



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:55 PM UTC

PDB ID : 5TAM / pdb_00005tam
EMDB ID : EMD-8379
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

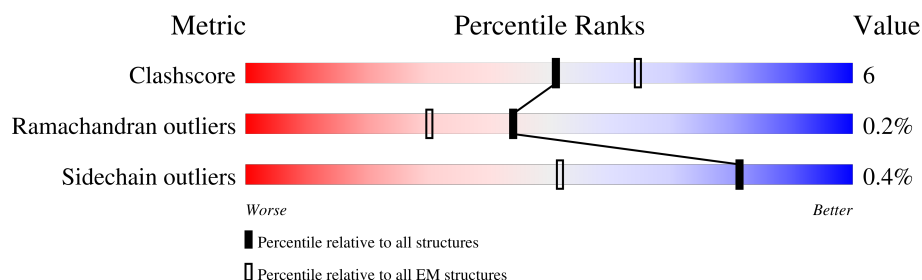
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	79% 20% .
1	F	108	79% 20% .
1	H	108	79% 20% .
1	J	108	79% 20% .
2	B	4416	83% 11% 5%
2	E	4416	83% 11% 5%
2	G	4416	83% 11% 5%
2	I	4416	83% 11% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-
4	CFF	I	5102	-	X	-	-

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.

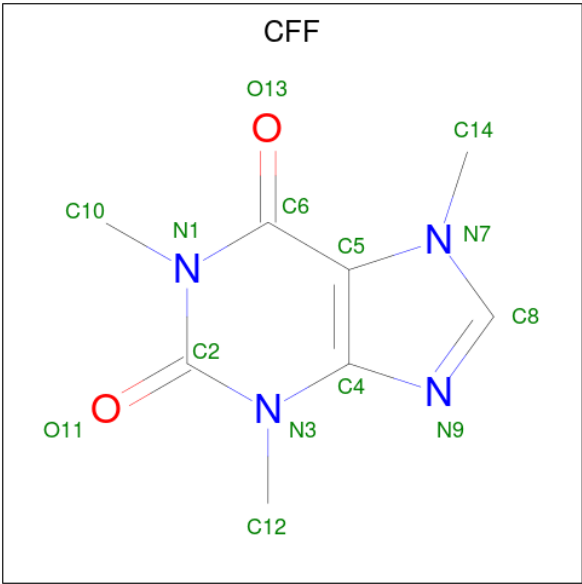
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 



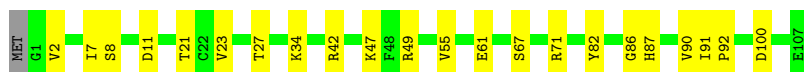
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 



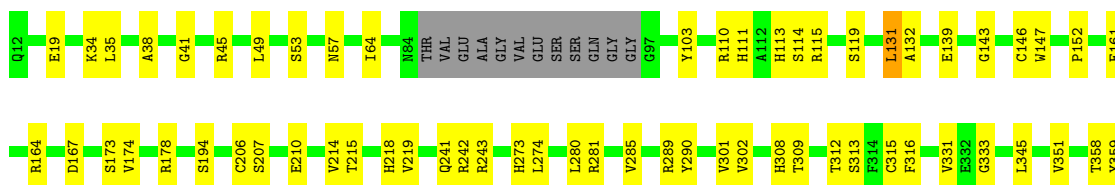
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

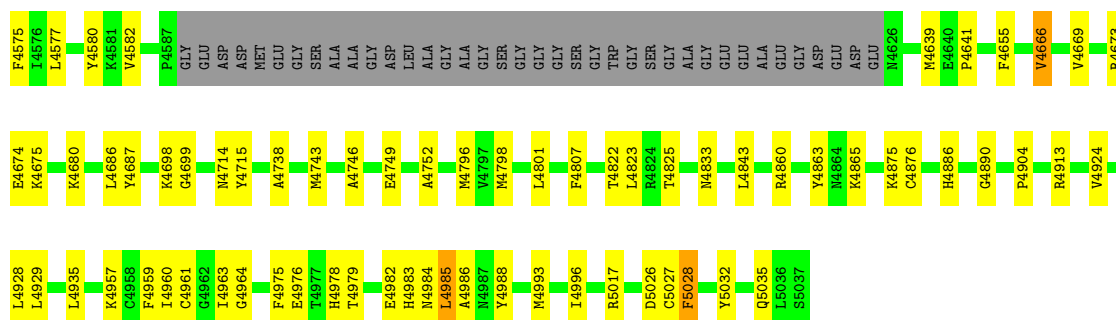


- Molecule 2: Ryanodine receptor 1

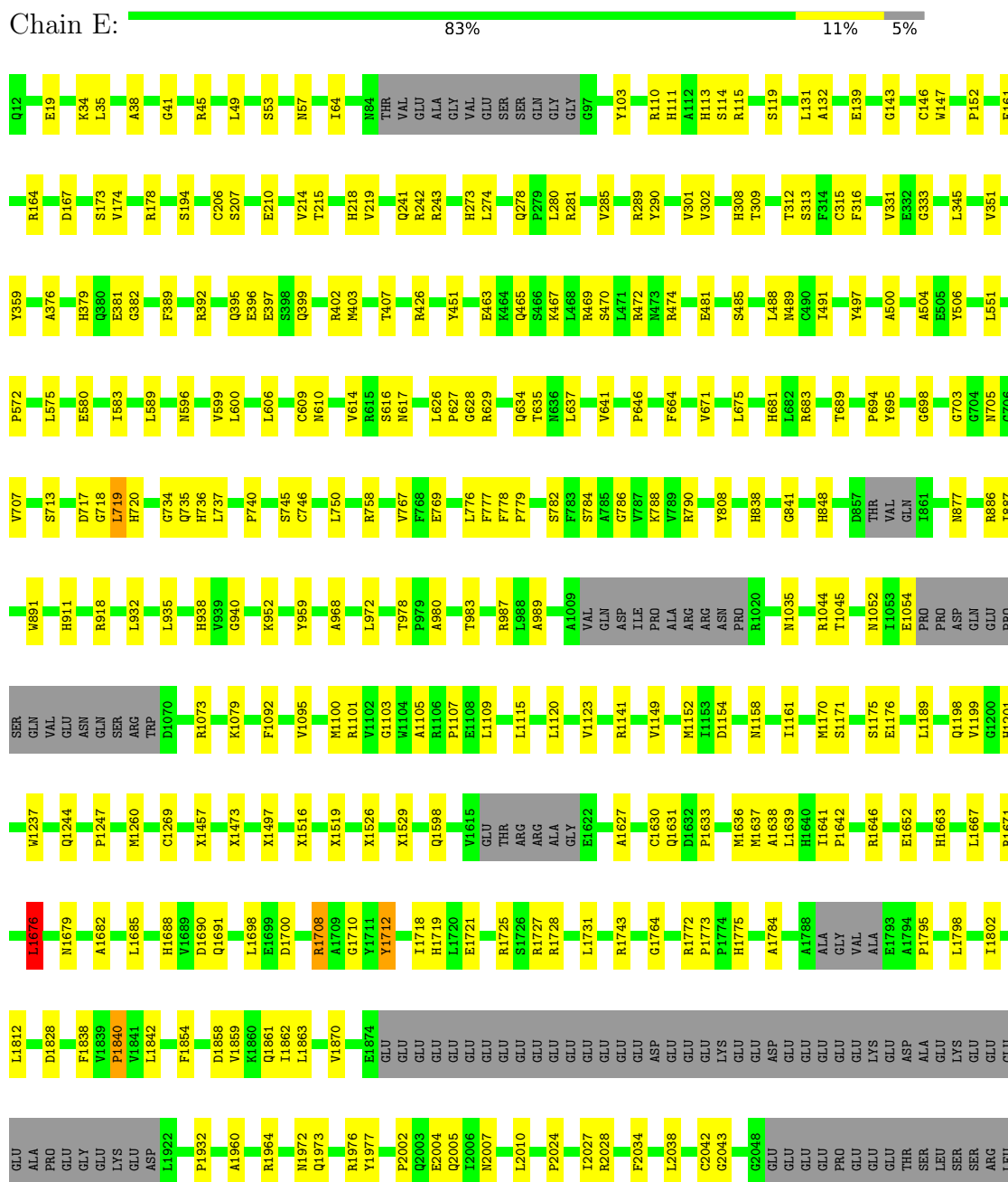
Chain B: 



E4032	N3741	S2261	L2466	LYS	VAL	PRO	F1838	D1690	P1247	GLU	H911	S713	L575	A376
V4036	GLY	M2267	L2469	LYS	ARG	GLU	V1839	Q1691	M1260	ASN	R918	D717	E580	H379
V4049	ALA	Q2268	I2469	THR	LEU	GLY	P1840	L1695	P1840	GLN	R932	G718	E583	Q380
D4063	GLU	Q2291	L2472	ARG	LYS	LYS	V1841	L1698	C1269	SER	L935	L719	L589	E381
L4066	ILE	D2294	X2493	SER	LYS	ASP	L1842	E1699	X1487	TRP	H938	H720	L606	G382
Y4080	GLN	L2295	X2502	GLN	GLU	L1922	F1854	D1700	X1473	D1070	G940	G734	L609	F389
D4083	ALA	V2299	X2517	ALA	PRG	P1932	D1858	A1708	X1497	R1073	V939	H735	N596	R392
P4084	GLN	A2303	X2521	GLN	GLU	A1960	V1859	G1710	X1516	E1078	K952	L737	V599	Q395
R4085	THR	C2326	X2674	THR	LEU	R1964	Q1861	Y1712	X1519	K1079	Y959	P740	L600	E396
G4086	PRG	G2327	X2675	ASP	PRG	M1972	I1863	H1719	X1526	S1080	A968	S745	L606	E397
A4096	ARG	R2330	X2676	ARG	ALA	Q1973	L1870	L1720	X1529	Y1081	C609	C746	N610	Q399
T4104	GLY	N2342	P2739	GLY	GLU	R1976	E1874	E1721	X1598	L572	L750	L750	V614	R402
P4106	GLU	G2343	P2748	GLU	GLU	Y1977	GLU	R1725	Q1598	M1100	V614	R758	R615	M403
E4126	VAL	V2346	L2751	GLU	GLU	P2003	GLU	S1726	Q1598	R1101	V615	T978	S616	T407
N4130	ARG	E2347	L2755	GLU	GLU	E2004	GLU	R1727	M1599	V1102	N617	V767	N617	
T4148	ARG	E2348	L2758	GLU	GLU	Q2005	GLU	R1728	L1600	G1103		F768	L626	R426
E4152	ARG	N2349	L2758	GLU	GLU	I2006	GLU	L1731	Y1615	A1105	T983	E769	P627	Y451
R4159	ASP	P2395	F2758	GLU	GLU	N2007	GLU	R1743	GLU	R1108	R987	L776	G628	E463
S4169	THR	VAL	T2762	GLU	GLU	L2010	GLU	G1764	ARG	P1107	L988	F777	R629	K464
Y4173	ARG	ARG	H2763	GLU	GLU	L2024	GLU	A1784	ALA	L1115	T983	P779	Q634	Q465
T3910	GLU	ARG	E2764	GLU	GLU	I2027	GLU	A1788	GLY	L1120	R987	L776	T635	S466
T3911	GLU	ASP	K2770	GLU	GLU	R2028	GLU	ALA	E1632	L1120	A989	F777	K636	K467
I3915	GLU	ARG	L2775	GLU	GLU	C2042	GLU	VAL	GLY	L1123	L988	F777	L637	R469
T3919	GLU	GLU	N2775	GLU	GLU	G2043	GLU	ALA	ALA	V1129	A989	P779	P646	S470
S3929	GLU	GLU	N2780	GLU	GLU	G2048	GLU	ALA	ALA	V1149	T983	P779	F664	R472
Y3937	GLU	GLU	T2787	GLU	GLU	G2048	GLU	ALA	ALA	M1152	T983	P779	F664	M473
M3955	GLU	GLU	L2787	GLU	GLU	G2048	GLU	ALA	ALA	I1153	T983	P779	F664	R474
Q3960	GLU	GLU	P2793	GLU	GLU	G2048	GLU	ALA	ALA	D1154	T983	P779	F664	S485
E4228	GLU	GLU	E2803	GLU	GLU	G2048	GLU	ALA	ALA	M1158	T983	P779	F664	L488
F4229	GLU	GLU	R2806	GLU	GLU	G2048	GLU	ALA	ALA	I1161	T983	P779	F664	M489
R4231	GLU	GLU	W2807	GLU	GLU	G2048	GLU	ALA	ALA	M1170	T983	P779	F664	C490
S4236	GLU	GLU	N2414	GLU	GLU	G2048	GLU	ALA	ALA	E1652	T983	P779	F664	I491
Y4560	GLU	GLU	H2420	GLU	GLU	G2048	GLU	ALA	ALA	R1671	T983	P779	F664	Y497
F4571	GLU	GLU	H2420	GLU	GLU	G2048	GLU	ALA	ALA	L1189	T983	P779	F664	A500
	GLU	GLU	H2420	GLU	GLU	G2048	GLU	ALA	ALA	Q1198	T983	P779	F664	A504
	GLU	GLU	H2420	GLU	GLU	G2048	GLU	ALA	ALA	V1199	T983	P779	F664	E505
	GLU	GLU	H2420	GLU	GLU	G2048	GLU	ALA	ALA	G1200	T983	P779	F664	Y506
	GLU	GLU	H2420	GLU	GLU	G2048	GLU	ALA	ALA	H1201	T983	P779	F664	L551
	GLU	GLU	H2420	GLU	GLU	G2048	GLU	ALA	ALA	W1237	T983	P779	F664	P572
	GLU	GLU	H2420	GLU	GLU	G2048	GLU	ALA	ALA	Q1244	T983	P779	F664	



