



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 01:13 pm GMT

PDB ID : 5TAP
EMDB ID: : EMD-8381
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.40 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

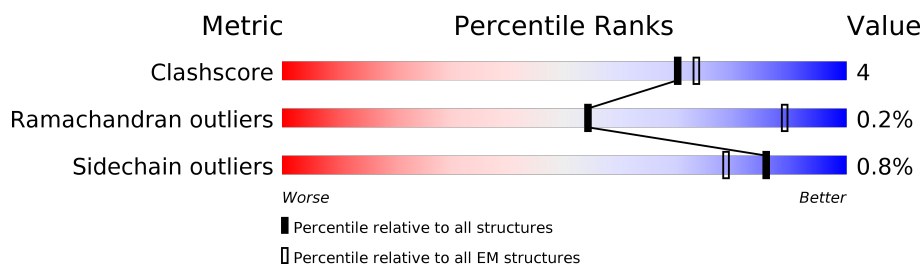
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

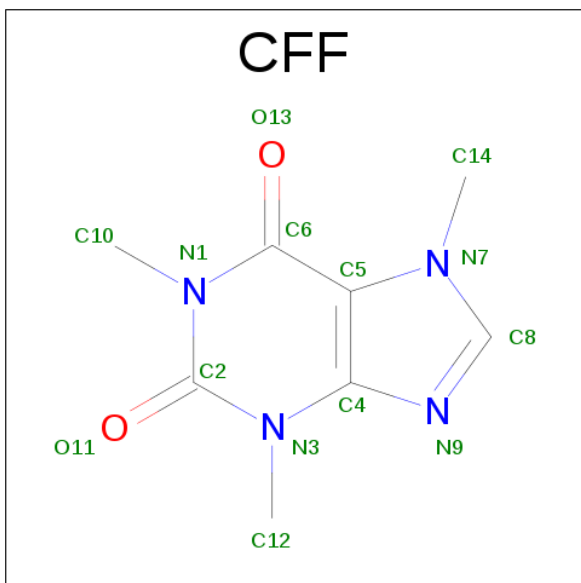
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is 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	E	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	G	1	Total 31	C 10	N 5	O 13	P 3	0

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



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


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

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

3 Residue-property plots


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

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

Chain F: 




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

Chain A: 




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

Chain H: 




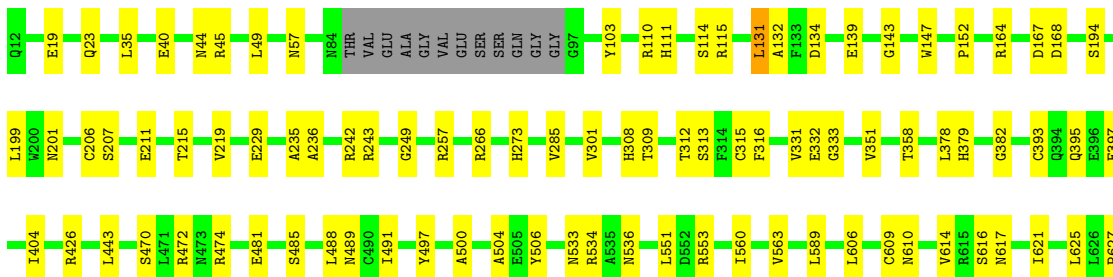
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

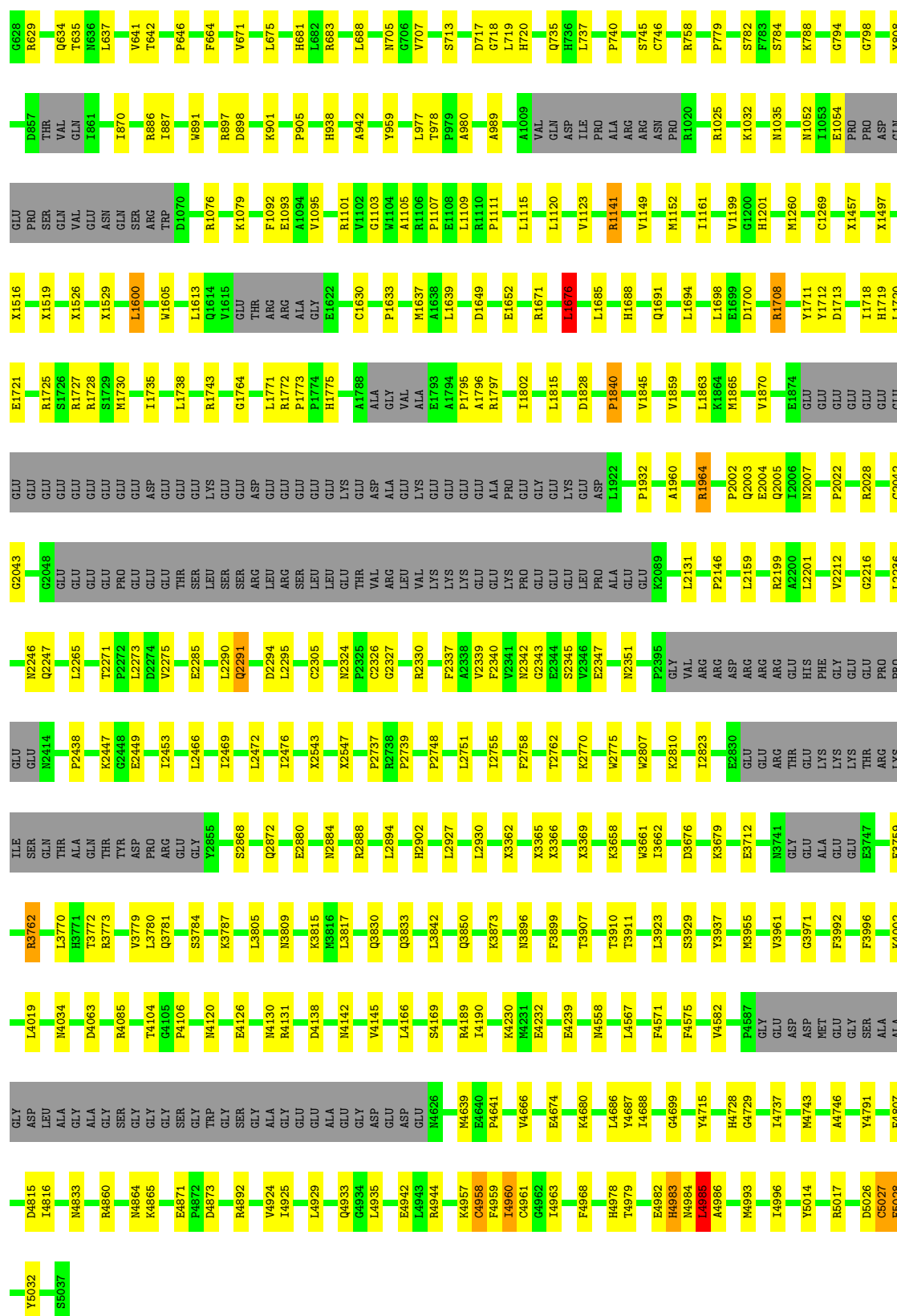
Chain J: 



