22	2.00	0.42
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.52	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.42
2:G:4658:ILE:HD11	2:G:4796:MET:HG3	2.00	0.42
2:I:1817:GLU:O	2:I:1821:ASP:N	2.49	0.42
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.01	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.02	0.42
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	2.01	0.42
2:I:181:HIS:CE1	2:I:195:PHE:HB2	2.54	0.42
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	2.00	0.42
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.01	0.42
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.01	0.42
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.48	0.42
2:G:4892:ARG:NH2	2:E:4899:ASP:OD1	2.52	0.42
1:F:23:VAL:H	1:F:105:ASN:HB3	1.85	0.42
2:G:1739:THR:H	2:G:1742:THR:HB	1.84	0.42
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.43	0.42
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.85	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
1:A:23:VAL:H	1:A:105:ASN:HB3	1.84	0.42
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.53	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.52	0.42
2:E:2107:GLN:NE2	2:E:3680:ALA:O	2.52	0.42
2:E:475:GLN:NE2	2:E:531:ARG:O	2.42	0.42
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.53	0.42
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	2.02	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.02	0.42
1:J:34:LYS:HE3	2:I:634:GLN:HB3	2.00	0.42
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.02	0.42
2:B:4017:LEU:HD22	2:B:4139:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1078:GLU:HB2	2:E:1235:THR:HG22	2.02	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:E:4017:LEU:HD22	2:E:4139:ILE:HG12	2.02	0.42
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.85	0.42
2:G:475:GLN:NE2	2:G:531:ARG:O	2.42	0.42
2:G:792:LEU:HD22	2:G:799:GLU:H	1.83	0.42
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.53	0.42
2:I:1739:THR:H	2:I:1742:THR:HB	1.85	0.42
2:I:286:THR:HA	2:I:405:HIS:HB2	2.00	0.42
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.42	0.42
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.42
2:B:471:LEU:O	2:B:475:GLN:N	2.47	0.42
2:B:540:PHE:HD2	2:B:567:VAL:HG11	1.85	0.42
2:B:792:LEU:HD22	2:B:799:GLU:H	1.83	0.42
2:E:1739:THR:H	2:E:1742:THR:HB	1.85	0.42
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	2.02	0.42
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.02	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.52	0.42
2:G:4231:MET:HE3	2:G:4960:ILE:HA	2.02	0.42
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.84	0.42
1:H:23:VAL:H	1:H:105:ASN:HB3	1.85	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.88	0.42
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.42
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.53	0.42
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.85	0.42
2:G:4017:LEU:HD22	2:G:4139:ILE:HG12	2.02	0.42
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	2.00	0.42
2:I:540:PHE:HD2	2:I:567:VAL:HG11	1.85	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.02	0.42
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.85	0.42
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.84	0.42
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.01	0.42
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.48	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.42
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.85	0.42
2:E:54:ASN:O	2:E:58:VAL:N	2.44	0.42
2:E:792:LEU:HD22	2:E:799:GLU:H	1.83	0.42
2:G:730:VAL:O	2:G:735:GLN:NE2	2.53	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1747:LEU:HD13	2:I:1760:HIS:CE1	2.55	0.42
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.02	0.42
2:I:924:MET:O	2:I:928:THR:OG1	2.34	0.42
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.02	0.42
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.85	0.41
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.41
2:B:730:VAL:O	2:B:735:GLN:NE2	2.53	0.41
2:E:730:VAL:O	2:E:735:GLN:NE2	2.53	0.41
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.52	0.41
2:B:1078:GLU:HB2	2:B:1235:THR:HG22	2.02	0.41
2:B:1747:LEU:HD13	2:B:1760:HIS:CE1	2.55	0.41
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.86	0.41
2:G:1817:GLU:O	2:G:1821:ASP:N	2.49	0.41
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.02	0.41
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.41
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.03	0.41
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.41
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.85	0.41
2:I:3677:LEU:O	2:I:3698:LEU:N	2.51	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.52	0.41
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.49	0.41
2:E:4658:ILE:HD11	2:E:4796:MET:HG3	2.01	0.41
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.49	0.41
2:G:540:PHE:HD2	2:G:567:VAL:HG11	1.85	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:I:792:LEU:HD22	2:I:799:GLU:H	1.83	0.41
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.02	0.41
2:B:4231:MET:HE3	2:B:4960:ILE:HA	2.02	0.41
2:B:475:GLN:NE2	2:B:531:ARG:O	2.42	0.41
2:E:3847:PHE:HD1	2:E:3850:GLN:HE21	1.69	0.41
2:G:4899:ASP:OD1	2:I:4892:ARG:NH2	2.52	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.41
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	2.02	0.41