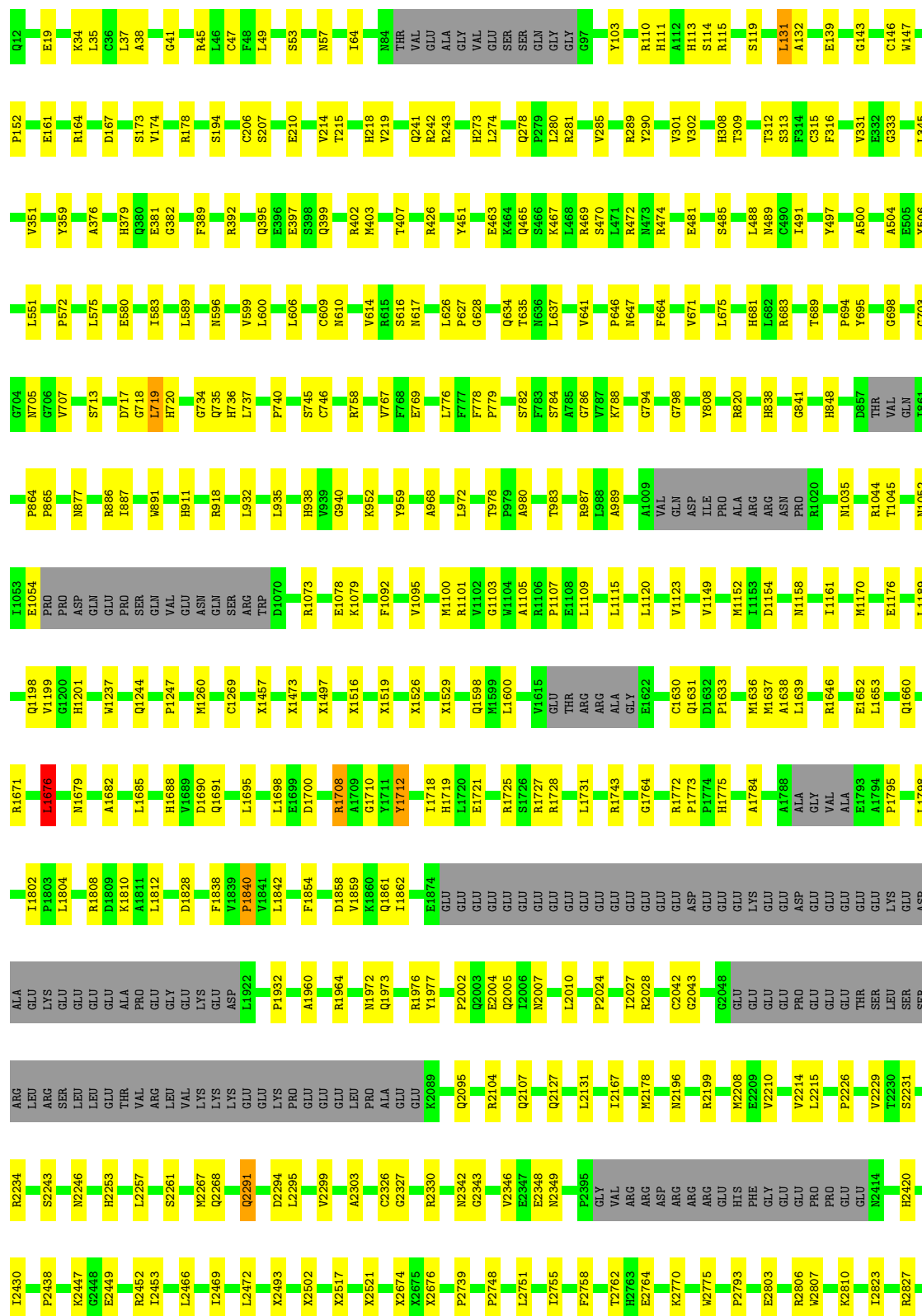
• Molecule 2: Ryanodine receptor 1



V4924	K4680	L4577	E4032	GLY	THR	L2472	Q2291	LYS	GLU	V1841	Q1691	X1473	ASN	H891
L4928	L4686	Y4580	V4036	ALA	ARG	X2493	D2294	LYS	ASP	L1842	L1698	X1497	GLN	H911
L4935	Y4687	V4582	GLU	ILE	GLU	L2295	L2295	GLU	L1922	F1854	E1699	H911	SER	H911
K4698	K4698	P4587	M4047	GLN	GLN	X2502	V2299	LYS	P1932	D1858	D1700	X1516	TRP	R918
C4968	G4699	GLY	L4048	THR	ALA	X2517	A2303	PRO	A1960	V1859	R1708	X1519	D1070	R918
F4959	N4714	ASP	D4063	GLN	ALA	X2521	C2326	GLU	R1964	Q1860	A1709	X1526	R1073	L932
C4961	Y4715	ASP	C2327	THR	THR	X2674	Q2327	GLU	N1972	K1861	G1710	X1526	K1079	L935
G4962	A4738	MET	L4066	ASP	ASP	X2675	R2330	PRO	Q1973	L1863	Y1712	X1529	F1092	H938
I4963	M4743	GLY	D4083	PRO	PRO	X2676	R2340	ALA	R1976	V1870	I1718	Q1598	V1095	H938
G4964	P4084	ALA	P4084	ARG	ARG	P2739	N2342	GLU	Y1977	E1874	H1719	Q1599	M1100	G940
A4746	G4086	ALA	G4086	GLY	GLY	P2748	G2343	GLU	P2002	GLU	E1721	L1600	R1101	K952
E4976	T4104	GLY	T4104	H2856	H2856	P2751	V2346	Q2095	Q2005	GLU	R1725	V1615	A1105	Y959
T4977	ASP	ASP	L3804	P2857	P2857	L2751	F2347	Q2095	Q2005	GLU	S1726	GLU	R1106	Y959
H4978	LEU	LEU	L3805	L2862	L2862	I2755	E2348	R2104	L2010	GLU	R1727	THR	A1105	A968
T4979	ALA	ALA	P4106	L2862	L2862	F2758	N2349	Q2107	L2010	GLU	R1728	ARG	R1106	A968
E4982	G4763	ALA	E4126	S2868	S2868	F2758	P2395	Q2127	P2024	GLU	L1731	ALA	L1109	L972
H4983	T4766	GLY	N4130	Q2872	Q2872	T2762	GLY	Q2127	I2027	GLU	R1743	E1622	L1115	T978
L4985	G4796	GLY	F3829	N2884	N2884	H2763	ARG	L2131	R2028	GLU	G1764	C1630	L1120	A980
A4986	V4797	GLY	Q3830	L2927	L2927	E2764	ASP	I2167	F2034	GLU	R1772	Q1631	V1149	T983
Y4988	M4798	SER	Q3833	K2928	K2928	K2770	ARG	M2178	L2038	GLU	P1773	P1633	P1149	T983
M4989	G4801	TRP	L3842	F2929	F2929	W2775	ARG	M2196	C2042	ASP	P1774	M1636	M1152	R987
F4990	F4807	GLY	Q3850	L2930	L2930	N2780	HIS	W2199	G2043	GLU	H1775	M1637	L1153	A1009
M4993	F4807	SER	Q3850	Q2931	Q2931	T2787	PHE	R2199	G2043	GLU	A1784	M1638	D1154	VAL
I4996	T4822	GLY	K3873	V2937	V2937	T2787	GLY	E2208	G2048	GLU	A1788	L1639	N1158	GLN
G5005	L4824	GLY	Q3889	X3362	X3362	P2783	GLU	M2209	G2048	LYS	ALA	R1646	I1161	ASP
R5017	T4825	GLU	T3910	X3365	X3365	E2803	PRO	V2210	GLU	GLU	GLY	R1646	I1161	ILE
D5026	N4833	ALA	T3911	X3366	X3366	E2806	PRO	P2226	PRO	ASP	VAL	E1652	M170	ALA
C5027	L4843	GLY	I3915	X3369	X3369	W2807	GLU	V2229	GLU	GLU	ALA	E1653	ARG	ARG
F5028	V4848	ASP	Q4209	X3369	X3369	R2807	N2414	T2230	GLU	GLU	E1793	Q1660	ASN	ASN
Y5032	T4852	GLU	R4215	H3647	H3647	K2810	H2420	S2231	THR	GLU	P1795	H1663	L1189	PRO
Q5035	R4860	M4626	A4228	N3651	N3651	K2814	T2430	R2234	SER	LYS	L1798	H1663	Q1198	R1044
L5036	E4229	E4640	E4229	N3651	N3651	K2814	T2430	R2234	LEU	GLU	I1802	L1667	V1199	T1045
S5037	Y4863	M4641	K4230	K3658	K3658	I2823	P2438	S2243	SER	ASP	P1803	R1671	G1200	N1052
	M4864	P4641	M4231	K3661	K3661	R2827	K2447	N2246	ARG	GLU	L1804	L1676	H1201	N1053
	K4865	F4665	E4232	I3662	I3662	E2830	G2448	N2246	LEU	LYS	L1807	N1679	W1237	E1054
	K4875	V4666	S4236	L3710	L3710	GLU	E2449	H2283	SER	GLU	R1808	N1679	Q1244	PRO
	C4876	Y4560	Y4560	T3711	T3711	ARG	R2452	L2257	LEU	GLU	L1812	A1682	P1247	ASP
	P4904	F4571	F4571	E3712	E3712	THR	I2453	S2261	THR	ALA	D1828	L1685	M1260	GLN
	R4913	F4575	F4575	Y3722	Y3722	GLU	L2466	M2287	VAL	GLU	F1838	H1688	C1269	SER
		I4576	I4576	L3741	L3741	LYS	I2469	Q2268	ARG	GLY	V1839	V1689	GLN	VAL
						LYS			VAL	LYS	P1840	D1690	X1457	GLU

● Molecule 2: Ryanodine receptor 1

Chain G:  83% 11% 5%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.23	0/25428	0.53	3/34534 (0.0%)
2	E	0.23	0/25428	0.53	3/34534 (0.0%)
2	G	0.23	0/25428	0.53	3/34534 (0.0%)
2	I	0.23	0/25428	0.53	3/34534 (0.0%)
All	All	0.23	0/105048	0.53	12/142628 (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	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4639	MET	CA-C-N	5.09	134.21	121.80
2	G	4639	MET	C-N-CA	5.09	134.21	121.80
2	B	4639	MET	CA-C-N	5.08	134.21	121.80
2	B	4639	MET	C-N-CA	5.08	134.21	121.80
2	I	4639	MET	CA-C-N	5.08	134.20	121.80
2	I	4639	MET	C-N-CA	5.08	134.20	121.80
2	E	131	LEU	CA-CB-CG	5.08	134.07	116.30
2	G	131	LEU	CA-CB-CG	5.08	134.07	116.30
2	E	4639	MET	CA-C-N	5.07	134.17	121.80
2	E	4639	MET	C-N-CA	5.07	134.17	121.80
2	B	131	LEU	CA-CB-CG	5.07	134.04	116.30
2	I	131	LEU	CA-CB-CG	5.05	133.99	116.30

There are no chirality outliers.