- Molecule 2: Ryanodine receptor 1

Chain B: 



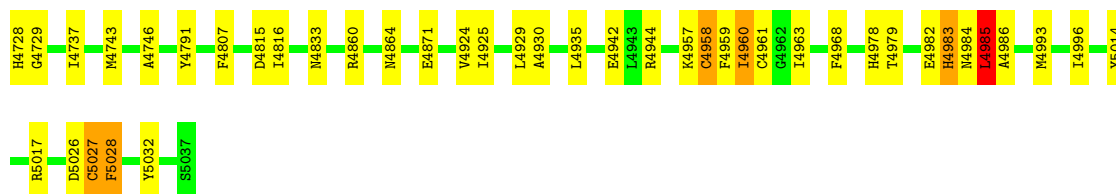


- Molecule 2: Ryanodine receptor 1

Chain E:

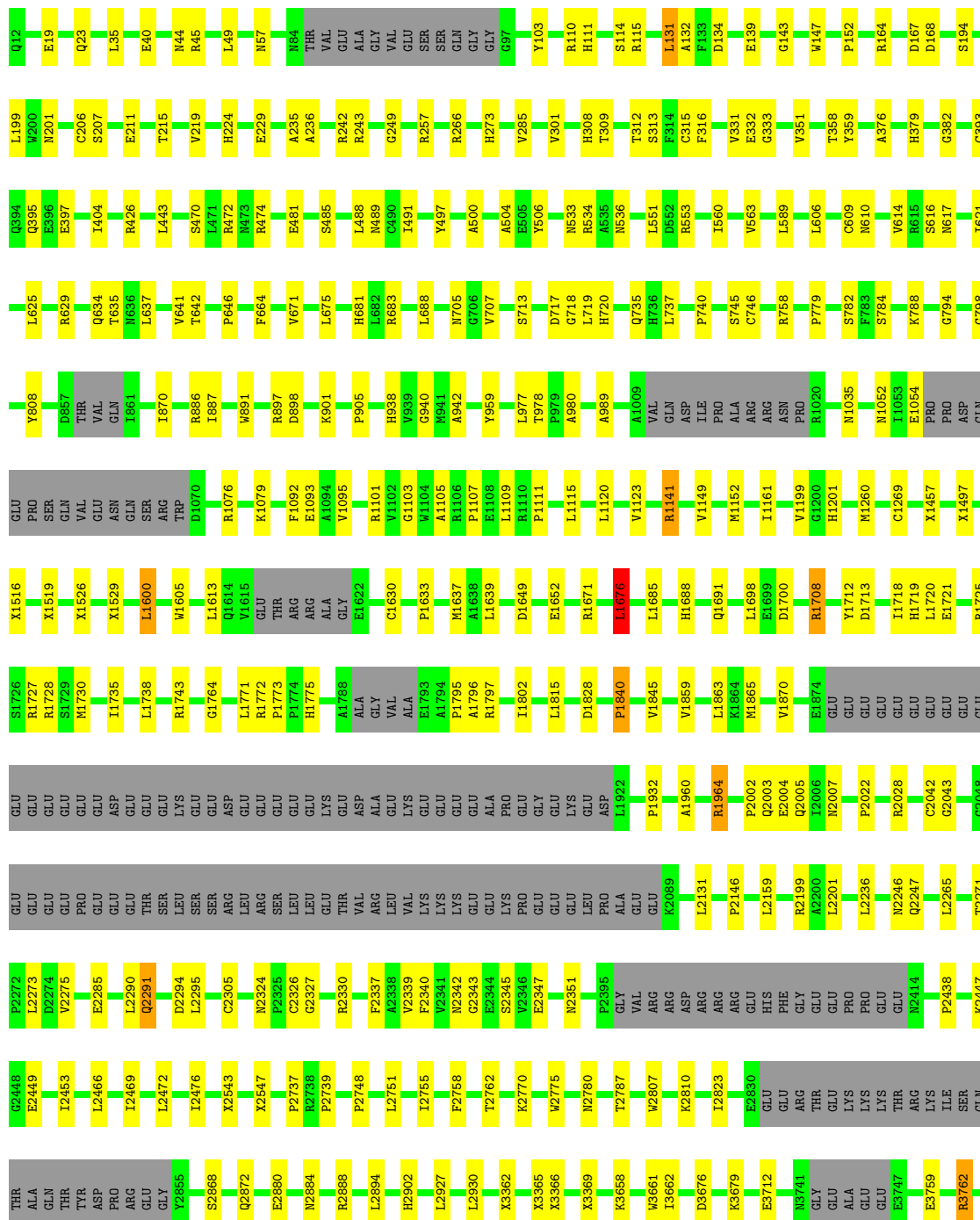




• Molecule 2: Ryanodine receptor 1

Chain I: 86% 9% 5%





L2236	C2042	GLU	I1718	X1497	SER	THR	T635	E397	C206	Q12
N2246	G2043	GLU	H1719	X1516	VAL	VAL	H636	S207	E19	
Q2247	G2048	GLU	E1721	X1519	GLU	GLU	L637	E211	Q23	
L2257	GLU	GLU	R1725	X1526	ASN	ASN	V641	R426	E40	
L2265	GLU	GLU	S1726	X1529	GLN	GLN	T642	L443	N44	
T2271	PRO	GLU	R1727	X1529	ARG	ARG	P646	S470	R445	
P2272	GLU	GLU	S1729	D1070	THR	THR	F664	L471	H224	
L2273	GLU	ASP	M1730	L1600	GLU	GLU	R897	R472	E229	
D2274	THR	GLU	I1735	W1605	R1073	R1073	V671	W473	N57	
V2275	SER	GLU	L1738	M1608	R1076	R1076	L675	R474	N54	
A2276	LEU	GLU	L1738	M1608	LYS	LYS	P905	E481	THR	
E2285	SER	GLU	R1743	L1613	K1079	K1079	H681	S485	VAL	
L2290	ARG	ASP	G1764	Q1614	E1092	H938	L682	R242	GLU	
Q2291	LEU	GLU	GLU	V1615	E1093	V939	R683	R243	ALA	
D2294	SER	GLU	L1771	THR	GLU	GLU	L689	L488	GLY	
L2295	LEU	GLU	R1772	ARG	V1095	H941	G940	M489	VAL	
L2295	LEU	GLU	P1773	ARG	ARG	A942	N705	C490	GLU	
C2326	GLU	LYS	P1774	ALA	R1101	Y959	G706	I491	SER	
G2327	THR	GLU	H1775	GLY	G1103	Y959	V707	Y497	SER	
R2330	VAL	ASP	A1788	E1632	W1104	L977	S713	A500	GLN	
F2337	ARG	GLU	ALA	C1630	A1105	T978	D717	H273	GLY	
A2338	LEU	LYS	GLY	P1633	R1106	P979	G718	V285	G97	
Z2339	VAL	GLU	VAL	GLU	P1107	A980	L719	Y301	Y103	
V2341	LYS	GLU	ALA	P1693	E1108	A989	H720	R534	R110	
N2342	PRO	GLU	R1797	M1637	R1110	A1009	Q735	H308	H111	
C2343	GLU	GLU	E1793	A1638	P1111	VAL	H736	T309	S114	
E2344	GLU	ALA	P1795	L1639	L1115	GLN	L737	T312	R115	
S2345	PRO	GLU	A1796	D1649	L1120	ASP	P740	S313	L131	
V2346	GLU	GLU	I1802	E1652	L1123	ILE	L575	F314	F133	
E2347	LYS	GLU	L1815	R1671	V1123	PRO	S745	C315	D134	
N2351	PRO	ASP	D1828	R1676	R1141	ARG	C746	L589	E139	
P2395	ALA	L1922	L1676	L1676	VAL	ASN	R758	L606	G43	
GLY	GLU	P1932	G1677	V1149	V1149	PRO	P779	E332	W147	
VAL	GLU	A1960	L1685	M1152	M1152	R1020	N610	G333	P152	
ARG	L2131	V1845	H1688	I1161	I1161	R1025	S782	V351	R164	
ARG	P2146	V1859	Q1691	V1199	V1199	K1032	F783	T358	D168	
ARG	L2159	L1863	L1698	H1201	H1201	M1035	S784	Y359	P152	
ARG	Q2003	Q2003	E1699	G1200	G1200	M1052	K788	A376	R164	
GLU	R2199	E2004	D1700	E1699	E1699	N1053	G794	I621	D167	
HIS	A2200	L2066	E1674	D1700	T1236	I1053	G798	H379	D168	
PHE	L2201	N2007	GLU	R1708	M1280	E1054	L625	L825	S194	
GLY	V2212	P2022	GLU	Y1711	C1269	PRO	P627	L625	L199	
GLU	G2216	R2028	GLU	Y1712	GLU	ASP	Y808	G628	W200	
PRO			GLU	D1713	X1457	GLN	G541	R629	N201	
			GLU			GLU	Y857	Y624	N201	

D4873	ALA	P4106	V3779	SER	GLU
V4924	GLY	M4120	L3780	GLN	GLU
I4925	GLU	M4126	Q3781	THR	N2414
L4929	ALA	E4126	S3784	ALA	P2438
A4930	GLY	M4130	K3787	GLN	K2447
Q4933	GLY	R4131	L3805	TYR	G2446
G4934	ASP	D4138	N3809	ASP	E2449
L4935	GLU	M4142	K3815	PRO	I2453
E4942	ASP	V4145	M3816	ARG	GLY
L4945	GLU	L4166	L3817	GLY	L2466
R4944	P4641	S4169	Q3830	Y2855	I2469
K4951	V4666	R4189	Q3833	Q2872	L2472
K4957	E4674	I4190	L3842	N2884	I2476
C4958	K4680	K4230	Q3850	R2889	P2737
I4960	L4686	L4567	K3873	L2927	R2738
C4961	Y4687	F4571	N3896	L2930	P2739
G4962	I4688	F4575	F3899	L2742	T2742
