



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 30, 2017 – 09:17 PM EST

PDB ID : 5GOA
EMDB ID: : EMD-9529
Title : Cryo-EM structure of RyR2 in open state
Authors : Peng, W.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-26
Resolution : 4.20 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

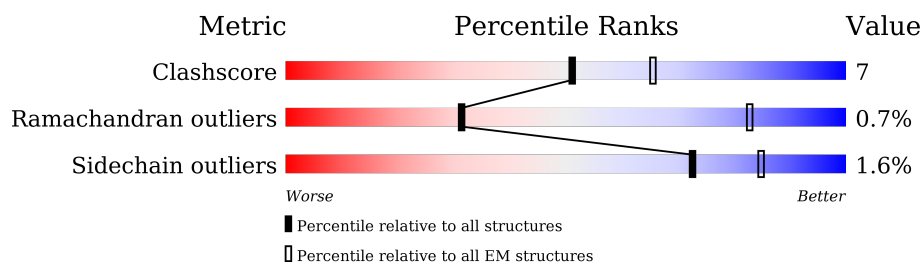
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4968	
1	B	4968	
1	C	4968	
1	D	4968	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105072 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	B	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	C	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	D	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		

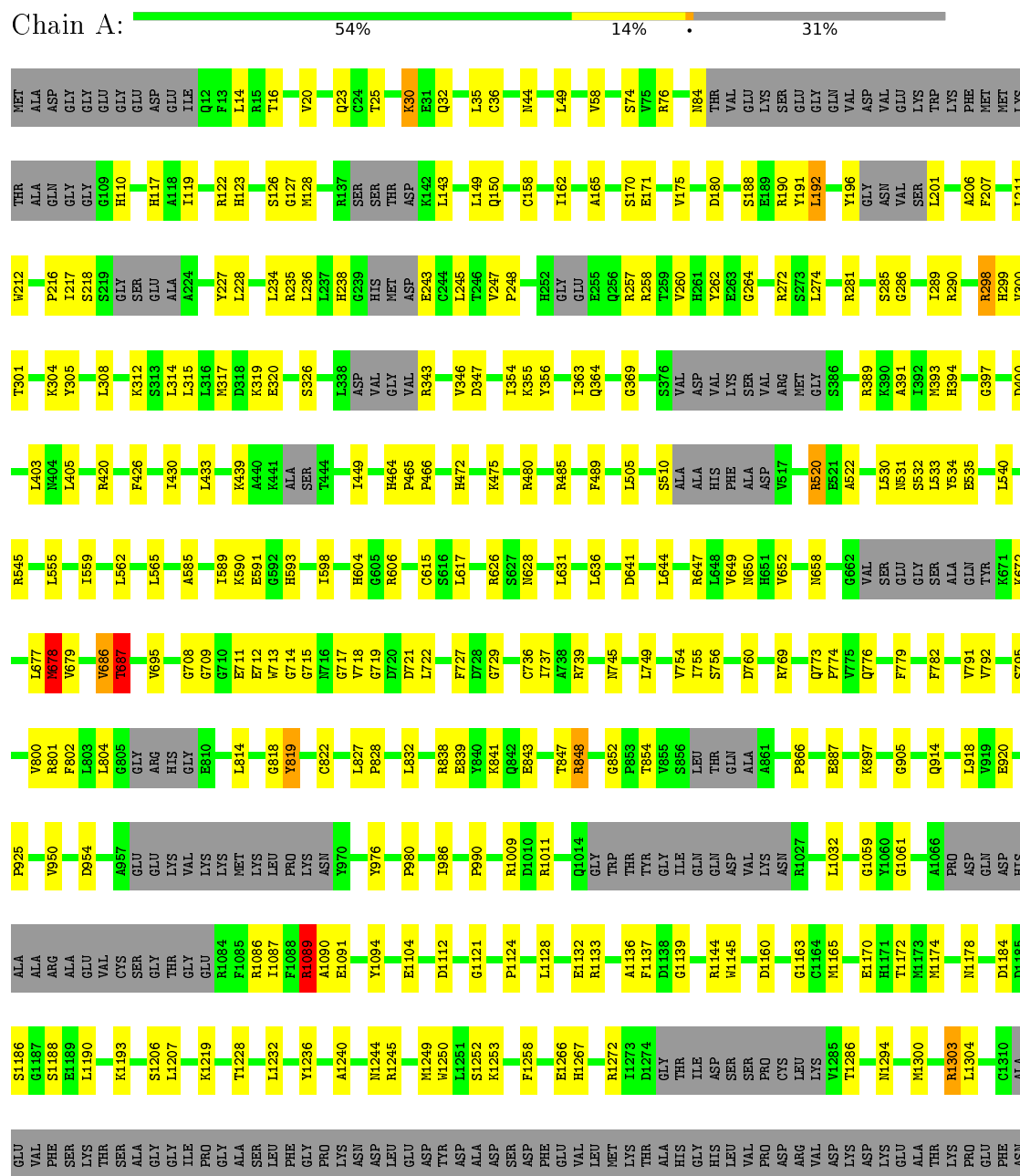
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Zn	0
			1	1	
2	A	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