All (72) 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	1690	ASP	Peptide
2	B	1712	TYR	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	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
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	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	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

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Mol	Chain	Res	Type	Group
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	15	0
1	F	818	0	824	14	0
1	H	818	0	824	13	0
1	J	818	0	824	15	0
2	B	29499	0	24747	302	0
2	E	29499	0	24747	303	0
2	G	29499	0	24747	304	0
2	I	29499	0	24748	304	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	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
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	102373	1235	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 (1235) 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:B:4975:PHE:O	2:B:4979:THR:HG23	1.85	0.77
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.85	0.76
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.86	0.76
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.86	0.76
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.78	0.71
2:G:4231:MET:HE1	2:G:4960:ILE:HG23	1.72	0.71
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.78	0.71
2:E:4231:MET:HE1	2:E:4960:ILE:HG23	1.72	0.71
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.78	0.71
2:B:4231:MET:HE1	2:B:4960:ILE:HG23	1.72	0.71
2:I:4231:MET:HE1	2:I:4960:ILE:HG23	1.72	0.70
2:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.78	0.70
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.57	0.70
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.57	0.70
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.57	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.57	0.67
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.60	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.60	0.66
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.60	0.66
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.78	0.66
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.78	0.66
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.78	0.66
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.78	0.66
2:G:173:SER:HB3	2:G:178:ARG:H	1.61	0.65
2:B:173:SER:HB3	2:B:178:ARG:H	1.61	0.65
2:I:173:SER:HB3	2:I:178:ARG:H	1.61	0.65
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.60	0.65
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.78	0.65
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.79	0.65
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.79	0.65
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.86	0.64
2:G:379:HIS:HD2	2:G:382:GLY:H	1.46	0.64
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.86	0.64
2:I:331:VAL:HG12	2:I:333:GLY:H	1.62	0.64
2:I:379:HIS:HD2	2:I:382:GLY:H	1.46	0.64
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.79	0.64
2:E:379:HIS:HD2	2:E:382:GLY:H	1.46	0.63
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.81	0.63
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.80	0.63
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.86	0.63
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:173:SER:HB3	2:E:178:ARG:H	1.61	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.80	0.63
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.79	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.80	0.63
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.81	0.63
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.86	0.63
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.79	0.63
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.80	0.63
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.79	0.63
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.79	0.63
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.81	0.63
2:G:331:VAL:HG12	2:G:333:GLY:H	1.62	0.63
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.31	0.63
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.63
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.80	0.63
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.80	0.63
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.79	0.63
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.80	0.62
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.81	0.62
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.80	0.62
2:B:379:HIS:HD2	2:B:382:GLY:H	1.46	0.62
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.81	0.62
2:E:331:VAL:HG12	2:E:333:GLY:H	1.63	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.62	0.62
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.80	0.62
2:I:111:HIS:HD2	2:I:114:SER:H	1.48	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.81	0.62
2:G:111:HIS:HD2	2:G:114:SER:H	1.48	0.62
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.81	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:B:111:HIS:HD2	2:B:114:SER:H	1.48	0.61
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.81	0.61
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.34	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.34	0.61
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.34	0.61
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.66	0.61
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.34	0.61
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.83	0.61
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.83	0.60
2:E:111:HIS:HD2	2:E:114:SER:H	1.48	0.60
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.66	0.60
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.34	0.60
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.34	0.60
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.34	0.60
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.66	0.60
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.66	0.60
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.34	0.60
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.34	0.60
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.34	0.60
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.83	0.59
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.84	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.83	0.59
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.85	0.59
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.85	0.59
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.84	0.59
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.85	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.84	0.59
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.85	0.59
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.85	0.59
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.85	0.59
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.85	0.58
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.68	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.84	0.58
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.34	0.58
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.77	0.58
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.58
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.77	0.58
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.68	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.84	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.77	0.58
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.85	0.58
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.84	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.85	0.58
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	2.21	0.58
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.84	0.58
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.77	0.58
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.69	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.69	0.58
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.37	0.58
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	2.21	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.58
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.85	0.58
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.86	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.84	0.58
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.85	0.58
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	2.21	0.58
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	2.21	0.58
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.86	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.57
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.68	0.57
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.86	0.57
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.37	0.57
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.57
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.57
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.85	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.68	0.57
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.38	0.57
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.69	0.57
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.86	0.57
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.57
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.86	0.57
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.85	0.57
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.57
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.86	0.57
2:I:2178:MET:HE1	2:I:2210:VAL:HG11	1.87	0.57
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.85	0.57
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.85	0.57
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:G:2178:MET:HE1	2:G:2210:VAL:HG11	1.87	0.57
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.57
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.38	0.57
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.86	0.57
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.86	0.57
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.38	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.86	0.57
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.86	0.57
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.85	0.57
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.38	0.57
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.86	0.57
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.38	0.57
2:B:2178:MET:HE1	2:B:2210:VAL:HG11	1.87	0.56
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.56
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.69	0.56
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.38	0.56
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.38	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.39	0.56
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.56
2:E:2178:MET:HE1	2:E:2210:VAL:HG11	1.87	0.56
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.38	0.56
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.71	0.56
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.38	0.56
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.88	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.79	0.56
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.88	0.56
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.39	0.56
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.88	0.56
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.88	0.56
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.88	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.38	0.56
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.88	0.56
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.88	0.55
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.39	0.55
2:B:111:HIS:CD2	2:B:114:SER:H	2.25	0.55
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.71	0.55
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.38	0.55
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.39	0.55
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.40	0.55
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.71	0.55
2:I:111:HIS:CD2	2:I:114:SER:H	2.25	0.55
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.38	0.55
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.72	0.55
2:G:315:CYS:SG	2:G:316:PHE:N	2.79	0.55
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.72	0.55
2:G:4983:HIS:HB2	2:G:4988:TYR:HE2	1.72	0.55
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.89	0.55
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.89	0.55
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.89	0.55
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.88	0.55
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.40	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.55
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.89	0.55
2:G:111:HIS:CD2	2:G:114:SER:H	2.25	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.88	0.55
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.38	0.55
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.40	0.55
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.88	0.55
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.39	0.55
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.40	0.55
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.89	0.55
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.71	0.55
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.88	0.55
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.80	0.55
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.89	0.55
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.89	0.55
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.39	0.55
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.88	0.55
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.40	0.55
2:I:4983:HIS:HB2	2:I:4988:TYR:HE2	1.72	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.80	0.55
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.88	0.54
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.40	0.54
2:E:4983:HIS:HB2	2:E:4988:TYR:HE2	1.72	0.54
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.39	0.54
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.89	0.54
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.89	0.54
2:B:614:VAL:HG22	2:B:616:SER:H	1.73	0.54
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.40	0.54
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.88	0.54
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.88	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.72	0.54
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.90	0.54
2:E:4228:ALA:O	2:E:4232:GLU:N	2.40	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.40	0.54
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.40	0.54
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.56	0.54
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.40	0.54
2:B:4983:HIS:HB2	2:B:4988:TYR:HE2	1.72	0.54
2:E:614:VAL:HG22	2:E:616:SER:H	1.73	0.54
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.89	0.54
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.90	0.54
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.40	0.54
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.40	0.54
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.90	0.54
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.40	0.54
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.40	0.54
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.80	0.54
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.89	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.73	0.54
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.54
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.90	0.54
2:G:395:GLN:HG3	2:G:397:GLU:H	1.73	0.54
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.89	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.72	0.54
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.90	0.54
2:G:689:THR:H	2:G:778:PHE:HE2	1.55	0.54
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.90	0.54
2:G:4982:GLU:OE1	2:G:4982:GLU:HA	2.08	0.54
2:B:689:THR:H	2:B:778:PHE:HE2	1.55	0.54
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.90	0.54
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.40	0.54
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.56	0.54
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.90	0.53
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.53
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.90	0.53
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.89	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.88	0.53
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.90	0.53
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.42	0.53
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.89	0.53
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.90	0.53
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.90	0.53
2:E:313:SER:HB3	2:E:351:VAL:HB	1.91	0.53
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.89	0.53
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.41	0.53
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.53
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.90	0.53
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.89	0.53
2:E:111:HIS:CD2	2:E:114:SER:H	2.25	0.53
2:I:689:THR:H	2:I:778:PHE:HE2	1.55	0.53
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.91	0.53
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.42	0.53
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.42	0.53
2:B:4231:MET:HE1	2:B:4960:ILE:HA	1.91	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.40	0.53
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.91	0.53
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.89	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.91	0.53
2:I:614:VAL:HG22	2:I:616:SER:H	1.73	0.53
2:B:315:CYS:SG	2:B:316:PHE:N	2.79	0.53
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.90	0.53
2:B:4982:GLU:OE1	2:B:4982:GLU:HA	2.08	0.53
2:E:4982:GLU:OE1	2:E:4982:GLU:HA	2.08	0.53
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.90	0.53
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.90	0.53
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.91	0.53
2:I:395:GLN:HG3	2:I:397:GLU:H	1.73	0.53
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.40	0.53
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.56	0.53
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.42	0.53
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.91	0.53
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.90	0.53
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.91	0.53
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.44	0.53
2:E:315:CYS:SG	2:E:316:PHE:N	2.79	0.53
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.91	0.53
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.44	0.53
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.89	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.90	0.53
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.91	0.53
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.90	0.53
2:B:313:SER:HB3	2:B:351:VAL:HB	1.91	0.53
2:B:395:GLN:HG3	2:B:397:GLU:H	1.73	0.53
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.53
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.91	0.53
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.44	0.53
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.90	0.52
2:I:911:HIS:O	2:I:918:ARG:NH2	2.42	0.52
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.52
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.91	0.52
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.44	0.52
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.91	0.52
2:B:911:HIS:O	2:B:918:ARG:NH2	2.42	0.52
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.91	0.52
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.89	0.52
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.92	0.52
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.91	0.52
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.91	0.52
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.92	0.52
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.91	0.52
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.89	0.52
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.90	0.52
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.90	0.52
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.91	0.52
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.91	0.52
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.52
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.75	0.52
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.92	0.52
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.75	0.52
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.92	0.52
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.90	0.52
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.92	0.52
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.92	0.52
2:I:4982:GLU:OE1	2:I:4982:GLU:HA	2.08	0.52
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.75	0.52
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.92	0.52
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.91	0.52
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.52
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.90	0.52
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.91	0.52
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.90	0.52
2:G:614:VAL:HG22	2:G:616:SER:H	1.73	0.52
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.92	0.52
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.43	0.52
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.90	0.52
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.91	0.52
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.90	0.52
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.92	0.52
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.91	0.52
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.91	0.52
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.92	0.52
2:G:4231:MET:HE1	2:G:4960:ILE:HA	1.91	0.52
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.52