I4963	Q4700	V4582	T3907	X3362	P2748
F4968	W4701	P4587	T3910	X3365	L2751
H4978	Y4715	GLY	T3911	X3366	L2755
T4979	H4728	GLU	L3923	X3369	F2758
E4982	G4729	ASP	S3929	K3658	T2762
H4983	I4737	ASP	Y3937	W3661	K2770
M4984	M4743	MET	M3955	D3676	W2775
A4986	A4746	GLU	V3961	K3679	W2807
M4993	Y4791	GLY	G3971	E3712	K2810
I4996	F4807	ASP	K4002	N3741	E2811
D5026	D4815	LEU	L4019	GLY	I2823
C5027	I4816	ALA	M4034	GLU	E2830
F5028	M4833	GLY	D4063	ALA	GLU
Y5032	R4860	SER	R4085	GLU	ARG
S5037	M4864	GLY	T4104	E3747	THR
	K4865	GLY	G4105	THR	ARG
	E4871	TRP		E3759	LYS
	P4872	GLY		R3762	LYS
		SER		L3770	THR
		GLY		H3771	ARG
				T3772	LYS
				R3773	ILE

4 Experimental information

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.32	0/834	0.51	0/1123
1	F	0.32	0/834	0.51	0/1123
1	H	0.32	0/834	0.51	0/1123
1	J	0.32	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.54	36/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	15
2	E	0	15
2	G	0	15
2	I	0	15
All	All	0	64

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2476	ILE	C-N	5.37	1.44	1.34
2	B	2476	ILE	C-N	5.34	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2476	ILE	C-N	5.33	1.44	1.34
2	G	2476	ILE	C-N	5.30	1.44	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.29	134.37	115.30
2	G	131	LEU	CA-CB-CG	8.28	134.35	115.30
2	B	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	E	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	G	1600	LEU	CA-CB-CG	7.05	131.52	115.30
2	I	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	E	1600	LEU	CA-CB-CG	7.03	131.48	115.30
2	I	1676	LEU	CA-CB-CG	6.55	130.37	115.30
2	B	1676	LEU	CA-CB-CG	6.54	130.33	115.30
2	G	1676	LEU	CA-CB-CG	6.52	130.31	115.30
2	E	1676	LEU	CA-CB-CG	6.51	130.28	115.30
2	I	4985	LEU	CA-CB-CG	6.23	129.63	115.30
2	G	4985	LEU	CA-CB-CG	6.23	129.63	115.30
2	B	4985	LEU	CA-CB-CG	6.22	129.60	115.30
2	E	4985	LEU	CA-CB-CG	6.22	129.60	115.30
2	G	977	LEU	CA-CB-CG	5.37	127.64	115.30
2	G	688	LEU	CA-CB-CG	5.36	127.63	115.30
2	B	977	LEU	CA-CB-CG	5.35	127.61	115.30
2	I	977	LEU	CA-CB-CG	5.35	127.61	115.30
2	I	688	LEU	CA-CB-CG	5.35	127.60	115.30
2	E	977	LEU	CA-CB-CG	5.34	127.59	115.30
2	B	688	LEU	CA-CB-CG	5.33	127.57	115.30
2	E	688	LEU	CA-CB-CG	5.33	127.57	115.30
2	E	3770	LEU	CA-CB-CG	5.12	127.07	115.30
2	B	3770	LEU	CA-CB-CG	5.12	127.06	115.30
2	G	3770	LEU	CA-CB-CG	5.11	127.04	115.30
2	I	3770	LEU	CA-CB-CG	5.10	127.03	115.30
2	I	2290	LEU	CA-CB-CG	5.08	126.97	115.30
2	E	2290	LEU	CA-CB-CG	5.07	126.95	115.30
2	B	2290	LEU	CA-CB-CG	5.06	126.95	115.30
2	G	2290	LEU	CA-CB-CG	5.06	126.94	115.30
2	I	4639	MET	C-N-CA	5.05	134.32	121.70
2	G	4639	MET	C-N-CA	5.03	134.27	121.70
2	E	4639	MET	C-N-CA	5.03	134.27	121.70
2	B	4639	MET	C-N-CA	5.03	134.26	121.70

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts [i](#)

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	8	0
1	F	818	0	824	8	0
1	H	818	0	824	9	0
1	J	818	0	824	8	0
2	B	29499	0	24749	236	0
2	E	29499	0	24749	235	0
2	G	29499	0	24749	231	0
2	I	29499	0	24749	233	0
3	B	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	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
All	All	121452	0	102380	949	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 4.