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.86	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.03	0.41
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:E:1747:LEU:HD13	2:E:1760:HIS:CE1	2.55	0.41
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.03	0.41
2:G:3847:PHE:HD1	2:G:3850:GLN:HE21	1.69	0.41
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.48	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.41
2:I:3847:PHE:HD1	2:I:3850:GLN:HE21	1.69	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.41
1:J:7:ILE:N	1:J:71:ARG:O	2.47	0.41
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.41
2:B:4821:LYS:HB3	2:B:4821:LYS:HE2	1.95	0.41
2:E:4848:VAL:O	2:E:4852:THR:OG1	2.28	0.41
2:E:4928:LEU:HA	2:E:4928:LEU:HD13	1.90	0.41
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.41
2:G:1078:GLU:HB2	2:G:1235:THR:HG22	2.02	0.41
2:G:1747:LEU:HD13	2:G:1760:HIS:CE1	2.55	0.41
2:I:1078:GLU:HB2	2:I:1235:THR:HG22	2.02	0.41
2:I:4658:ILE:HD11	2:I:4796:MET:HG3	2.01	0.41
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	2.02	0.41
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.03	0.41
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.85	0.41
2:I:4017:LEU:HD22	2:I:4139:ILE:HG12	2.02	0.41
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.85	0.41
2:I:892:THR:N	2:I:902:ARG:O	2.52	0.41
2:B:1739:THR:H	2:B:1742:THR:HB	1.85	0.41
2:B:4222:VAL:HG23	2:B:4950:VAL:HG12	2.02	0.41
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.41
2:E:540:PHE:HD2	2:E:567:VAL:HG11	1.85	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.03	0.41
2:I:1716:ILE:HG23	2:I:1720:LEU:HD13	2.03	0.41
2:I:3771:HIS:O	2:I:3774:GLY:N	2.48	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.03	0.41
2:B:3677:LEU:O	2:B:3698:LEU:N	2.51	0.41
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.03	0.41
2:E:2034:PHE:O	2:E:2038:LEU:N	2.54	0.41
1:F:7:ILE:N	1:F:71:ARG:O	2.47	0.41
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.86	0.41
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.54	0.41
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.33	0.41
2:I:730:VAL:O	2:I:735:GLN:NE2	2.53	0.41
2:B:3676:ASP:N	2:B:3676:ASP:OD1	2.54	0.41
2:B:3847:PHE:HD1	2:B:3850:GLN:HE21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.44	0.41
2:E:3677:LEU:O	2:E:3698:LEU:N	2.51	0.41
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.38	0.41
2:G:119:SER:HA	2:G:146:CYS:HA	2.03	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.02	0.41
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.54	0.41
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.49	0.41
2:B:1657:LEU:HD13	2:B:1657:LEU:HA	1.95	0.40
2:B:4822:THR:O	2:B:4825:THR:OG1	2.31	0.40
2:B:512:ALA:HA	2:B:515:TRP:HB2	2.03	0.40
2:B:16:THR:OG1	2:B:97:GLY:O	2.39	0.40
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.02	0.40
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.86	0.40
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.40
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.41	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.85	0.40
2:I:1641:ILE:HA	2:I:1642:PRO:HD3	1.92	0.40
2:I:16:THR:OG1	2:I:97:GLY:O	2.39	0.40
2:B:2029:GLN:O	2:B:2033:ASP:N	2.50	0.40
2:B:4697:VAL:O	2:B:4701:TRP:N	2.50	0.40
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.02	0.40
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.04	0.40
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.04	0.40
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.40
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.03	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.50	0.40
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.40
2:B:1685:LEU:HD22	2:B:1718:ILE:HG21	2.03	0.40
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.86	0.40
2:B:2437:ALA:HA	2:B:2438:PRO:HD3	1.95	0.40
2:B:4710:SER:HB3	2:B:4713:SER:HB3	2.03	0.40
2:G:983:THR:O	2:G:987:ARG:N	2.52	0.40
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	2.03	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.47	0.40
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.04	0.40
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.86	0.40
2:E:4984:ASN:C	2:E:4986:ALA:H	2.23	0.40
2:G:1592:PRO:HA	2:G:1593:PRO:HD3	1.98	0.40
2:G:1716:ILE:HG23	2:G:1720:LEU:HD13	2.03	0.40
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.86	0.40
2:G:512:ALA:HA	2:G:515:TRP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.04	0.40
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.86	0.40
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.40
2:I:983:THR:O	2:I:987:ARG:N	2.52	0.40
2:B:119:SER:HA	2:B:146:CYS:HA	2.03	0.40
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.03	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.55	0.40
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.87	0.40
2:B:907:LEU:O	2:B:963:ASN:ND2	2.40	0.40
2:E:2029:GLN:O	2:E:2033:ASP:N	2.50	0.40
2:E:321:GLU:HB3	2:E:322:LYS:H	1.76	0.40
2:E:472:ARG:HA	2:E:475:GLN:HB2	2.03	0.40
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.40
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.40
2:I:2034:PHE:O	2:I:2038:LEU:N	2.54	0.40
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	338 (10%)	7 (0%)	52	86
2	E	3235/4416 (73%)	2888 (89%)	340 (10%)	7 (0%)	52	86
2	G	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	52	86
All	All	13360/18096 (74%)	11932 (89%)	1400 (10%)	28 (0%)	56	86