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.92	0.52
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.92	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.91	0.52
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.92	0.51
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.93	0.51
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.91	0.51
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.92	0.51
2:E:689:THR:H	2:E:778:PHE:HE2	1.55	0.51
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.56	0.51
2:E:4798:MET:HA	2:E:4801:LEU:HB2	1.91	0.51
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.91	0.51
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.92	0.51
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.92	0.51
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.75	0.51
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.92	0.51
2:E:470:SER:O	2:E:474:ARG:NE	2.40	0.51
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.40	0.51
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.92	0.51
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.91	0.51
2:I:1516:UNK:N	2:I:1529:UNK:O	2.43	0.51
2:G:309:THR:O	2:G:313:SER:OG	2.28	0.51
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.91	0.51
2:G:4798:MET:HA	2:G:4801:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.92	0.51
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.40	0.51
2:E:309:THR:O	2:E:313:SER:OG	2.28	0.51
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.92	0.51
2:I:164:ARG:N	2:I:167:ASP:OD2	2.44	0.51
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.51
2:G:911:HIS:O	2:G:918:ARG:NH2	2.42	0.51
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.93	0.51
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	2.29	0.51
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.91	0.51
2:B:4798:MET:HA	2:B:4801:LEU:HB2	1.91	0.51
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.93	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.51
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.92	0.51
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.51
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.92	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.37	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.92	0.51
2:I:4798:MET:HA	2:I:4801:LEU:HB2	1.91	0.51
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.91	0.51
2:B:309:THR:O	2:B:313:SER:OG	2.29	0.51
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.92	0.51
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	2.29	0.51
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.92	0.51
2:E:1516:UNK:N	2:E:1529:UNK:O	2.43	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.43	0.51
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.91	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.93	0.51
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.93	0.51
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.92	0.51
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.40	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.92	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:B:34:LYS:H	2:B:53:SER:HG	1.57	0.51
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.92	0.51
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.43	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.50
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.45	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.94	0.50
1:A:82:TYR:O	1:A:86:GLY:N	2.45	0.50
2:B:164:ARG:N	2:B:167:ASP:OD2	2.44	0.50
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.93	0.50
1:F:21:THR:HA	1:F:49:ARG:HA	1.94	0.50
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.93	0.50
2:E:241:GLN:O	2:E:289:ARG:NH1	2.38	0.50
2:E:359:TYR:HA	2:E:376:ALA:HA	1.94	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.50
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.45	0.50
2:I:470:SER:O	2:I:474:ARG:NE	2.40	0.50
2:G:359:TYR:HA	2:G:376:ALA:HA	1.93	0.50
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.92	0.50
1:J:82:TYR:O	1:J:86:GLY:N	2.45	0.50
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.45	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.42	0.50
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.45	0.50
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	2.29	0.50
2:I:309:THR:O	2:I:313:SER:OG	2.29	0.50
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.45	0.50
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.45	0.50
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.83	0.50
2:I:243:ARG:NH1	2:I:301:VAL:O	2.39	0.50
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.44	0.50
1:F:11:ASP:OD1	1:F:67:SER:OG	2.29	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.94	0.49
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.45	0.49
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.77	0.49
2:B:4976:GLU:HA	2:B:4979:THR:HG23	1.94	0.49
2:E:243:ARG:NH1	2:E:301:VAL:O	2.39	0.49
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.94	0.49
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.94	0.49
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.94	0.49
2:G:470:SER:O	2:G:474:ARG:NE	2.40	0.49
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.94	0.49
1:H:82:TYR:O	1:H:86:GLY:N	2.45	0.49
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.94	0.49
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.49
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.40	0.49
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.95	0.49
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.93	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.49
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.49
2:I:4228:ALA:O	2:I:4232:GLU:N	2.40	0.49
2:G:164:ARG:N	2:G:167:ASP:OD2	2.44	0.49
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.40	0.49
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.94	0.49
2:B:241:GLN:O	2:B:289:ARG:NH1	2.38	0.49
2:B:470:SER:O	2:B:474:ARG:NE	2.40	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.44	0.49
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.93	0.49
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.94	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.49
1:H:11:ASP:OD1	1:H:67:SER:OG	2.29	0.49
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.49
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.94	0.49
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.95	0.49
2:G:4976:GLU:HA	2:G:4979:THR:HG23	1.94	0.49
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.95	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.77	0.49
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.95	0.49
2:I:500:ALA:HB1	2:I:504:ALA:HB2	1.95	0.49
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.40	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.49
2:I:4904:PRO:HB3	2:I:4913:ARG:HD2	1.95	0.49
2:G:4904:PRO:HB3	2:G:4913:ARG:HD2	1.95	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.94	0.49
2:B:290:TYR:O	2:B:302:VAL:N	2.46	0.49
2:E:164:ARG:N	2:E:167:ASP:OD2	2.44	0.49
2:G:500:ALA:HB1	2:G:504:ALA:HB2	1.95	0.49
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.78	0.49
1:F:82:TYR:O	1:F:86:GLY:N	2.45	0.49
2:I:359:TYR:HA	2:I:376:ALA:HA	1.93	0.49
2:B:359:TYR:HA	2:B:376:ALA:HA	1.93	0.49
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.94	0.49
2:I:4976:GLU:HA	2:I:4979:THR:HG23	1.94	0.49
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.78	0.49
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.61	0.49
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.95	0.49
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.78	0.49
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.49
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.95	0.49
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.95	0.48
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.78	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.48
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	2.29	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.78	0.48
2:B:485:SER:O	2:B:489:ASN:N	2.37	0.48
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.48
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.94	0.48
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.95	0.48
2:I:978:THR:HB	2:I:980:ALA:H	1.78	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.83	0.48
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.96	0.48
2:B:4904:PRO:HB3	2:B:4913:ARG:HD2	1.95	0.48
2:E:290:TYR:O	2:E:302:VAL:N	2.46	0.48
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.78	0.48
2:E:4976:GLU:HA	2:E:4979:THR:HG23	1.94	0.48
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.95	0.48
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.78	0.48
2:I:290:TYR:O	2:I:302:VAL:N	2.46	0.48
2:I:2346:VAL:HG13	2:I:2349:ASN:H	1.79	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.47	0.48
2:G:243:ARG:NH1	2:G:301:VAL:O	2.39	0.48
2:G:4228:ALA:O	2:G:4232:GLU:N	2.40	0.48
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.61	0.48
2:B:978:THR:HB	2:B:980:ALA:H	1.78	0.48
2:B:2346:VAL:HG13	2:B:2349:ASN:H	1.79	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.47	0.48
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.96	0.48
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.47	0.48
2:E:4904:PRO:HB3	2:E:4913:ARG:HD2	1.95	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.94	0.48
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.95	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.48
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.79	0.48
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.54	0.48
1:J:11:ASP:OD1	1:J:67:SER:OG	2.29	0.48
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.94	0.48
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.96	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.95	0.48
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.48
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.79	0.48
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.54	0.48
2:E:978:THR:HB	2:E:980:ALA:H	1.78	0.48
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.48
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.79	0.48
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.94	0.48
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.96	0.48
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.47	0.48
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.95	0.48
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.95	0.48
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.95	0.48
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.78	0.48
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.79	0.48
2:G:2346:VAL:HG13	2:G:2349:ASN:H	1.79	0.48
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.79	0.48
2:E:500:ALA:HB1	2:E:504:ALA:HB2	1.95	0.48
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.96	0.48
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.48
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.79	0.48
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.54	0.48
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.48
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.54	0.48
2:G:3770:LEU:HD21	2:G:3775:ALA:HB3	1.96	0.48
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.79	0.48
2:B:3915:ILE:O	2:B:3919:THR:N	2.45	0.48
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.95	0.48
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.78	0.48
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.96	0.48
2:B:500:ALA:HB1	2:B:504:ALA:HB2	1.95	0.47
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.79	0.47
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.47
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.78	0.47
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.78	0.47
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4822:THR:O	2:I:4825:THR:OG1	2.27	0.47
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.95	0.47
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.79	0.47
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.96	0.47
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.79	0.47
2:G:3915:ILE:O	2:G:3919:THR:N	2.45	0.47
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:G:290:TYR:O	2:G:302:VAL:N	2.46	0.47
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.47
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.96	0.47
2:B:4228:ALA:O	2:B:4232:GLU:N	2.40	0.47
2:B:4822:THR:O	2:B:4825:THR:OG1	2.27	0.47
2:E:3915:ILE:O	2:E:3919:THR:N	2.45	0.47
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.45	0.47
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.48	0.47
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.79	0.47
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.36	0.47
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.78	0.47
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.47	0.47
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.61	0.47
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.48	0.47
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.96	0.47
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.97	0.47
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.79	0.47
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.78	0.47
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.48	0.47
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.96	0.47
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.79	0.47
1:F:34:LYS:HE3	2:E:634:GLN:HB3	1.95	0.47
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.44	0.47
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.36	0.47
2:E:4822:THR:O	2:E:4825:THR:OG1	2.27	0.47
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.79	0.47
2:I:451:TYR:O	2:I:474:ARG:NH1	2.47	0.47
2:G:241:GLN:O	2:G:289:ARG:NH1	2.38	0.47
1:A:11:ASP:OD1	1:A:67:SER:OG	2.29	0.47
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.80	0.47
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.97	0.47
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.80	0.47
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.44	0.47
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.46
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.46
2:B:403:MET:O	2:B:407:THR:N	2.49	0.46
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.97	0.46
2:B:4863:TYR:HD2	2:B:4875:LYS:HB2	1.79	0.46
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.80	0.46
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.97	0.46
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	1.96	0.46
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.32	0.46
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.46
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.78	0.46
2:G:451:TYR:O	2:G:474:ARG:NH1	2.47	0.46
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.49	0.46
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.83	0.46
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.97	0.46
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.46
1:J:34:LYS:HE3	2:I:634:GLN:HB3	1.97	0.46
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.80	0.46
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.81	0.46
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	1.96	0.46
2:E:1105:ALA:N	2:E:1189:LEU:O	2.49	0.46
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.81	0.46
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.34	0.46
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.51	0.46
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.97	0.46
2:E:4571:PHE:O	2:E:4575:PHE:N	2.49	0.46
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.46
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.49	0.46
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.49	0.46
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.80	0.46
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.98	0.46
2:B:451:TYR:O	2:B:474:ARG:NH1	2.47	0.46
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.49	0.46
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	1.98	0.46
2:I:403:MET:O	2:I:407:THR:N	2.49	0.46
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.48	0.46
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	1.96	0.46
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.98	0.46
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.80	0.46
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	1.98	0.46
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.33	0.46
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.49	0.46
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.34	0.46
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46
2:E:2346:VAL:HG13	2:E:2349:ASN:H	1.79	0.46
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.46
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.97	0.46
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.34	0.46
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	1.98	0.46
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.97	0.46
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.49	0.46
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.51	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.46
1:H:87:HIS:H	1:H:91:ILE:HB	1.81	0.46
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.98	0.46
2:B:1105:ALA:N	2:B:1189:LEU:O	2.49	0.46
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.33	0.46
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.98	0.46
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	1.98	0.46
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.36	0.46
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.80	0.46
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.98	0.46
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.98	0.46
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.61	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.34	0.46
2:G:4571:PHE:O	2:G:4575:PHE:N	2.49	0.46
2:B:606:LEU:O	2:B:617:ASN:ND2	2.49	0.46
2:E:403:MET:O	2:E:407:THR:N	2.49	0.46
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.32	0.46
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.81	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.51	0.46
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.81	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.34	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.49	0.46
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.98	0.46
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.98	0.46
2:E:218:HIS:HB3	2:E:392:ARG:HD3	1.98	0.46
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.98	0.46
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.49	0.46
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.98	0.46
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.97	0.46
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.98	0.45
2:B:243:ARG:NH1	2:B:301:VAL:O	2.39	0.45
2:E:983:THR:O	2:E:987:ARG:N	2.48	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.34	0.45
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.80	0.45
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.97	0.45
1:F:87:HIS:H	1:F:91:ILE:HB	1.81	0.45
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.98	0.45
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.98	0.45
2:E:3362:UNK:O	2:E:3366:UNK:N	2.50	0.45
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.33	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.90	0.45
2:I:606:LEU:O	2:I:617:ASN:ND2	2.49	0.45
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.97	0.45
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.99	0.45
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.99	0.45
2:I:3362:UNK:O	2:I:3366:UNK:N	2.50	0.45
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.98	0.45
2:G:403:MET:O	2:G:407:THR:N	2.49	0.45
2:G:3362:UNK:O	2:G:3366:UNK:N	2.50	0.45
2:B:218:HIS:HB3	2:B:392:ARG:HD3	1.98	0.45
2:B:1457:UNK:N	2:B:1497:UNK:O	2.49	0.45
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.99	0.45
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.32	0.45
2:E:1457:UNK:N	2:E:1497:UNK:O	2.49	0.45
2:I:218:HIS:HB3	2:I:392:ARG:HD3	1.98	0.45
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.97	0.45
2:I:4571:PHE:O	2:I:4575:PHE:N	2.49	0.45
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.49	0.45
2:B:206:CYS:SG	2:B:207:SER:N	2.89	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.34	0.45
2:B:1973:GLN:O	2:B:1977:TYR:N	2.45	0.45
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	1.98	0.45
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.98	0.45
2:E:3842:LEU:O	2:E:3929:SER:OG	2.34	0.45
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.98	0.45
2:G:206:CYS:SG	2:G:207:SER:N	2.89	0.45
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:606:LEU:O	2:G:617:ASN:ND2	2.49	0.45
2:G:1105:ALA:N	2:G:1189:LEU:O	2.49	0.45
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.99	0.45
2:G:3842:LEU:O	2:G:3929:SER:OG	2.34	0.45
2:G:4822:THR:O	2:G:4825:THR:OG1	2.27	0.45
2:E:206:CYS:SG	2:E:207:SER:N	2.90	0.45
2:I:1457:UNK:N	2:I:1497:UNK:O	2.49	0.45
2:G:1457:UNK:N	2:G:1497:UNK:O	2.49	0.45
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.97	0.45
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.98	0.45
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.98	0.45
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	1.99	0.45
2:B:3362:UNK:O	2:B:3366:UNK:N	2.50	0.45
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.98	0.45
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.97	0.45
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.98	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.34	0.45
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.98	0.45
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	1.98	0.45
2:B:4984:ASN:C	2:B:4986:ALA:N	2.75	0.45
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.33	0.45
2:G:218:HIS:HB3	2:G:392:ARG:HD3	1.98	0.45
1:A:87:HIS:H	1:A:91:ILE:HB	1.81	0.45
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.97	0.45
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.98	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.34	0.45