All (949) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.38	0.88
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.38	0.88
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.38	0.87
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.38	0.87
2:B:4983:HIS:H	2:B:4983:HIS:CD2	1.94	0.86
2:G:4983:HIS:H	2:G:4983:HIS:CD2	1.94	0.86
2:I:4983:HIS:CD2	2:I:4983:HIS:H	1.94	0.84
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	1.92	0.83
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	1.92	0.82
2:E:4983:HIS:H	2:E:4983:HIS:CD2	1.94	0.82
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	1.92	0.82
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.15	0.81
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	1.92	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.15	0.80
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.29	0.79
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.29	0.77
2:I:4983:HIS:HD2	2:I:4983:HIS:H	1.29	0.77
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.29	0.77
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.77	0.73
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.77	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.77	0.72
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.77	0.72
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.04	0.72
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.04	0.71
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.04	0.71
2:B:4960:ILE:HD13	2:B:4960:ILE:N	2.04	0.71
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.61	0.69
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.61	0.68
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.61	0.68
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.61	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.67
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.67
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.67
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.78	0.66
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.78	0.66
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.61	0.65
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.61	0.65
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.61	0.64
2:G:379:HIS:HD2	2:G:382:GLY:H	1.45	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.62	0.64
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.78	0.64
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.80	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.61	0.64
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.80	0.64
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.78	0.64
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.63	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.80	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.63
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.81	0.63
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.81	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.80	0.63
2:E:379:HIS:HD2	2:E:382:GLY:H	1.45	0.63
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.81	0.63
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.64	0.63
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.64	0.63
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.81	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.63	0.63
2:B:379:HIS:HD2	2:B:382:GLY:H	1.45	0.63
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.64	0.62
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.81	0.62
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.81	0.62
2:G:4982:GLU:HB3	2:G:4983:HIS:HD2	1.65	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.63	0.62
2:E:4982:GLU:HB3	2:E:4983:HIS:HD2	1.65	0.62
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.62
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.81	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.33	0.62
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.64	0.61
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.61
2:B:4982:GLU:HB3	2:B:4983:HIS:HD2	1.65	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.81	0.61
2:I:4982:GLU:HB3	2:I:4983:HIS:HD2	1.65	0.61
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.61
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.65	0.61
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.61
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.61
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.33	0.61
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.66	0.61
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	2.14	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.33	0.60
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.83	0.60
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	2.14	0.60
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.66	0.60
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.60
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.33	0.60
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.60
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.60
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.60
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.65	0.60
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	2.14	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.60
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.60
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	2.14	0.60
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.83	0.59
2:B:4979:THR:HG22	3:B:5101:ATP:H2	1.67	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4979:THR:HG22	3:I:5101:ATP:H2	1.67	0.59
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.65	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.83	0.59
2:B:132:ALA:HA	2:B:194:SER:HB2	1.84	0.59
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.85	0.59
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.67	0.59
2:E:132:ALA:HA	2:E:194:SER:HB2	1.84	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.85	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.85	0.59
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.85	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.58
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.86	0.58
2:I:4190:ILE:HD13	2:I:5026:ASP:CG	2.24	0.58
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.22	0.58
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.22	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.58
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.85	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.85	0.58
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.85	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.58
2:G:4979:THR:HG22	3:G:5101:ATP:H2	1.67	0.58
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.85	0.58
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.22	0.58
2:E:4979:THR:HG22	3:E:5101:ATP:H2	1.67	0.58
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:E:4190:ILE:HD13	2:E:5026:ASP:CG	2.24	0.58
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.57
2:B:4190:ILE:HD13	2:B:5026:ASP:CG	2.24	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.86	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.57
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.86	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.85	0.57
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.85	0.57
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.57
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.22	0.57
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.86	0.57
2:G:132:ALA:HA	2:G:194:SER:HB2	1.84	0.57
2:G:4190:ILE:HD13	2:G:5026:ASP:CG	2.24	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.57
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.86	0.57
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.78	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.87	0.57
2:I:132:ALA:HA	2:I:194:SER:HB2	1.84	0.57
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.87	0.57
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.87	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.78	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.87	0.57
2:E:4968:PHE:CZ	2:E:4978:HIS:ND1	2.73	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.87	0.57
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.86	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.56
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.86	0.56
2:B:4968:PHE:CZ	2:B:4978:HIS:ND1	2.73	0.56
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.86	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.56
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.87	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.70	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.78	0.56
2:G:4968:PHE:CZ	2:G:4978:HIS:ND1	2.73	0.56
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.88	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.86	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.56
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.56
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.86	0.56
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.87	0.56
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.86	0.56
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.88	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.56
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	2.54	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.56
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.88	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.86	0.56
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.88	0.56
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.56
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.86	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.88	0.56
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.88	0.56
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.56
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.56
2:I:4968:PHE:CZ	2:I:4978:HIS:ND1	2.73	0.56
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.55
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.95	0.55
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.88	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.71	0.55
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.88	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.55
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.88	0.55
2:E:4190:ILE:CD1	2:E:5026:ASP:OD2	2.54	0.55
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.55
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.55
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.95	0.55
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.88	0.55
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.71	0.55
2:I:4190:ILE:CD1	2:I:5026:ASP:OD2	2.54	0.55
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.55
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.88	0.55
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.71	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.71	0.55
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	2.54	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.89	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.55
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.95	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.89	0.54
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.54
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.89	0.54
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.88	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.88	0.54
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.81	0.54
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.88	0.54
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.95	0.54
2:E:4190:ILE:CD1	2:E:5026:ASP:CG	2.76	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.41	0.54
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.88	0.54
2:I:4190:ILE:CD1	2:I:5026:ASP:CG	2.76	0.54
2:B:4190:ILE:CD1	2:B:5026:ASP:CG	2.76	0.54
2:G:4190:ILE:CD1	2:G:5026:ASP:CG	2.76	0.54
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.54
2:E:331:VAL:HG12	2:E:333:GLY:H	1.73	0.54
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.81	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.56	0.54
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.81	0.54
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.54
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.56	0.54
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.70	0.54
2:G:111:HIS:HD2	2:G:114:SER:H	1.56	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.90	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.26	0.53
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.26	0.53
2:G:794:GLY:H	2:G:798:GLY:HA3	1.73	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.53
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.90	0.53
2:I:794:GLY:H	2:I:798:GLY:HA3	1.73	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.53
2:B:331:VAL:HG12	2:B:333:GLY:H	1.73	0.53
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.91	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.56	0.53
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.41	0.53
2:B:794:GLY:H	2:B:798:GLY:HA3	1.73	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.91	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.90	0.53
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.53
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.73	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.91	0.53
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.26	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.53
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.53
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.74	0.53
2:E:794:GLY:H	2:E:798:GLY:HA3	1.74	0.53
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.53
2:G:331:VAL:HG12	2:G:333:GLY:H	1.73	0.53
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.26	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.73	0.53
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.92	0.52
2:B:2868:SER:O	2:B:2872:GLN:N	2.41	0.52
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.90	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.82	0.52
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.39	0.52
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.75	0.52
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.52
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.52
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.75	0.52
2:E:313:SER:HB3	2:E:351:VAL:HB	1.91	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.75	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.52
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.92	0.52
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.92	0.52
2:B:313:SER:HB3	2:B:351:VAL:HB	1.91	0.52
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.90	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.91	0.52
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.52