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU
2	B	4962	GLY
2	B	4985	LEU
2	G	4641	PRO
2	G	4962	GLY
2	G	4985	LEU
2	I	4641	PRO
2	I	4962	GLY
2	I	4985	LEU
2	E	4962	GLY
2	B	1840	PRO
2	B	4641	PRO
2	G	1840	PRO
2	I	1840	PRO
2	E	1840	PRO
2	E	4641	PRO
2	B	2291	GLN
2	G	2291	GLN
2	I	2291	GLN
2	E	2291	GLN
2	B	1932	PRO
2	G	1932	PRO
2	I	1932	PRO
2	E	1932	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%)	2474 (99%)	19 (1%)	86	93
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	89	94

All (76) 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	978	THR
2	B	1076	ARG
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	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4166	LEU
2	B	4961	CYS
2	B	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG

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Mol	Chain	Res	Type
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
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	4166	LEU
2	G	4961	CYS
2	G	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	978	THR
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	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4166	LEU
2	I	4961	CYS
2	I	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU

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Mol	Chain	Res	Type
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4166	LEU
2	E	4961	CYS
2	E	4983	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) 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	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	725	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1691	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN

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Mol	Chain	Res	Type
2	B	3960	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4806	ASN
2	B	4833	ASN
2	B	4978	HIS
2	B	4983	HIS
2	B	5003	HIS
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN
2	G	479	GLN
2	G	725	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1691	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3900	GLN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4806	ASN
2	G	4833	ASN
2	G	4978	HIS
2	G	4983	HIS
2	G	5003	HIS

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Mol	Chain	Res	Type
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	479	GLN
2	I	725	HIS
2	I	838	HIS
2	I	1598	GLN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3900	GLN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4806	ASN
2	I	4833	ASN
2	I	4978	HIS
2	I	4983	HIS
2	I	5003	HIS
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	479	GLN
2	E	725	HIS
2	E	838	HIS
2	E	1598	GLN