2:E:4959:PHE:O	2:E:4959:PHE:CG	2.70	0.45
2:I:215:THR:HG22	2:I:273:HIS:HA	1.99	0.45
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.98	0.45
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.81	0.45
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.98	0.45
2:G:4959:PHE:O	2:G:4959:PHE:CG	2.70	0.45
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.45
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.99	0.45
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	1.98	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.47	0.45
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.81	0.45
2:I:626:LEU:HG	2:I:628:GLY:H	1.82	0.45
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	1.99	0.45
1:F:27:THR:HB	1:F:100:ASP:HB3	1.99	0.44
1:A:27:THR:HB	1:A:100:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.82	0.44
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.83	0.44
2:E:4848:VAL:O	2:E:4852:THR:OG1	2.34	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.00	0.44
1:J:27:THR:HB	1:J:100:ASP:HB3	1.99	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.51	0.44
2:E:215:THR:HG22	2:E:273:HIS:HA	2.00	0.44
2:E:606:LEU:O	2:E:617:ASN:ND2	2.49	0.44
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.99	0.44
2:E:4047:MET:HE3	2:E:4047:MET:HB2	1.89	0.44
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.98	0.44
2:E:4984:ASN:C	2:E:4986:ALA:H	2.25	0.44
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.83	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.44
2:I:4984:ASN:C	2:I:4986:ALA:H	2.25	0.44
2:G:215:THR:HG22	2:G:273:HIS:HA	2.00	0.44
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.83	0.44
2:E:626:LEU:HG	2:E:628:GLY:H	1.82	0.44
2:I:1105:ALA:N	2:I:1189:LEU:O	2.49	0.44
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.99	0.44
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.99	0.44
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.82	0.44
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.82	0.44
2:G:210:GLU:H	2:G:273:HIS:CE1	2.36	0.44
2:G:626:LEU:HG	2:G:628:GLY:H	1.82	0.44
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.82	0.44
2:G:4984:ASN:C	2:G:4986:ALA:H	2.25	0.44
1:J:87:HIS:H	1:J:91:ILE:HB	1.81	0.44
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	1.99	0.44
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.47	0.44
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.00	0.44
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.00	0.44
2:G:1804:LEU:O	2:G:1808:ARG:N	2.49	0.44
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.44
1:H:34:LYS:HE3	2:G:634:GLN:HB3	1.98	0.44
2:B:215:THR:HG22	2:B:273:HIS:HA	1.99	0.44
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.51	0.44
2:B:626:LEU:HG	2:B:628:GLY:H	1.82	0.44
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.99	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.70	0.44
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.99	0.44
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.81	0.44
2:E:4843:LEU:HD12	2:G:4823:LEU:HD23	2.00	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	2.00	0.44
2:I:3915:ILE:O	2:I:3919:THR:N	2.45	0.44
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.00	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.51	0.44
2:I:210:GLU:H	2:I:273:HIS:CE1	2.36	0.44
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	1.98	0.44
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.99	0.44
2:I:2299:VAL:O	2:I:2303:ALA:N	2.50	0.44
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.51	0.44
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.99	0.44
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.00	0.44
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.98	0.44
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	2.00	0.44
2:G:4959:PHE:O	2:G:4959:PHE:CD1	2.70	0.44
2:G:5028:PHE:CG	2:G:5028:PHE:O	2.70	0.44
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.00	0.44
2:B:1101:ARG:HH21	2:B:1115:LEU:H	1.66	0.44
2:E:210:GLU:H	2:E:273:HIS:CE1	2.36	0.44
2:E:4215:ARG:NH2	3:E:5101:ATP:O1A	2.51	0.44
2:I:485:SER:O	2:I:489:ASN:N	2.37	0.44
2:I:647:ASN:ND2	2:I:820:ARG:O	2.50	0.44
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	1.99	0.44
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.98	0.44
2:I:2758:PHE:O	2:I:2762:THR:N	2.51	0.44
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.83	0.44
2:G:4229:GLU:HA	2:G:4232:GLU:HB3	1.99	0.44
2:B:34:LYS:N	2:B:53:SER:OG	2.40	0.44
2:E:4959:PHE:O	2:E:4959:PHE:CD1	2.70	0.44
2:I:241:GLN:O	2:I:289:ARG:NH1	2.38	0.44
2:I:1663:HIS:O	2:I:1667:LEU:N	2.49	0.44
2:I:2257:LEU:O	2:I:2261:SER:N	2.51	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CG	2.70	0.44
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.99	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.51	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	1.99	0.43
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	2.00	0.43
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.43
2:I:119:SER:HA	2:I:146:CYS:HA	2.00	0.43
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.51	0.43
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.99	0.43
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.43
2:I:4229:GLU:HA	2:I:4232:GLU:HB3	1.99	0.43
2:G:2758:PHE:O	2:G:2762:THR:N	2.51	0.43
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.47	0.43
2:G:4215:ARG:NH2	3:G:5101:ATP:O1A	2.51	0.43
2:B:4215:ARG:NH2	3:B:5101:ATP:O1A	2.51	0.43
2:E:34:LYS:N	2:E:53:SER:OG	2.40	0.43
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	2.00	0.43
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.52	0.43
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	2.00	0.43
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.00	0.43
1:H:27:THR:HB	1:H:100:ASP:HB3	1.99	0.43
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.81	0.43
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	2.00	0.43
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.82	0.43
2:E:1663:HIS:O	2:E:1667:LEU:N	2.49	0.43
2:E:4229:GLU:HA	2:E:4232:GLU:HB3	1.99	0.43
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.99	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.84	0.43
2:B:210:GLU:H	2:B:273:HIS:CE1	2.36	0.43
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.32	0.43
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.51	0.43
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.99	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.51	0.43
2:B:4229:GLU:HA	2:B:4232:GLU:HB3	1.99	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.01	0.43
2:G:1101:ARG:HH21	2:G:1115:LEU:H	1.65	0.43
1:A:34:LYS:HE3	2:B:634:GLN:HB3	2.00	0.43
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.00	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.00	0.43
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.01	0.43
2:B:4984:ASN:C	2:B:4986:ALA:H	2.25	0.43
2:E:119:SER:HA	2:E:146:CYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.01	0.43
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.00	0.43
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.01	0.43
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.52	0.43
2:G:776:LEU:HG	2:G:848:HIS:HA	2.01	0.43
2:G:864:PRO:HA	2:G:865:PRO:HD3	1.92	0.43
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.01	0.43
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.43
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.00	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.01	0.43
2:E:2758:PHE:O	2:E:2762:THR:N	2.51	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.84	0.43
2:E:5028:PHE:O	2:E:5028:PHE:CG	2.70	0.43
2:I:1973:GLN:O	2:I:1977:TYR:N	2.45	0.43
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.01	0.43
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.54	0.43
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.99	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.84	0.43
2:B:119:SER:HA	2:B:146:CYS:HA	2.01	0.43
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.84	0.43
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.49	0.43
2:E:4984:ASN:C	2:E:4986:ALA:N	2.75	0.43
2:I:103:TYR:HB3	2:I:152:PRO:HD3	2.01	0.43
2:I:1854:PHE:HD1	2:I:1858:ASP:HB3	1.84	0.43
2:I:4215:ARG:NH2	3:I:5101:ATP:O1A	2.51	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.01	0.43
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.01	0.43
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.01	0.43
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.99	0.43
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	2.00	0.43
2:B:4983:HIS:CB	2:B:4988:TYR:HE2	2.32	0.43
2:E:734:GLY:O	2:E:736:HIS:ND1	2.51	0.43
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.00	0.43
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.01	0.43
2:I:4984:ASN:C	2:I:4986:ALA:N	2.75	0.43
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.01	0.43
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.43
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	2.00	0.43
2:G:4984:ASN:C	2:G:4986:ALA:N	2.75	0.43
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.01	0.43
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	2.00	0.43
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	2.00	0.43
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.51	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.01	0.43
2:E:838:HIS:HA	2:E:1201:HIS:HB3	2.00	0.43
2:E:1101:ARG:HH21	2:E:1115:LEU:H	1.66	0.43
2:E:2257:LEU:O	2:E:2261:SER:N	2.51	0.43
2:I:776:LEU:HG	2:I:848:HIS:HA	2.01	0.43
2:I:4993:MET:HA	2:I:4996:ILE:HD12	2.00	0.43
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.49	0.43
2:G:2299:VAL:O	2:G:2303:ALA:N	2.50	0.43
2:G:4929:LEU:HD13	2:G:4929:LEU:HA	1.91	0.43
2:B:103:TYR:HB3	2:B:152:PRO:HD3	2.01	0.42
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	2.00	0.42
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.00	0.42
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.54	0.42
2:E:4983:HIS:CB	2:E:4988:TYR:HE2	2.32	0.42
2:E:4993:MET:HA	2:E:4996:ILE:HD12	2.01	0.42
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.01	0.42
2:I:1101:ARG:HH21	2:I:1115:LEU:H	1.66	0.42
2:I:2780:ASN:O	2:I:2787:THR:OG1	2.34	0.42
2:I:4983:HIS:CB	2:I:4988:TYR:HE2	2.32	0.42
2:G:485:SER:O	2:G:489:ASN:N	2.37	0.42
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.51	0.42
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.54	0.42
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	2.00	0.42
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	2.00	0.42
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.00	0.42
2:G:4833:ASN:ND2	2:G:4935:LEU:O	2.52	0.42
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.52	0.42
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.42
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.02	0.42
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.34	0.42
2:B:38:ALA:HB1	2:B:64:ILE:HG13	2.02	0.42
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.00	0.42
2:B:1804:LEU:O	2:B:1808:ARG:N	2.49	0.42
2:B:2257:LEU:O	2:B:2261:SER:N	2.51	0.42
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.84	0.42
2:I:38:ALA:HB1	2:I:64:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:38:ALA:HB1	2:G:64:ILE:HG13	2.02	0.42
2:G:119:SER:HA	2:G:146:CYS:HA	2.01	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.54	0.42
2:G:4047:MET:HE3	2:G:4047:MET:HB2	1.89	0.42
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.01	0.42
2:B:4993:MET:HA	2:B:4996:ILE:HD12	2.00	0.42
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.42
2:E:4833:ASN:ND2	2:E:4935:LEU:O	2.52	0.42
2:I:1269:CYS:HA	2:I:1473:UNK:HA	2.01	0.42
2:G:1973:GLN:O	2:G:1977:TYR:N	2.45	0.42
2:B:2517:UNK:O	2:B:2521:UNK:N	2.53	0.42
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.01	0.42
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.02	0.42
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.32	0.42
2:G:940:GLY:O	2:G:1052:ASN:N	2.53	0.42
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.52	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.48	0.42
2:I:983:THR:O	2:I:987:ARG:N	2.48	0.42
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.49	0.42
2:G:34:LYS:N	2:G:53:SER:OG	2.40	0.42
2:G:103:TYR:HB3	2:G:152:PRO:HD3	2.01	0.42
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.42
2:G:4190:ILE:HD11	2:G:5026:ASP:CG	2.45	0.42
2:G:4983:HIS:CB	2:G:4988:TYR:HE2	2.32	0.42
2:G:4993:MET:HA	2:G:4996:ILE:HD12	2.01	0.42
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.42
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.32	0.42
2:E:38:ALA:HB1	2:E:64:ILE:HG13	2.02	0.42
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.51	0.42
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.42
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.42
2:I:4047:MET:HE3	2:I:4047:MET:HB2	1.89	0.42
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.42
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.01	0.42
2:E:1237:TRP:HH2	2:E:1652:GLU:HA	1.85	0.42
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.49	0.42
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.02	0.42
2:I:940:GLY:O	2:I:1052:ASN:N	2.53	0.42
2:I:1804:LEU:O	2:I:1808:ARG:N	2.49	0.42
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.00	0.42
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.42
2:G:2517:UNK:O	2:G:2521:UNK:N	2.53	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.51	0.42
2:B:776:LEU:HG	2:B:848:HIS:HA	2.01	0.42
2:B:4929:LEU:HD13	2:B:4929:LEU:HA	1.91	0.42
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.00	0.42
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.84	0.42
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.51	0.42
2:E:4190:ILE:HD11	2:E:5026:ASP:CG	2.45	0.42
2:I:4066:LEU:HD11	2:I:4173:TYR:HB2	2.02	0.42
2:G:399:GLN:HG2	2:G:403:MET:HE3	2.02	0.42
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.42
2:B:1695:LEU:HB3	2:B:1810:LYS:HZ2	1.85	0.41
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.01	0.41
2:I:3647:HIS:O	2:I:3651:ASN:ND2	2.53	0.41
2:I:4190:ILE:HD11	2:I:5026:ASP:CG	2.45	0.41
2:G:734:GLY:O	2:G:736:HIS:ND1	2.51	0.41
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.02	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.02	0.41
2:G:4066:LEU:HD11	2:G:4173:TYR:HB2	2.02	0.41
2:B:4066:LEU:HD11	2:B:4173:TYR:HB2	2.02	0.41
2:G:1154:ASP:O	2:G:1158:ASN:N	2.53	0.41
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.52	0.41
2:B:1237:TRP:HH2	2:B:1652:GLU:HA	1.85	0.41
2:B:4833:ASN:ND2	2:B:4935:LEU:O	2.52	0.41
2:E:1171:SER:OG	2:E:1175:SER:N	2.44	0.41
2:E:2517:UNK:O	2:E:2521:UNK:N	2.53	0.41
2:E:3647:HIS:O	2:E:3651:ASN:ND2	2.53	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.01	0.41
2:I:2674:UNK:O	2:I:2676:UNK:N	2.53	0.41
2:I:4084:PRO:HD2	2:I:4085:ARG:NH1	2.36	0.41
2:I:4823:LEU:HD23	2:G:4843:LEU:HD12	2.01	0.41
2:I:4929:LEU:HD13	2:I:4929:LEU:HA	1.91	0.41
2:G:2674:UNK:O	2:G:2676:UNK:N	2.54	0.41
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.02	0.41
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.01	0.41
2:B:4655:PHE:HD1	2:B:4796:MET:HE1	1.86	0.41
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.41
2:E:776:LEU:HG	2:E:848:HIS:HA	2.01	0.41
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.03	0.41
2:E:4655:PHE:HD1	2:E:4796:MET:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1154:ASP:O	2:I:1158:ASN:N	2.53	0.41
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.41
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.86	0.41
1:A:2:VAL:HG21	1:A:61:GLU:HB2	2.02	0.41
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.86	0.41
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.03	0.41
2:B:4148:THR:HG21	2:B:4178:LEU:HD21	2.02	0.41
2:E:1973:GLN:O	2:E:1977:TYR:N	2.45	0.41
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.85	0.41
2:I:3722:TYR:CZ	2:I:3782:MET:HE3	2.56	0.41
2:G:1237:TRP:HH2	2:G:1652:GLU:HA	1.85	0.41
2:G:3647:HIS:O	2:G:3651:ASN:ND2	2.53	0.41
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.55	0.41
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.86	0.41
2:E:4066:LEU:HD11	2:E:4173:TYR:HB2	2.02	0.41
2:E:4084:PRO:HD2	2:E:4085:ARG:NH1	2.36	0.41
2:E:4112:LEU:O	2:E:4115:SER:OG	2.38	0.41
2:E:4148:THR:HG21	2:E:4178:LEU:HD21	2.02	0.41
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.41
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.01	0.41
2:I:4848:VAL:O	2:I:4852:THR:OG1	2.34	0.41
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.55	0.41
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	2.03	0.41
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.55	0.41
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.03	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.41
2:B:2299:VAL:O	2:B:2303:ALA:N	2.50	0.41
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.85	0.41
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.52	0.41
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.93	0.41
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.86	0.41
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.41
2:I:399:GLN:HG2	2:I:403:MET:HE3	2.02	0.41
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.03	0.41
2:G:983:THR:O	2:G:987:ARG:N	2.48	0.41
2:B:2780:ASN:O	2:B:2787:THR:OG1	2.34	0.41
2:E:103:TYR:HB3	2:E:152:PRO:HD3	2.01	0.41
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.86	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.53	0.41
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.55	0.41
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2810:LYS:O	2:I:2814:LYS:N	2.45	0.41
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.03	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.52	0.41
1:F:2:VAL:HG21	1:F:61:GLU:HB2	2.02	0.41
1:A:7:ILE:N	1:A:71:ARG:O	2.50	0.41
1:J:7:ILE:N	1:J:71:ARG:O	2.50	0.41
2:B:767:VAL:HG12	2:B:769:GLU:HG3	2.03	0.41
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.85	0.41
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.41
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.03	0.41
2:B:3647:HIS:O	2:B:3651:ASN:ND2	2.53	0.41
2:B:4084:PRO:HD2	2:B:4085:ARG:NH1	2.36	0.41
2:B:4960:ILE:HD11	2:B:4985:LEU:CD2	2.51	0.41
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.86	0.41
2:E:1154:ASP:O	2:E:1158:ASN:N	2.53	0.41
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.03	0.41
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.86	0.41
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.47	0.41
2:I:4655:PHE:HD1	2:I:4796:MET:HE1	1.86	0.41
2:I:4833:ASN:ND2	2:I:4935:LEU:O	2.52	0.41
2:G:647:ASN:ND2	2:G:820:ARG:O	2.50	0.41
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.86	0.41
1:H:2:VAL:HG21	1:H:61:GLU:HB2	2.02	0.41
1:J:2:VAL:HG21	1:J:61:GLU:HB2	2.02	0.41
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.03	0.41
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.41
2:B:4190:ILE:HD11	2:B:5026:ASP:CG	2.45	0.41
2:E:767:VAL:HG12	2:E:769:GLU:HG3	2.03	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.03	0.41
2:E:4957:LYS:HG2	2:E:4964:GLY:CA	2.51	0.41
2:I:2517:UNK:O	2:I:2521:UNK:N	2.53	0.41
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.86	0.41
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.32	0.41
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.85	0.41
2:G:2208:MET:HE2	2:G:2208:MET:HB3	1.97	0.41
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.03	0.41
2:G:4655:PHE:HD1	2:G:4796:MET:HE1	1.86	0.41
2:B:4886:HIS:O	2:B:4890:GLY:N	2.52	0.40
2:E:4976:GLU:HA	2:E:4979:THR:CG2	2.52	0.40
2:I:864:PRO:HD2	2:I:867:LEU:HD12	2.03	0.40
2:I:1237:TRP:HH2	2:I:1652:GLU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.03	0.40
2:I:4148:THR:HG21	2:I:4178:LEU:HD21	2.02	0.40
2:G:37:LEU:HD11	2:G:47:CYS:HB3	2.04	0.40
2:G:1695:LEU:HB3	2:G:1810:LYS:HZ2	1.86	0.40
2:G:2095:GLN:HA	2:G:2127:GLN:NE2	2.37	0.40
2:G:3722:TYR:CZ	2:G:3782:MET:HE3	2.56	0.40
2:E:399:GLN:HG2	2:E:403:MET:HE3	2.02	0.40
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.02	0.40
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.04	0.40
2:I:4960:ILE:HD11	2:I:4985:LEU:CD2	2.51	0.40
2:G:767:VAL:HG12	2:G:769:GLU:HG3	2.03	0.40
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	2.04	0.40
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.04	0.40
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.86	0.40
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	2.04	0.40
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.86	0.40
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.56	0.40
2:E:2034:PHE:O	2:E:2038:LEU:N	2.55	0.40
2:I:37:LEU:HD11	2:I:47:CYS:HB3	2.03	0.40
2:G:4976:GLU:HA	2:G:4979:THR:CG2	2.52	0.40
2:B:399:GLN:HG2	2:B:403:MET:HE3	2.02	0.40
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.86	0.40
2:B:1154:ASP:O	2:B:1158:ASN:N	2.53	0.40
2:E:786:GLY:HA2	2:E:1631:GLN:HA	2.03	0.40
2:E:2095:GLN:HA	2:E:2127:GLN:NE2	2.36	0.40
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.03	0.40
2:E:3722:TYR:CZ	2:E:3782:MET:HE3	2.56	0.40
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.40
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.86	0.40
2:I:2034:PHE:O	2:I:2038:LEU:N	2.55	0.40
2:I:4987:ASN:HA	2:I:4990:PHE:HD2	1.87	0.40
2:G:786:GLY:HA2	2:G:1631:GLN:HA	2.03	0.40
2:G:1078:GLU:HG3	2:G:1237:TRP:HE1	1.87	0.40
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.86	0.40
2:G:4987:ASN:HA	2:G:4990:PHE:HD2	1.87	0.40
2:B:2095:GLN:HA	2:B:2127:GLN:NE2	2.37	0.40
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	2.03	0.40
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.86	0.40
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	2.04	0.40
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.03	0.40
2:I:2095:GLN:HA	2:I:2127:GLN:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:794:GLY:H	2:G:798:GLY:HA3	1.87	0.40
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.03	0.40
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.86	0.40
2:G:4148:THR:HG21	2:G:4178:LEU:HD21	2.02	0.40
2:G:4156:HIS:CE1	2:G:5036:LEU:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	J	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	43	77
2	E	3235/4416 (73%)	2892 (89%)	338 (10%)	5 (0%)	43	77
2	G	3235/4416 (73%)	2890 (89%)	340 (10%)	5 (0%)	43	77
2	I	3235/4416 (73%)	2889 (89%)	340 (10%)	6 (0%)	43	77
All	All	13360/18096 (74%)	11954 (90%)	1384 (10%)	22 (0%)	44	77