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.92	0.52
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.90	0.52
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.52
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.52
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:G:4979:THR:HG22	3:G:5101:ATP:C2	2.45	0.51
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.75	0.51
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.51
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.51
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.75	0.51
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:B:4979:THR:HG22	3:B:5101:ATP:C2	2.45	0.51
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.51
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.82	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.39	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.82	0.51
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.41	0.51
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.41	0.51
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.39	0.51
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.75	0.51
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.46	0.51
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.92	0.51
1:A:27:THR:HB	1:A:100:ASP:HB3	1.93	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.93	0.51
2:B:614:VAL:HG22	2:B:616:SER:H	1.75	0.51
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.82	0.51
2:E:4979:THR:HG22	3:E:5101:ATP:C2	2.45	0.51
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.93	0.51
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:G:614:VAL:HG22	2:G:616:SER:H	1.75	0.51
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.46	0.50
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.45	0.50
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.93	0.50
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.45	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.94	0.50
2:I:4979:THR:HG22	3:I:5101:ATP:C2	2.45	0.50
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.94	0.50
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.50
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.93	0.50
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.50
2:I:614:VAL:HG22	2:I:616:SER:H	1.75	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.41	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.50
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.93	0.50
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.30	0.50
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.50
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.50
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.50
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.50
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.50
2:E:614:VAL:HG22	2:E:616:SER:H	1.75	0.50
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.50
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.41	0.50
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.93	0.50
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.49
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.93	0.49
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.30	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.49
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.94	0.49
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.49
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.95	0.49
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.30	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.94	0.49
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.49
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.94	0.49
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.93	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.49
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.95	0.49
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.94	0.49
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.49
2:E:629:ARG:HD3	2:E:634:GLN:HG2	1.94	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.49
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.94	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.49
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.95	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.95	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.49
2:I:642:THR:HG23	2:I:1613:LEU:HD12	1.95	0.49
2:B:642:THR:HG23	2:B:1613:LEU:HD12	1.95	0.49
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.45	0.49
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.95	0.49
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.46	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.95	0.49
2:I:629:ARG:HD3	2:I:634:GLN:HG2	1.94	0.49
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.41	0.49
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.45	0.49
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.43	0.49
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.45	0.49
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.49
2:G:629:ARG:HD3	2:G:634:GLN:HG2	1.94	0.49
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.94	0.49
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.95	0.49
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.31	0.49
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.46	0.49
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.94	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.94	0.48
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.48
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.48
2:G:3842:LEU:O	2:G:3929:SER:OG	2.31	0.48
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.95	0.48
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.95	0.48
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.31	0.48
2:I:2868:SER:O	2:I:2872:GLN:N	2.41	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.45	0.48
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.96	0.48
2:I:2342:ASN:N	2:I:2342:ASN:OD1	2.45	0.48
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:B:629:ARG:HD3	2:B:634:GLN:HG2	1.94	0.48
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.95	0.48
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.46	0.48
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.93	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.32	0.48
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.95	0.48
2:G:642:THR:HG23	2:G:1613:LEU:HD12	1.95	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.48
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.30	0.48
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.96	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.46	0.48
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.96	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.48
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.96	0.48
2:I:3842:LEU:O	2:I:3929:SER:OG	2.31	0.48
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.95	0.48
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.45	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.94	0.48
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.79	0.48
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.46	0.48
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.95	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.31	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.32	0.48
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.79	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.31	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.94	0.47
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.47
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.79	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.96	0.47
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.96	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.47
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.28	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.46	0.47
2:E:3842:LEU:O	2:E:3929:SER:OG	2.31	0.47
2:E:642:THR:HG23	2:E:1613:LEU:HD12	1.95	0.47
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.39	0.47
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.80	0.47
2:E:111:HIS:CD2	2:E:114:SER:H	2.32	0.47
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.96	0.47
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.79	0.47
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.47
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.47
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.79	0.47
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.96	0.47
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.96	0.47
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.96	0.47
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.96	0.47
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.97	0.47
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.97	0.47
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.79	0.47
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.97	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.47
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.96	0.47
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.97	0.47
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.47
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.97	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:3676:ASP:HA	2:B:3679:LYS:HB3	1.97	0.47
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.97	0.47
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.96	0.47
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.96	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.79	0.47
2:I:3676:ASP:HA	2:I:3679:LYS:HB3	1.97	0.47
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.79	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.96	0.47
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.79	0.46
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.96	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.79	0.46
2:G:395:GLN:HG3	2:G:397:GLU:H	1.80	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.79	0.46
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.28	0.46
2:B:1738:LEU:HB3	2:B:2146:PRO:HG3	1.97	0.46
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.31	0.46
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.97	0.46
2:E:395:GLN:HG3	2:E:397:GLU:H	1.80	0.46
2:G:3676:ASP:HA	2:G:3679:LYS:HB3	1.97	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.97	0.46
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.97	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.96	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.79	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.97	0.46
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.46
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.97	0.46
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.98	0.46
2:B:134:ASP:OD1	2:B:134:ASP:N	2.48	0.46
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.96	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.49	0.46
2:G:1738:LEU:HB3	2:G:2146:PRO:HG3	1.97	0.46
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.98	0.46
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.46
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.46	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.97	0.46
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.96	0.46
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.97	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.39	0.46
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.97	0.46
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.98	0.46
2:E:1738:LEU:HB3	2:E:2146:PRO:HG3	1.97	0.46
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.46
2:I:1738:LEU:HB3	2:I:2146:PRO:HG3	1.97	0.46
2:E:134:ASP:OD1	2:E:134:ASP:N	2.48	0.46
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.34	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.98	0.46
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:B:395:GLN:HG3	2:B:397:GLU:H	1.80	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.98	0.45
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.45
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.45
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.79	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.97	0.45
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.43	0.45
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:B:621:ILE:O	2:B:625:LEU:N	2.48	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.48	0.45
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.98	0.45
2:I:395:GLN:HG3	2:I:397:GLU:H	1.80	0.45
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.45
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.97	0.45
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.45
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.98	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.45
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.98	0.45
2:E:3676:ASP:HA	2:E:3679:LYS:HB3	1.97	0.45
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.39	0.45
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.57	0.45
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.97	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	1.98	0.45
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.57	0.45
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.45
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.98	0.45
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.45
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.70	0.45
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.99	0.45
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.99	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:4571:PHE:O	2:B:4575:PHE:N	2.50	0.45
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.45
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.99	0.45
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.45
2:E:4571:PHE:O	2:E:4575:PHE:N	2.50	0.45
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.99	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:B:1516:UNK:N	2:B:1529:UNK:O	2.50	0.45
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.45
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.45
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.45
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.57	0.45
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.34	0.45
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.28	0.44
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.99	0.44
2:G:1516:UNK:N	2:G:1529:UNK:O	2.50	0.44
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.99	0.44
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.44
2:B:3910:THR:HG23	2:B:3911:THR:HG23	2.00	0.44
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.49	0.44
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.00	0.44
2:E:164:ARG:N	2:E:167:ASP:OD2	2.51	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.34	0.44
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.44
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.49	0.44