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Mol	Chain	Res	Type
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2127	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4806	ASN
2	E	4833	ASN
2	E	4978	HIS
2	E	4983	HIS
2	E	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 16 ligands modelled in this entry, 8 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	-	26,33,33	0.92	1 (3%)	26,52,52	1.58	2 (7%)
4	CFF	B	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.23	1 (12%)
3	ATP	E	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.59	2 (7%)
4	CFF	E	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.22	1 (12%)
3	ATP	G	5101	-	26,33,33	0.92	1 (3%)	26,52,52	1.58	2 (7%)
4	CFF	G	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.23	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.58	2 (7%)
4	CFF	I	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.22	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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C4-N3	-4.43	1.34	1.39
4	B	5102	CFF	C4-N3	-4.42	1.34	1.39
4	I	5102	CFF	C4-N3	-4.42	1.34	1.39
4	G	5102	CFF	C4-N3	-4.39	1.34	1.39
4	G	5102	CFF	C6-N1	-4.10	1.32	1.38
4	B	5102	CFF	C6-N1	-4.07	1.32	1.38
4	E	5102	CFF	C6-N1	-4.07	1.32	1.38
4	I	5102	CFF	C6-N1	-4.06	1.32	1.38
4	I	5102	CFF	O13-C6	-2.38	1.18	1.24
4	B	5102	CFF	O13-C6	-2.35	1.18	1.24
4	G	5102	CFF	O13-C6	-2.35	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	O13-C6	-2.34	1.18	1.24
3	G	5101	ATP	C5-C4	2.94	1.47	1.40
3	E	5101	ATP	C5-C4	2.95	1.47	1.40
3	B	5101	ATP	C5-C4	2.95	1.47	1.40
3	I	5101	ATP	C5-C4	2.96	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-5.95	124.20	128.87
3	B	5101	ATP	N3-C2-N1	-5.91	124.23	128.87
3	G	5101	ATP	N3-C2-N1	-5.89	124.25	128.87
3	I	5101	ATP	N3-C2-N1	-5.88	124.26	128.87
4	E	5102	CFF	C14-N7-C8	-2.56	111.94	125.31
4	B	5102	CFF	C14-N7-C8	-2.56	111.96	125.31
4	G	5102	CFF	C14-N7-C8	-2.55	111.98	125.31
4	I	5102	CFF	C14-N7-C8	-2.55	111.99	125.31
3	G	5101	ATP	C4'-O4'-C1'	2.24	112.02	109.64
3	B	5101	ATP	C4'-O4'-C1'	2.26	112.04	109.64
3	I	5101	ATP	C4'-O4'-C1'	2.29	112.07	109.64
3	E	5101	ATP	C4'-O4'-C1'	2.30	112.08	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	E	5101	ATP	1	0
3	G	5101	ATP	1	0
3	I	5101	ATP	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	73.47
1	G	4345:UNK	C	4540:PHE	N	73.47
1	I	4345:UNK	C	4540:PHE	N	73.47
1	E	4345:UNK	C	4540:PHE	N	73.47
1	B	3613:UNK	C	3639:THR	N	45.62
1	G	3613:UNK	C	3639:THR	N	45.62
1	I	3613:UNK	C	3639:THR	N	45.62
1	E	3613:UNK	C	3639:THR	N	45.62
1	B	4253:GLU	C	4320:UNK	N	27.90
1	G	4253:GLU	C	4320:UNK	N	27.90
1	I	4253:GLU	C	4320:UNK	N	27.90
1	E	4253:GLU	C	4320:UNK	N	27.90
1	B	3163:UNK	C	3170:UNK	N	15.83
1	G	3163:UNK	C	3170:UNK	N	15.83
1	I	3163:UNK	C	3170:UNK	N	15.83
1	E	3163:UNK	C	3170:UNK	N	15.83
1	B	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.87
1	I	3063:UNK	C	3134:UNK	N	14.87
1	E	3063:UNK	C	3134:UNK	N	14.87
1	B	3468:UNK	C	3511:UNK	N	14.52
1	G	3468:UNK	C	3511:UNK	N	14.52
1	I	3468:UNK	C	3511:UNK	N	14.52
1	E	3468:UNK	C	3511:UNK	N	14.52
1	B	2703:UNK	C	2734:ASN	N	13.45
1	G	2703:UNK	C	2734:ASN	N	13.45
1	I	2703:UNK	C	2734:ASN	N	13.45
1	E	2703:UNK	C	2734:ASN	N	13.45
1	B	3236:UNK	C	3241:UNK	N	12.87
1	G	3236:UNK	C	3241:UNK	N	12.87
1	I	3236:UNK	C	3241:UNK	N	12.87
1	E	3236:UNK	C	3241:UNK	N	12.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1564:UNK	C	1573:MET	N	12.40
1	G	1564:UNK	C	1573:MET	N	12.40
1	I	1564:UNK	C	1573:MET	N	12.40
1	E	1564:UNK	C	1573:MET	N	12.40
1	B	2976:UNK	C	2995:UNK	N	12.24
1	G	2976:UNK	C	2995:UNK	N	12.24
1	I	2976:UNK	C	2995:UNK	N	12.24
1	E	2976:UNK	C	2995:UNK	N	12.24
1	B	3254:UNK	C	3261:UNK	N	8.57
1	G	3254:UNK	C	3261:UNK	N	8.57
1	I	3254:UNK	C	3261:UNK	N	8.57
1	E	3254:UNK	C	3261:UNK	N	8.57
1	B	1297:UNK	C	1430:UNK	N	5.81
1	G	1297:UNK	C	1430:UNK	N	5.81
1	I	1297:UNK	C	1430:UNK	N	5.81
1	E	1297:UNK	C	1430:UNK	N	5.81
1	B	2939:ARG	C	2942:UNK	N	3.33
1	G	2939:ARG	C	2942:UNK	N	3.33
1	I	2939:ARG	C	2942:UNK	N	3.33
1	E	2939:ARG	C	2942:UNK	N	3.33
1	B	2479:LEU	C	2487:UNK	N	3.30
1	G	2479:LEU	C	2487:UNK	N	3.30
1	I	2479:LEU	C	2487:UNK	N	3.30
1	E	2479:LEU	C	2487:UNK	N	3.30