All (22) 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	1932	PRO

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

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	2033/3022 (67%)	2026 (100%)	7 (0%)	86	84
2	E	1878/3022 (62%)	1871 (100%)	7 (0%)	84	82
2	G	2470/3022 (82%)	2461 (100%)	9 (0%)	84	82
2	I	2016/3022 (67%)	2007 (100%)	9 (0%)	84	82
All	All	8749/12444 (70%)	8717 (100%)	32 (0%)	81	82

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	1600	LEU
2	B	1676	LEU
2	B	2010	LEU
2	B	3663	LEU
2	B	3805	LEU
2	E	719	LEU
2	E	1676	LEU
2	E	2010	LEU
2	E	3663	LEU
2	E	3805	LEU
2	E	4960	ILE
2	E	4961	CYS
2	I	131	LEU
2	I	719	LEU
2	I	1600	LEU
2	I	1676	LEU
2	I	2010	LEU
2	I	3663	LEU
2	I	3805	LEU
2	I	4960	ILE
2	I	4961	CYS
2	G	131	LEU
2	G	719	LEU
2	G	1600	LEU
2	G	1676	LEU
2	G	2010	LEU
2	G	3663	LEU
2	G	3805	LEU
2	G	4960	ILE
2	G	4961	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	84	ASN
2	B	98	HIS

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Mol	Chain	Res	Type
2	B	113	HIS
2	B	151	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	520	ASN
2	B	582	HIS
2	B	725	HIS
2	B	765	GLN
2	B	812	HIS
2	B	838	HIS
2	B	877	ASN
2	B	1598	GLN
2	B	1678	ASN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1953	HIS
2	B	2005	GLN
2	B	2127	GLN
2	B	2772	GLN
2	B	2773	ASN
2	B	2788	HIS
2	B	2856	ASN
2	B	3809	ASN
2	B	3814	GLN
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4043	GLN
2	B	4142	ASN

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Mol	Chain	Res	Type
2	B	4209	GLN
2	B	4246	GLN
2	B	4806	ASN
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	399	GLN
2	E	405	HIS
2	E	413	GLN
2	E	479	GLN
2	E	520	ASN
2	E	582	HIS
2	E	725	HIS
2	E	765	GLN
2	E	812	HIS
2	E	838	HIS
2	E	877	ASN
2	E	1220	GLN
2	E	1678	ASN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1775	HIS
2	E	1953	HIS
2	E	2260	ASN
2	E	2772	GLN
2	E	2773	ASN
2	E	3761	GLN
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3882	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	4209	GLN
2	E	4246	GLN
2	E	4776	GLN

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Mol	Chain	Res	Type
2	E	4806	ASN
2	E	4946	GLN
2	E	4947	GLN
2	E	4983	HIS
2	E	4987	ASN
2	E	5003	HIS
2	I	84	ASN
2	I	98	HIS
2	I	113	HIS
2	I	151	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	413	GLN
2	I	582	HIS
2	I	725	HIS
2	I	765	GLN
2	I	812	HIS
2	I	838	HIS
2	I	866	HIS
2	I	877	ASN
2	I	1220	GLN
2	I	1598	GLN
2	I	1678	ASN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1953	HIS
2	I	2005	GLN
2	I	2772	GLN
2	I	2773	ASN
2	I	2856	ASN
2	I	3700	GLN
2	I	3761	GLN
2	I	3809	ASN
2	I	3814	GLN
2	I	3830	GLN

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Mol	Chain	Res	Type
2	I	3850	GLN
2	I	3882	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4054	ASN
2	I	4209	GLN
2	I	4246	GLN
2	I	4776	GLN
2	I	4806	ASN
2	I	4864	ASN
2	I	4946	GLN
2	I	4987	ASN
2	I	5003	HIS
2	G	57	ASN
2	G	84	ASN
2	G	98	HIS
2	G	113	HIS
2	G	151	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	399	GLN
2	G	405	HIS
2	G	413	GLN
2	G	582	HIS
2	G	725	HIS
2	G	765	GLN
2	G	838	HIS
2	G	866	HIS
2	G	877	ASN
2	G	1220	GLN
2	G	1598	GLN
2	G	1678	ASN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN

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Mol	Chain	Res	Type
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1953	HIS
2	G	2005	GLN
2	G	2127	GLN
2	G	2260	ASN
2	G	2772	GLN
2	G	2773	ASN
2	G	2856	ASN
2	G	3761	GLN
2	G	3809	ASN
2	G	3814	GLN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4043	GLN
2	G	4054	ASN
2	G	4209	GLN
2	G	4246	GLN
2	G	4776	GLN
2	G	4806	ASN
2	G	4864	ASN
2	G	4946	GLN
2	G	4947	GLN
2	G	4983	HIS
2	G	4987	ASN
2	G	5003	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.66	9 (18%)
4	CFF	I	5102	-	15,15,15	1.99	7 (46%)	23,23,23	2.74	11 (47%)
4	CFF	B	5102	-	15,15,15	1.99	7 (46%)	23,23,23	2.74	11 (47%)
4	CFF	G	5102	-	15,15,15	1.99	7 (46%)	23,23,23	2.75	11 (47%)
3	ATP	G	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.67	9 (18%)
3	ATP	B	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.67	9 (18%)
3	ATP	I	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.67	9 (18%)
4	CFF	E	5102	-	15,15,15	1.99	7 (46%)	23,23,23	2.74	11 (47%)

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	E	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	I	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	4.46	1.47	1.39
3	I	5101	ATP	C5-C4	4.46	1.47	1.39
3	G	5101	ATP	C5-C4	4.43	1.47	1.39
3	E	5101	ATP	C5-C4	4.41	1.46	1.39
4	G	5102	CFF	C6-N1	-3.85	1.32	1.40
4	I	5102	CFF	C6-N1	-3.85	1.32	1.40
4	B	5102	CFF	C6-N1	-3.83	1.32	1.40
4	E	5102	CFF	C6-N1	-3.83	1.32	1.40
4	B	5102	CFF	C4-N3	-2.94	1.33	1.38
4	E	5102	CFF	C4-N3	-2.94	1.33	1.38
4	I	5102	CFF	C4-N3	-2.94	1.33	1.38
4	G	5102	CFF	C4-N3	-2.92	1.33	1.38
4	I	5102	CFF	C5-N7	-2.58	1.33	1.38
4	G	5102	CFF	C5-N7	-2.56	1.33	1.38
4	B	5102	CFF	C5-N7	-2.55	1.34	1.38
4	E	5102	CFF	C5-N7	-2.55	1.34	1.38
3	G	5101	ATP	C5-C6	2.49	1.47	1.41
3	B	5101	ATP	C5-C6	2.48	1.47	1.41
3	E	5101	ATP	C5-C6	2.48	1.47	1.41
3	I	5101	ATP	C5-C6	2.47	1.47	1.41
3	B	5101	ATP	C5-N7	-2.36	1.34	1.39
3	G	5101	ATP	C5-N7	-2.36	1.34	1.39
3	E	5101	ATP	C5-N7	-2.33	1.34	1.39
3	I	5101	ATP	C5-N7	-2.33	1.34	1.39
3	B	5101	ATP	C8-N7	2.27	1.36	1.31
3	E	5101	ATP	C8-N7	2.27	1.36	1.31
3	I	5101	ATP	C8-N7	2.27	1.36	1.31
3	G	5101	ATP	C8-N7	2.25	1.36	1.31
3	G	5101	ATP	C4-N9	-2.25	1.33	1.37
3	B	5101	ATP	C4-N9	-2.24	1.33	1.37
3	E	5101	ATP	C4-N9	-2.24	1.33	1.37
3	I	5101	ATP	C4-N9	-2.24	1.33	1.37
4	I	5102	CFF	C2-N3	-2.20	1.34	1.39
4	G	5102	CFF	C2-N3	-2.19	1.34	1.39
4	B	5102	CFF	C2-N3	-2.18	1.34	1.39
4	E	5102	CFF	C2-N3	-2.18	1.34	1.39
4	B	5102	CFF	O13-C6	-2.18	1.18	1.23
4	E	5102	CFF	O13-C6	-2.18	1.18	1.23
4	I	5102	CFF	O13-C6	-2.18	1.18	1.23
4	G	5102	CFF	O13-C6	-2.17	1.18	1.23
4	E	5102	CFF	C2-N1	-2.09	1.34	1.39
4	I	5102	CFF	C2-N1	-2.09	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	CFF	C2-N1	-2.08	1.34	1.39
4	G	5102	CFF	C2-N1	-2.08	1.34	1.39
4	G	5102	CFF	O11-C2	-2.03	1.18	1.22
4	B	5102	CFF	O11-C2	-2.01	1.18	1.22
4	E	5102	CFF	O11-C2	-2.01	1.18	1.22
4	I	5102	CFF	O11-C2	-2.01	1.18	1.22