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.00	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.44
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.99	0.44
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.57	0.44
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	2.00	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.44
2:E:3910:THR:HG23	2:E:3911:THR:HG23	2.00	0.44
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.00	0.44
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	2.00	0.44
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.44
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.00	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.51	0.44
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.99	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.44
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.99	0.44
2:G:164:ARG:N	2:G:167:ASP:OD2	2.51	0.44
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.99	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.49	0.44
2:I:1516:UNK:N	2:I:1529:UNK:O	2.50	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.44
2:I:266:ARG:NH1	2:I:332:GLU:OE2	2.51	0.44
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.44
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.44
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.44
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	1.99	0.44
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.99	0.44
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.44
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.00	0.44
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.44
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.00	0.44
2:E:621:ILE:O	2:E:625:LEU:N	2.48	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.44
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.00	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.44
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.44
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.44
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	1.99	0.44
2:I:224:HIS:N	2:I:229:GLU:O	2.46	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.44
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.44
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.83	0.43
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.43
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.70	0.43
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.00	0.43
2:G:497:TYR:HB3	2:G:500:ALA:HB2	2.00	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.43
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.50	0.43
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.43
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.99	0.43
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.99	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	1.98	0.43
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.84	0.43
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.00	0.43
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.00	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.43
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.84	0.43
2:G:266:ARG:NH1	2:G:332:GLU:OE2	2.51	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.43
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.00	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.34	0.43
2:E:497:TYR:HB3	2:E:500:ALA:HB2	2.00	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.43
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	1.98	0.43
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.43
2:G:4571:PHE:O	2:G:4575:PHE:N	2.50	0.43
2:G:621:ILE:O	2:G:625:LEU:N	2.48	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.99	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.43
2:B:4933:GLN:HG2	2:I:4930:ALA:HB2	2.00	0.43
2:B:5028:PHE:CG	2:B:5028:PHE:O	2.70	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.46	0.43
2:E:266:ARG:NH1	2:E:332:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.99	0.43
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.52	0.43
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.43
2:B:497:TYR:HB3	2:B:500:ALA:HB2	2.00	0.43
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.43
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.84	0.43
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.01	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	2.01	0.43
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.00	0.43
2:B:4984:ASN:C	2:B:4986:ALA:H	2.22	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.50	0.43
2:I:4960:ILE:N	2:I:4960:ILE:CD1	2.73	0.43
2:I:4984:ASN:C	2:I:4986:ALA:H	2.22	0.43
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.43
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.52	0.43
2:G:4982:GLU:HB3	2:G:4983:HIS:H	1.67	0.43
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:I:4571:PHE:O	2:I:4575:PHE:N	2.50	0.43
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.00	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.52	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.01	0.43
2:I:497:TYR:HB3	2:I:500:ALA:HB2	2.00	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.42
2:E:2103:VAL:O	2:E:2107:GLN:N	2.46	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.51	0.42
2:B:266:ARG:NH1	2:B:332:GLU:OE2	2.51	0.42
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.01	0.42
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.01	0.42
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.42
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.52	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.42
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.67	0.42
2:E:4984:ASN:C	2:E:4986:ALA:H	2.22	0.42
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.00	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.52	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.51	0.42
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.42
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.50	0.42
2:G:224:HIS:N	2:G:229:GLU:O	2.46	0.42
2:G:243:ARG:NH1	2:G:301:VAL:O	2.46	0.42
2:I:485:SER:O	2:I:489:ASN:N	2.39	0.42
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.50	0.42
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.52	0.42
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	1.99	0.42
2:G:4138:ASP:N	2:G:4138:ASP:OD1	2.52	0.42
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.42
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.01	0.42
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.42
2:G:4984:ASN:C	2:G:4986:ALA:H	2.22	0.42
2:B:4558:ASN:N	2:B:4558:ASN:OD1	2.51	0.42
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.53	0.42
2:I:4190:ILE:HD13	2:I:5026:ASP:OD2	2.19	0.42
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.01	0.42
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.53	0.42
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.01	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.51	0.42
2:B:3992:PHE:O	2:B:3996:PHE:N	2.42	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.42
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.02	0.42
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.01	0.42
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.53	0.42
2:I:621:ILE:O	2:I:625:LEU:N	2.48	0.42
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.02	0.41
2:B:206:CYS:SG	2:B:207:SER:N	2.93	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.02	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.83	0.41
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.02	0.41
2:E:4189:ARG:NH1	2:E:5032:TYR:OH	2.53	0.41
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.49	0.41
2:G:2212:VAL:O	2:G:2216:GLY:N	2.45	0.41
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.53	0.41
2:G:358:THR:HG21	2:G:382:GLY:HA2	2.02	0.41
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.41
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.53	0.41
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.41
2:B:4958:CYS:SG	2:B:4958:CYS:O	2.79	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.94	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:359:TYR:HA	2:E:376:ALA:HA	2.02	0.41
2:E:4958:CYS:SG	2:E:4958:CYS:O	2.79	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.41
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.03	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:E:206:CYS:SG	2:E:207:SER:N	2.93	0.41
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.47	0.41
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.36	0.41
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.03	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.36	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:B:4189:ARG:NH1	2:B:5032:TYR:OH	2.53	0.41
2:E:1595:LEU:HD23	2:E:1595:LEU:HA	1.96	0.41
2:G:206:CYS:SG	2:G:207:SER:N	2.93	0.41
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.54	0.41
2:G:2339:VAL:HG12	2:G:2345:SER:H	1.86	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.41
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.02	0.41
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.52	0.41
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.03	0.41
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.41
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.02	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.03	0.41
2:G:378:LEU:HA	2:G:378:LEU:HD23	1.88	0.41
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.02	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.70	0.41
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.03	0.41
2:B:168:ASP:HB3	2:B:199:LEU:HD22	2.02	0.41
2:B:2339:VAL:HG12	2:B:2345:SER:H	1.85	0.41
2:B:4865:LYS:HB2	2:B:4873:ASP:HB3	2.03	0.41
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.53	0.41
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.53	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:359:TYR:HA	2:G:376:ALA:HA	2.02	0.41
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	2.03	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.41
2:I:243:ARG:NH1	2:I:301:VAL:O	2.46	0.41
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	2.03	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.01	0.41
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.54	0.41
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.01	0.41
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.41
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.35	0.41
2:G:4951:LYS:HB3	2:G:4951:LYS:HE2	1.96	0.41
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.03	0.41
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.41
2:I:168:ASP:HB3	2:I:199:LEU:HD22	2.02	0.41
2:I:359:TYR:HA	2:I:376:ALA:HA	2.02	0.41
2:I:4958:CYS:O	2:I:4958:CYS:SG	2.79	0.41
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.02	0.41
2:E:224:HIS:N	2:E:229:GLU:O	2.46	0.41
2:E:2339:VAL:HG12	2:E:2345:SER:H	1.86	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:I:2543:UNK:O	2:I:2547:UNK:N	2.54	0.41
2:I:4982:GLU:N	2:I:4982:GLU:OE1	2.54	0.41
1:J:82:TYR:O	1:J:86:GLY:N	2.54	0.41
2:B:2305:CYS:O	2:B:2324:ASN:ND2	2.54	0.41
2:B:378:LEU:HD23	2:B:378:LEU:HA	1.88	0.41
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.94	0.41
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.49	0.41
2:E:168:ASP:HB3	2:E:199:LEU:HD22	2.03	0.41
2:E:2543:UNK:O	2:E:2547:UNK:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.86	0.41
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.41
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	2.03	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.50	0.41
2:G:4958:CYS:O	2:G:4958:CYS:SG	2.79	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.53	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.41	0.41
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.02	0.40
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	2.03	0.40
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.37	0.40
2:B:4982:GLU:N	2:B:4982:GLU:OE1	2.54	0.40
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.03	0.40
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.04	0.40
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.03	0.40
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.40
2:I:4933:GLN:HG2	2:G:4930:ALA:HB2	2.03	0.40
2:G:575:LEU:HD22	2:G:609:CYS:HB3	2.03	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.93	0.40
2:I:4982:GLU:HB3	2:I:4983:HIS:H	1.67	0.40
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	2.03	0.40
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.40
2:B:1865:MET:SD	2:B:1865:MET:N	2.95	0.40
2:B:4138:ASP:N	2:B:4138:ASP:OD1	2.52	0.40
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.40
2:E:4930:ALA:HB2	2:G:4933:GLN:HG2	2.03	0.40
2:G:168:ASP:HB3	2:G:199:LEU:HD22	2.02	0.40
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.02	0.40
1:H:82:TYR:O	1:H:86:GLY:N	2.54	0.40
2:I:1865:MET:SD	2:I:1865:MET:N	2.94	0.40
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.04	0.40
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	2.03	0.40
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.40
2:B:870:ILE:HA	2:B:870:ILE:HD12	1.92	0.40
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:378:LEU:HD23	2:E:378:LEU:HA	1.88	0.40
2:E:3992:PHE:O	2:E:3996:PHE:N	2.42	0.40
2:E:4982:GLU:N	2:E:4982:GLU:OE1	2.54	0.40
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	2.03	0.40
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.79	0.40
2:G:4865:LYS:HB2	2:G:4873:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.04	0.40
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.54	0.40
2:I:2339:VAL:HG12	2:I:2345:SER:H	1.86	0.40
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.02	0.40
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.94	0.40
2:I:4697:VAL:O	2:I:4701:TRP:N	2.50	0.40
2:I:560:ILE:HA	2:I:563:VAL:HG12	2.04	0.40
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.03	0.40
2:B:2543:UNK:O	2:B:2547:UNK:N	2.54	0.40
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.40
2:B:560:ILE:HA	2:B:563:VAL:HG12	2.04	0.40
2:E:2212:VAL:O	2:E:2216:GLY:N	2.45	0.40
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.04	0.40
2:G:4189:ARG:NH1	2:G:5032:TYR:OH	2.53	0.40
2:I:3992:PHE:O	2:I:3996:PHE:N	2.42	0.40
2:B:2212:VAL:O	2:B:2216:GLY:N	2.45	0.40
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.54	0.40
2:B:2880:GLU:O	2:B:2884:ASN:N	2.53	0.40
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.04	0.40
2:E:2305:CYS:O	2:E:2324:ASN:ND2	2.55	0.40
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.57	0.40
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	2.03	0.40
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.03	0.40
2:I:2305:CYS:O	2:I:2324:ASN:ND2	2.54	0.40
2:I:2780:ASN:O	2:I:2787:THR:OG1	2.31	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%)	96 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	51	85
2	E	3235/4416 (73%)	2908 (90%)	321 (10%)	6 (0%)	51	85
2	G	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	51	85
2	I	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	51	85
All	All	13360/18096 (74%)	12010 (90%)	1326 (10%)	24 (0%)	54	85