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	5102	CFF	C14-N7-C8	-7.78	111.73	126.28
4	B	5102	CFF	C14-N7-C8	-7.76	111.76	126.28
4	E	5102	CFF	C14-N7-C8	-7.76	111.76	126.28
4	G	5102	CFF	C14-N7-C8	-7.75	111.77	126.28
3	I	5101	ATP	C5-C4-N3	-5.48	119.17	126.72
3	B	5101	ATP	C5-C4-N3	-5.46	119.20	126.72
3	G	5101	ATP	C5-C4-N3	-5.45	119.21	126.72
3	E	5101	ATP	C5-C4-N3	-5.43	119.25	126.72
4	I	5102	CFF	C14-N7-C5	5.05	139.78	127.77
4	G	5102	CFF	C14-N7-C5	5.03	139.74	127.77
4	B	5102	CFF	C14-N7-C5	5.03	139.73	127.77
4	E	5102	CFF	C14-N7-C5	5.03	139.73	127.77
3	I	5101	ATP	N3-C4-N9	4.34	134.55	127.17
3	B	5101	ATP	N3-C4-N9	4.32	134.52	127.17
3	G	5101	ATP	N3-C4-N9	4.31	134.49	127.17
3	E	5101	ATP	N3-C4-N9	4.29	134.46	127.17
4	G	5102	CFF	C5-C6-N1	4.07	119.51	112.06
4	B	5102	CFF	C5-C6-N1	4.06	119.51	112.06
4	E	5102	CFF	C5-C6-N1	4.06	119.50	112.06
4	I	5102	CFF	C5-C6-N1	4.04	119.47	112.06
3	G	5101	ATP	C2-N3-C4	3.49	120.36	111.83
3	B	5101	ATP	C2-N3-C4	3.49	120.35	111.83
3	I	5101	ATP	C2-N3-C4	3.48	120.32	111.83
3	E	5101	ATP	C2-N3-C4	3.46	120.29	111.83
4	B	5102	CFF	C6-N1-C2	-3.24	120.39	125.66
4	E	5102	CFF	C6-N1-C2	-3.24	120.40	125.66
4	G	5102	CFF	C6-N1-C2	-3.22	120.42	125.66
4	I	5102	CFF	C6-N1-C2	-3.20	120.46	125.66
3	I	5101	ATP	C4-C5-N7	-3.20	106.92	110.58
3	B	5101	ATP	C4-C5-N7	-3.18	106.95	110.58
3	G	5101	ATP	C4-C5-N7	-3.17	106.96	110.58
3	E	5101	ATP	C4-C5-N7	-3.16	106.97	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-3.10	123.88	128.58
3	B	5101	ATP	N3-C2-N1	-3.09	123.90	128.58
3	I	5101	ATP	N3-C2-N1	-3.08	123.92	128.58
3	E	5101	ATP	N3-C2-N1	-3.07	123.93	128.58
4	G	5102	CFF	N7-C8-N9	-2.98	108.07	113.48
4	I	5102	CFF	N7-C8-N9	-2.97	108.10	113.48
4	E	5102	CFF	N7-C8-N9	-2.97	108.10	113.48
4	B	5102	CFF	N7-C8-N9	-2.96	108.11	113.48
4	G	5102	CFF	O13-C6-C5	-2.81	120.63	126.38
4	I	5102	CFF	O13-C6-C5	-2.79	120.67	126.38
4	B	5102	CFF	O13-C6-C5	-2.78	120.69	126.38
4	E	5102	CFF	O13-C6-C5	-2.78	120.69	126.38
3	I	5101	ATP	C4-N9-C8	2.72	108.60	105.74
3	B	5101	ATP	C4-N9-C8	2.69	108.56	105.74
3	E	5101	ATP	C4-N9-C8	2.69	108.56	105.74
4	G	5102	CFF	C6-C5-C4	-2.68	119.55	122.92
3	G	5101	ATP	C4-N9-C8	2.67	108.54	105.74
4	I	5102	CFF	C6-C5-C4	-2.66	119.57	122.92
4	B	5102	CFF	C6-C5-C4	-2.64	119.59	122.92
4	E	5102	CFF	C6-C5-C4	-2.64	119.59	122.92
4	G	5102	CFF	N3-C4-N9	2.59	130.34	126.27
4	E	5102	CFF	N3-C4-N9	2.59	130.34	126.27
4	B	5102	CFF	N3-C4-N9	2.59	130.33	126.27
4	I	5102	CFF	N3-C4-N9	2.59	130.33	126.27
4	B	5102	CFF	C10-N1-C6	2.39	121.34	117.64
4	E	5102	CFF	C10-N1-C6	2.39	121.34	117.64
4	G	5102	CFF	C10-N1-C6	2.38	121.33	117.64
4	I	5102	CFF	C10-N1-C6	2.36	121.30	117.64
4	G	5102	CFF	C12-N3-C2	2.26	121.27	117.33
4	I	5102	CFF	C12-N3-C2	2.25	121.25	117.33
4	B	5102	CFF	C12-N3-C2	2.24	121.24	117.33
4	E	5102	CFF	C12-N3-C2	2.24	121.24	117.33
3	I	5101	ATP	C5-N7-C8	2.23	106.95	103.45
3	G	5101	ATP	C5-N7-C8	2.21	106.93	103.45
3	B	5101	ATP	C5-N7-C8	2.21	106.93	103.45
3	E	5101	ATP	C3'-C2'-C1'	2.21	105.64	101.46
3	G	5101	ATP	C3'-C2'-C1'	2.21	105.64	101.46
3	B	5101	ATP	C3'-C2'-C1'	2.21	105.64	101.46
3	E	5101	ATP	C5-N7-C8	2.19	106.89	103.45
3	I	5101	ATP	C3'-C2'-C1'	2.18	105.59	101.46
3	B	5101	ATP	C6-C5-N7	2.11	136.15	132.09
4	B	5102	CFF	N3-C2-N1	2.10	119.76	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	C6-C5-N7	2.10	136.13	132.09
4	E	5102	CFF	N3-C2-N1	2.09	119.75	117.14
3	I	5101	ATP	C6-C5-N7	2.09	136.13	132.09
3	E	5101	ATP	C6-C5-N7	2.09	136.12	132.09
4	G	5102	CFF	N3-C2-N1	2.08	119.74	117.14
4	I	5102	CFF	N3-C2-N1	2.07	119.72	117.14

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C3'-C4'-C5'-O5'
3	E	5101	ATP	C3'-C4'-C5'-O5'
3	I	5101	ATP	C3'-C4'-C5'-O5'
3	G	5101	ATP	C3'-C4'-C5'-O5'
3	B	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

4 monomers are involved in 8 short contacts:

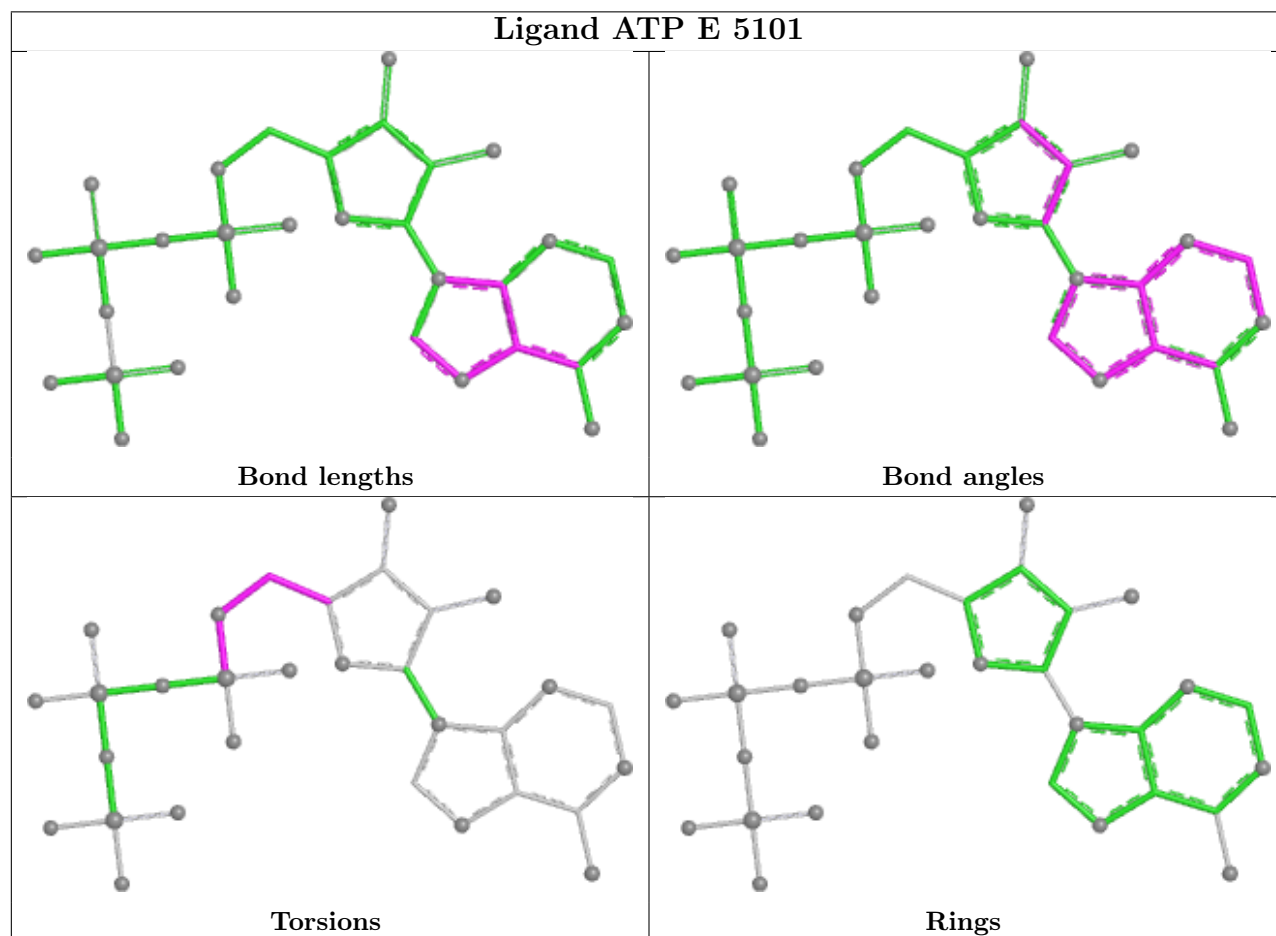
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	2	0

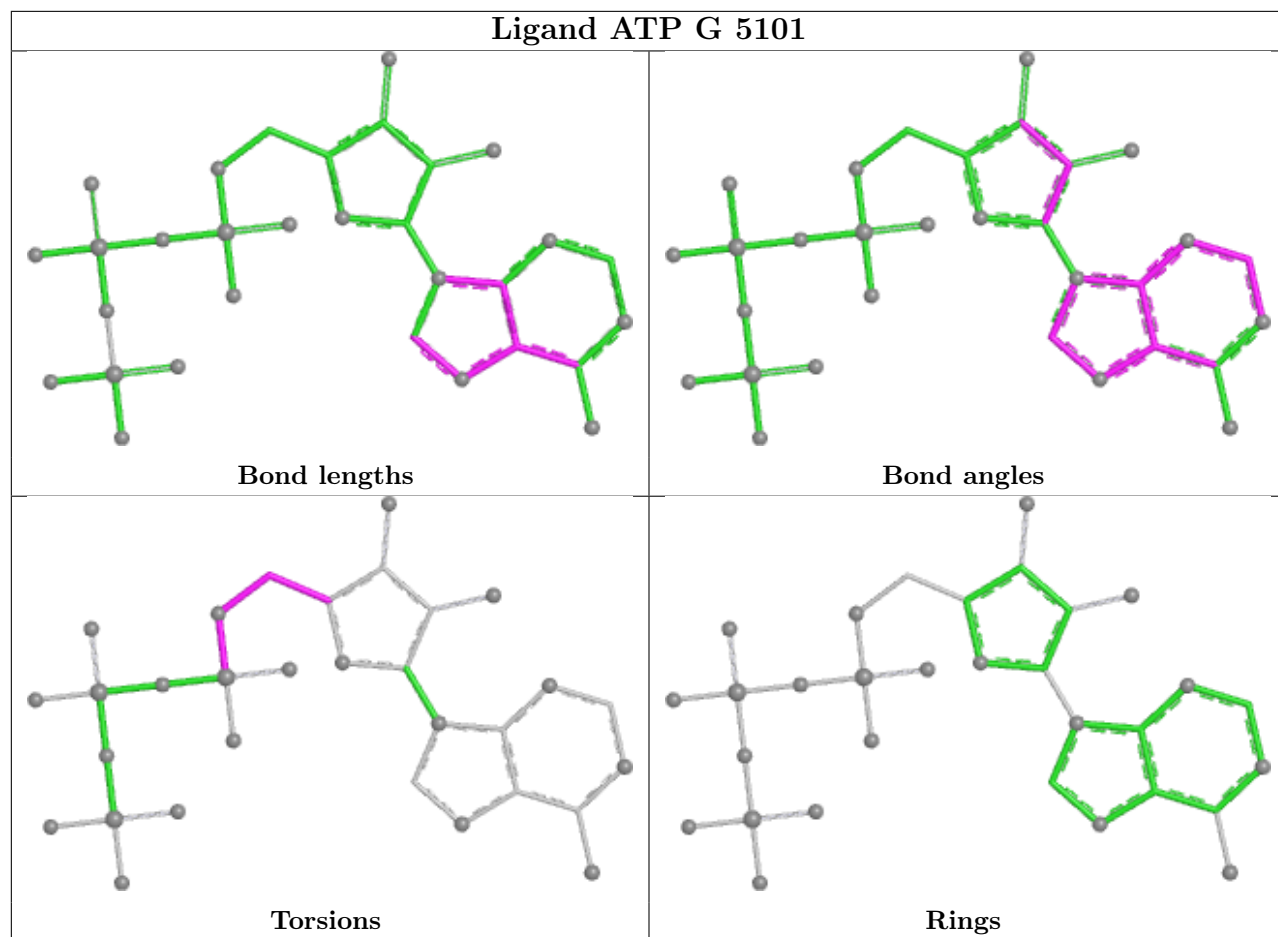
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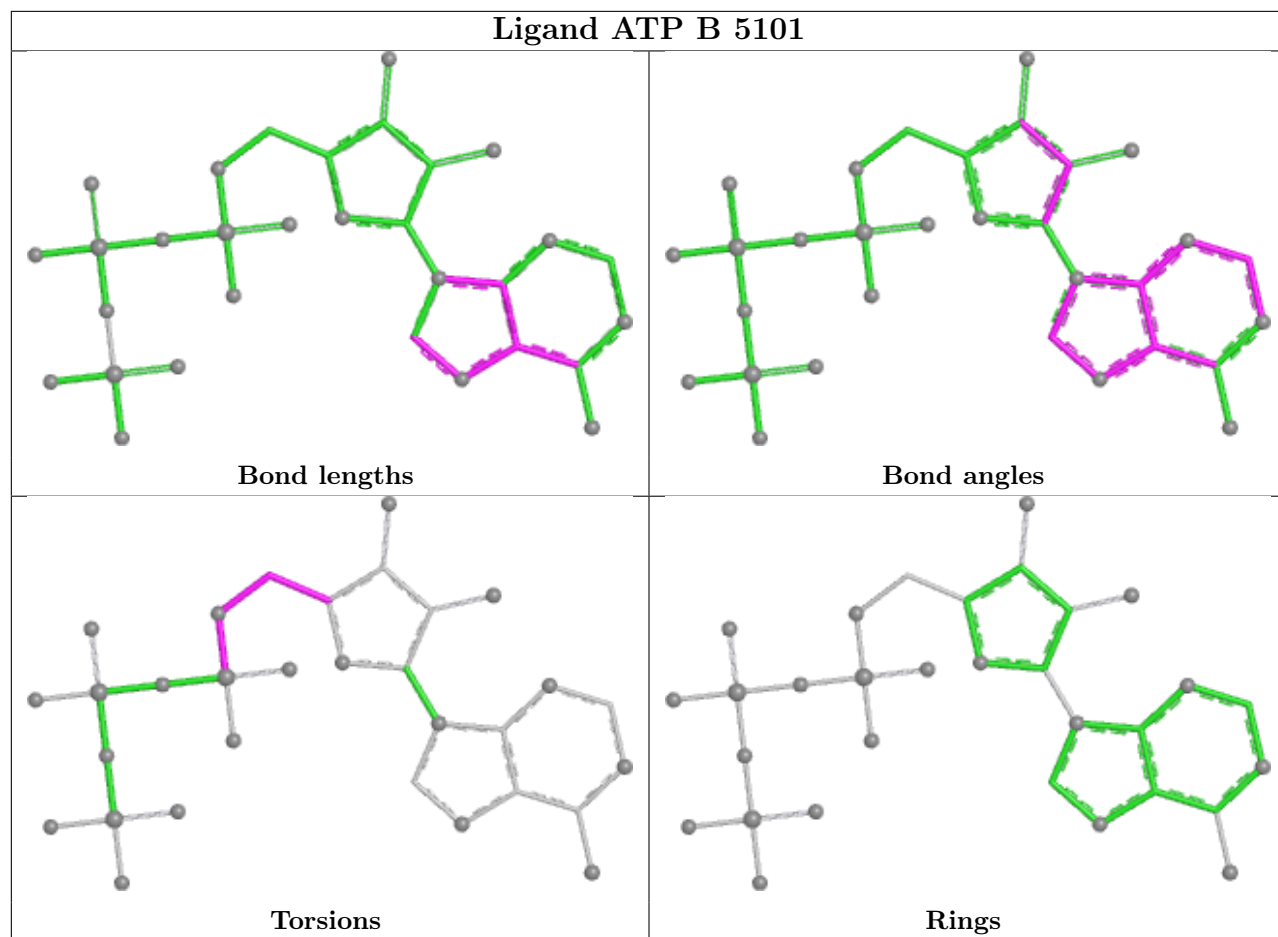
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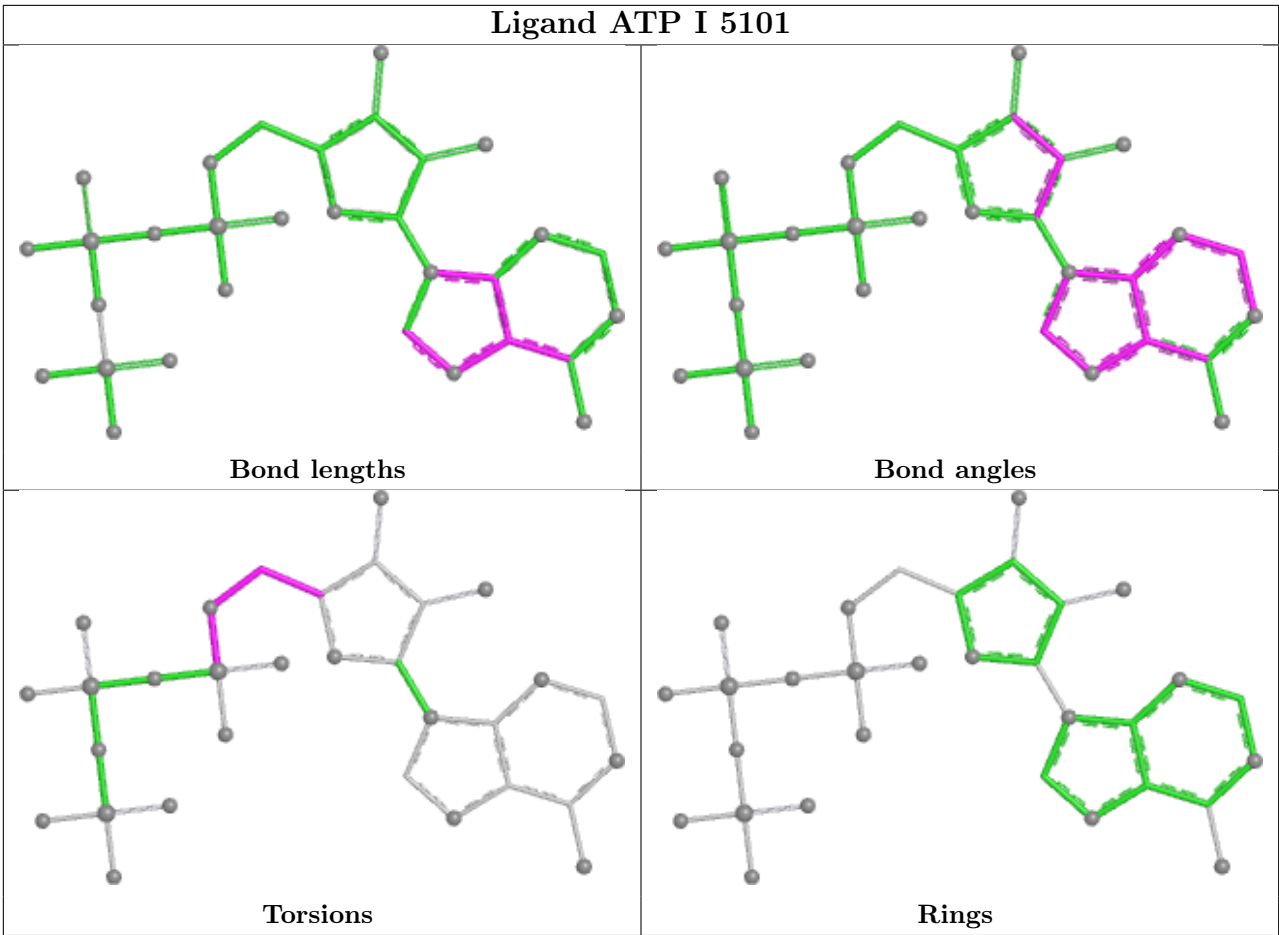
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5101	ATP	2	0
3	B	5101	ATP	2	0
3	I	5101	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	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	72.88
1	E	4345:UNK	C	4540:PHE	N	72.88

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.88
1	G	4345:UNK	C	4540:PHE	N	72.88
1	B	3613:UNK	C	3639:THR	N	43.44
1	E	3613:UNK	C	3639:THR	N	43.44
1	I	3613:UNK	C	3639:THR	N	43.44
1	G	3613:UNK	C	3639:THR	N	43.44
1	B	4253:GLU	C	4320:UNK	N	27.19
1	E	4253:GLU	C	4320:UNK	N	27.19
1	I	4253:GLU	C	4320:UNK	N	27.19
1	G	4253:GLU	C	4320:UNK	N	27.19
1	B	3163:UNK	C	3170:UNK	N	15.93
1	E	3163:UNK	C	3170:UNK	N	15.93
1	I	3163:UNK	C	3170:UNK	N	15.93
1	G	3163:UNK	C	3170:UNK	N	15.93
1	E	3063:UNK	C	3134:UNK	N	15.07
1	G	3063:UNK	C	3134:UNK	N	15.07
1	B	3063:UNK	C	3134:UNK	N	15.06
1	I	3063:UNK	C	3134:UNK	N	15.06
1	B	3468:UNK	C	3511:UNK	N	14.28
1	E	3468:UNK	C	3511:UNK	N	14.28
1	I	3468:UNK	C	3511:UNK	N	14.28
1	G	3468:UNK	C	3511:UNK	N	14.28
1	B	2703:UNK	C	2734:ASN	N	14.09
1	E	2703:UNK	C	2734:ASN	N	14.09
1	I	2703:UNK	C	2734:ASN	N	14.09
1	G	2703:UNK	C	2734:ASN	N	14.09
1	B	3236:UNK	C	3241:UNK	N	13.30
1	E	3236:UNK	C	3241:UNK	N	13.30
1	I	3236:UNK	C	3241:UNK	N	13.30
1	G	3236:UNK	C	3241:UNK	N	13.30
1	B	1564:UNK	C	1573:MET	N	12.36
1	E	1564:UNK	C	1573:MET	N	12.36
1	I	1564:UNK	C	1573:MET	N	12.36
1	G	1564:UNK	C	1573:MET	N	12.36
1	B	2976:UNK	C	2995:UNK	N	12.29
1	E	2976:UNK	C	2995:UNK	N	12.29
1	I	2976:UNK	C	2995:UNK	N	12.29
1	G	2976:UNK	C	2995:UNK	N	12.29
1	B	3254:UNK	C	3261:UNK	N	8.12
1	E	3254:UNK	C	3261:UNK	N	8.12
1	I	3254:UNK	C	3261:UNK	N	8.12
1	G	3254:UNK	C	3261:UNK	N	8.12

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	6.33
1	E	1297:UNK	C	1430:UNK	N	6.33
1	I	1297:UNK	C	1430:UNK	N	6.33
1	G	1297:UNK	C	1430:UNK	N	6.33
1	B	2939:ARG	C	2942:UNK	N	3.27
1	E	2939:ARG	C	2942:UNK	N	3.27
1	I	2939:ARG	C	2942:UNK	N	3.27
1	G	2939:ARG	C	2942:UNK	N	3.27
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

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8379. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.