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	B	4985	LEU
2	E	1708	ARG
2	E	4985	LEU
2	I	1708	ARG
2	I	4985	LEU
2	G	1708	ARG
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	PRO
2	B	4641	PRO
2	E	4641	PRO
2	I	4641	PRO
2	G	4641	PRO
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	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%)	2472 (99%)	21 (1%)	85	92
2	E	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
2	G	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
All	All	10324/12444 (83%)	10240 (99%)	84 (1%)	86	92

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3762	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4166	LEU
2	B	4957	LYS
2	B	4958	CYS
2	B	4960	ILE

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Mol	Chain	Res	Type
2	B	4983	HIS
2	B	5027	CYS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3762	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4166	LEU
2	E	4957	LYS
2	E	4958	CYS
2	E	4960	ILE
2	E	4983	HIS
2	E	5027	CYS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3762	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4166	LEU
2	I	4957	LYS
2	I	4958	CYS
2	I	4960	ILE

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Mol	Chain	Res	Type
2	I	4983	HIS
2	I	5027	CYS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3762	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4166	LEU
2	G	4957	LYS
2	G	4958	CYS
2	G	4960	ILE
2	G	4983	HIS
2	G	5027	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) 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	111	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	582	HIS

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Mol	Chain	Res	Type
2	B	1041	GLN
2	B	1598	GLN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2041	HIS
2	B	3809	ASN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4120	ASN
2	B	4806	ASN
2	B	4973	HIS
2	B	4983	HIS
2	E	57	ASN
2	E	111	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	582	HIS
2	E	1041	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2041	HIS
2	E	3781	GLN
2	E	3809	ASN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN

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Mol	Chain	Res	Type
2	E	4034	ASN
2	E	4120	ASN
2	E	4806	ASN
2	E	4973	HIS
2	E	4983	HIS
2	I	57	ASN
2	I	111	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	582	HIS
2	I	1041	GLN
2	I	1598	GLN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	2041	HIS
2	I	2884	ASN
2	I	3809	ASN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4120	ASN
2	I	4806	ASN
2	I	4973	HIS
2	I	4983	HIS
2	G	57	ASN
2	G	111	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	582	HIS
2	G	1041	GLN

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Mol	Chain	Res	Type
2	G	1598	GLN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	2041	HIS
2	G	3781	GLN
2	G	3809	ASN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4120	ASN
2	G	4806	ASN
2	G	4973	HIS
2	G	4983	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	B	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.60	3 (12%)
4	CFF	B	5102	-	7,15,15	1.99	2 (28%)	8,23,23	1.37	2 (25%)
3	ATP	E	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.61	3 (12%)
4	CFF	E	5102	-	7,15,15	1.99	2 (28%)	8,23,23	1.38	2 (25%)
3	ATP	G	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.62	3 (12%)
4	CFF	G	5102	-	7,15,15	2.00	2 (28%)	8,23,23	1.38	2 (25%)
3	ATP	I	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.60	3 (12%)
4	CFF	I	5102	-	7,15,15	2.01	2 (28%)	8,23,23	1.37	2 (25%)

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

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C6-N1	-4.07	1.32	1.38
4	G	5102	CFF	C6-N1	-4.02	1.32	1.38
4	B	5102	CFF	C6-N1	-4.02	1.32	1.38
4	E	5102	CFF	C6-N1	-4.01	1.32	1.38
4	G	5102	CFF	O13-C6	-2.42	1.18	1.24
4	I	5102	CFF	O13-C6	-2.41	1.18	1.24
4	B	5102	CFF	O13-C6	-2.41	1.18	1.24
4	E	5102	CFF	O13-C6	-2.38	1.18	1.24
3	I	5101	ATP	C5-C4	2.56	1.46	1.40
3	B	5101	ATP	C5-C4	2.58	1.46	1.40
3	G	5101	ATP	C5-C4	2.58	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5101	ATP	C5-C4	2.62	1.46	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-6.04	123.60	128.86
3	E	5101	ATP	N3-C2-N1	-6.01	123.62	128.86
3	B	5101	ATP	N3-C2-N1	-5.99	123.64	128.86
3	I	5101	ATP	N3-C2-N1	-5.94	123.69	128.86
4	I	5102	CFF	C14-N7-C8	-2.81	112.09	125.45
4	B	5102	CFF	C14-N7-C8	-2.81	112.09	125.45
4	E	5102	CFF	C14-N7-C8	-2.81	112.11	125.45
4	G	5102	CFF	C14-N7-C8	-2.80	112.14	125.45
3	G	5101	ATP	C4-C5-N7	-2.39	107.10	109.41
3	E	5101	ATP	C4-C5-N7	-2.38	107.11	109.41
3	B	5101	ATP	C4-C5-N7	-2.35	107.14	109.41
3	I	5101	ATP	C4-C5-N7	-2.31	107.18	109.41
3	G	5101	ATP	C4'-O4'-C1'	-2.05	107.59	109.77
3	I	5101	ATP	C4'-O4'-C1'	-2.05	107.59	109.77
3	B	5101	ATP	C4'-O4'-C1'	-2.04	107.60	109.77
3	E	5101	ATP	C4'-O4'-C1'	-2.01	107.63	109.77
4	I	5102	CFF	C5-C6-N1	2.02	120.59	118.28
4	B	5102	CFF	C5-C6-N1	2.03	120.60	118.28
4	G	5102	CFF	C5-C6-N1	2.06	120.64	118.28
4	E	5102	CFF	C5-C6-N1	2.06	120.64	118.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
3	I	5101	ATP	2	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	74.00
1	E	4345:UNK	C	4540:PHE	N	74.00
1	I	4345:UNK	C	4540:PHE	N	74.00
1	G	4345:UNK	C	4540:PHE	N	74.00
1	B	3613:UNK	C	3639:THR	N	43.80
1	E	3613:UNK	C	3639:THR	N	43.80
1	I	3613:UNK	C	3639:THR	N	43.80
1	G	3613:UNK	C	3639:THR	N	43.80
1	B	4253:GLU	C	4320:UNK	N	26.28
1	E	4253:GLU	C	4320:UNK	N	26.28
1	I	4253:GLU	C	4320:UNK	N	26.28
1	G	4253:GLU	C	4320:UNK	N	26.28
1	G	3163:UNK	C	3170:UNK	N	16.13
1	B	3163:UNK	C	3170:UNK	N	16.12
1	E	3163:UNK	C	3170:UNK	N	16.12
1	I	3163:UNK	C	3170:UNK	N	16.12
1	B	3063:UNK	C	3134:UNK	N	15.30
1	E	3063:UNK	C	3134:UNK	N	15.30
1	I	3063:UNK	C	3134:UNK	N	15.30
1	G	3063:UNK	C	3134:UNK	N	15.30
1	B	3468:UNK	C	3511:UNK	N	14.89
1	E	3468:UNK	C	3511:UNK	N	14.89
1	I	3468:UNK	C	3511:UNK	N	14.89
1	G	3468:UNK	C	3511:UNK	N	14.89
1	B	2703:UNK	C	2734:ASN	N	13.90
1	E	2703:UNK	C	2734:ASN	N	13.90
1	I	2703:UNK	C	2734:ASN	N	13.90
1	G	2703:UNK	C	2734:ASN	N	13.90
1	B	3236:UNK	C	3241:UNK	N	13.63
1	E	3236:UNK	C	3241:UNK	N	13.63
1	I	3236:UNK	C	3241:UNK	N	13.63
1	G	3236:UNK	C	3241:UNK	N	13.63

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2976:UNK	C	2995:UNK	N	12.77
1	E	2976:UNK	C	2995:UNK	N	12.77
1	I	2976:UNK	C	2995:UNK	N	12.77
1	G	2976:UNK	C	2995:UNK	N	12.77
1	B	1564:UNK	C	1573:MET	N	12.33
1	E	1564:UNK	C	1573:MET	N	12.33
1	I	1564:UNK	C	1573:MET	N	12.33
1	G	1564:UNK	C	1573:MET	N	12.33
1	B	3254:UNK	C	3261:UNK	N	8.26
1	E	3254:UNK	C	3261:UNK	N	8.26
1	I	3254:UNK	C	3261:UNK	N	8.26
1	G	3254:UNK	C	3261:UNK	N	8.26
1	E	1297:UNK	C	1430:UNK	N	6.06
1	G	1297:UNK	C	1430:UNK	N	6.06
1	B	1297:UNK	C	1430:UNK	N	6.05
1	I	1297:UNK	C	1430:UNK	N	6.05
1	B	2939:ARG	C	2942:UNK	N	3.63
1	E	2939:ARG	C	2942:UNK	N	3.63
1	I	2939:ARG	C	2942:UNK	N	3.63
1	G	2939:ARG	C	2942:UNK	N	3.63
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24