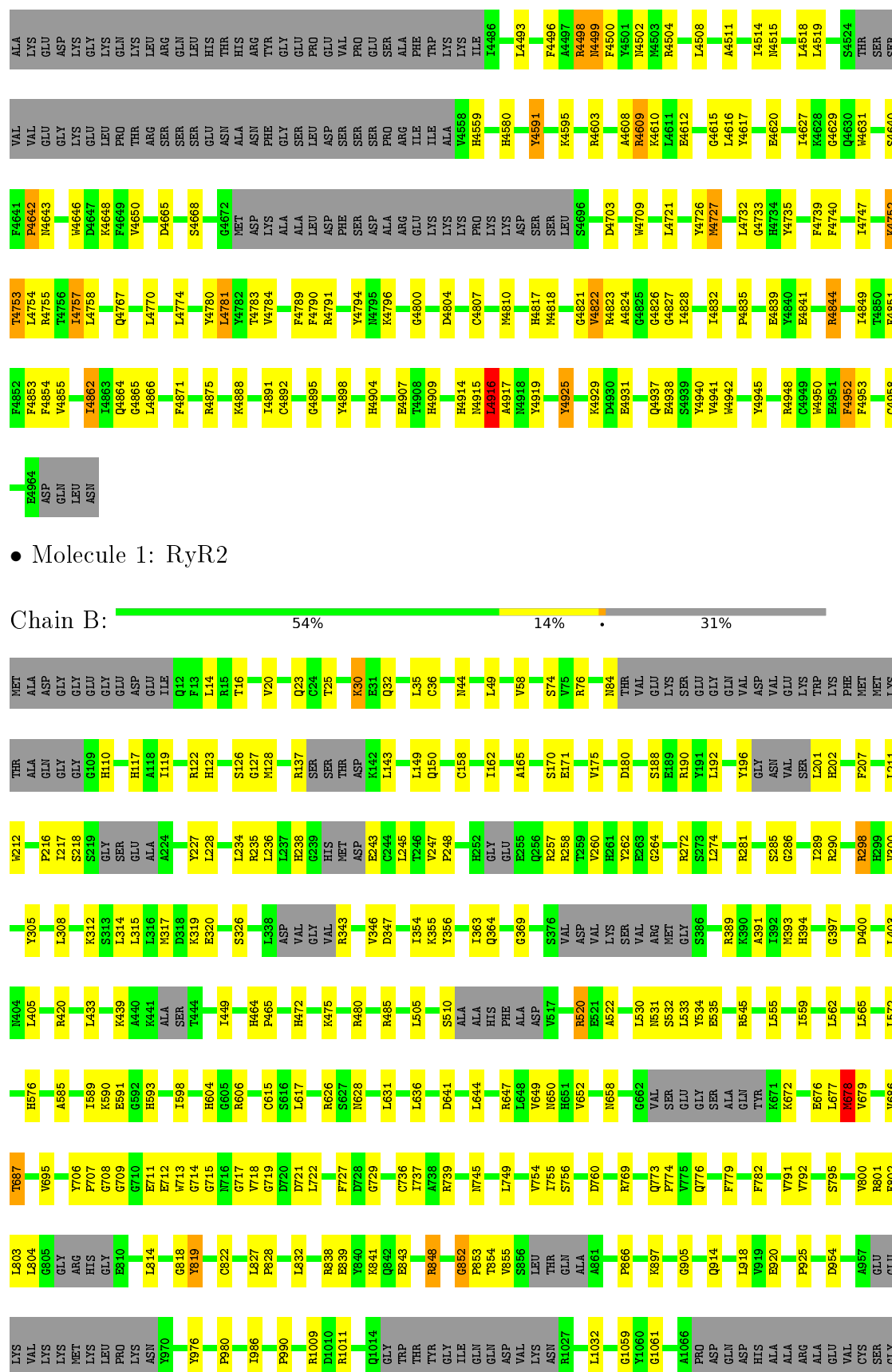
- Molecule 1: RyR2





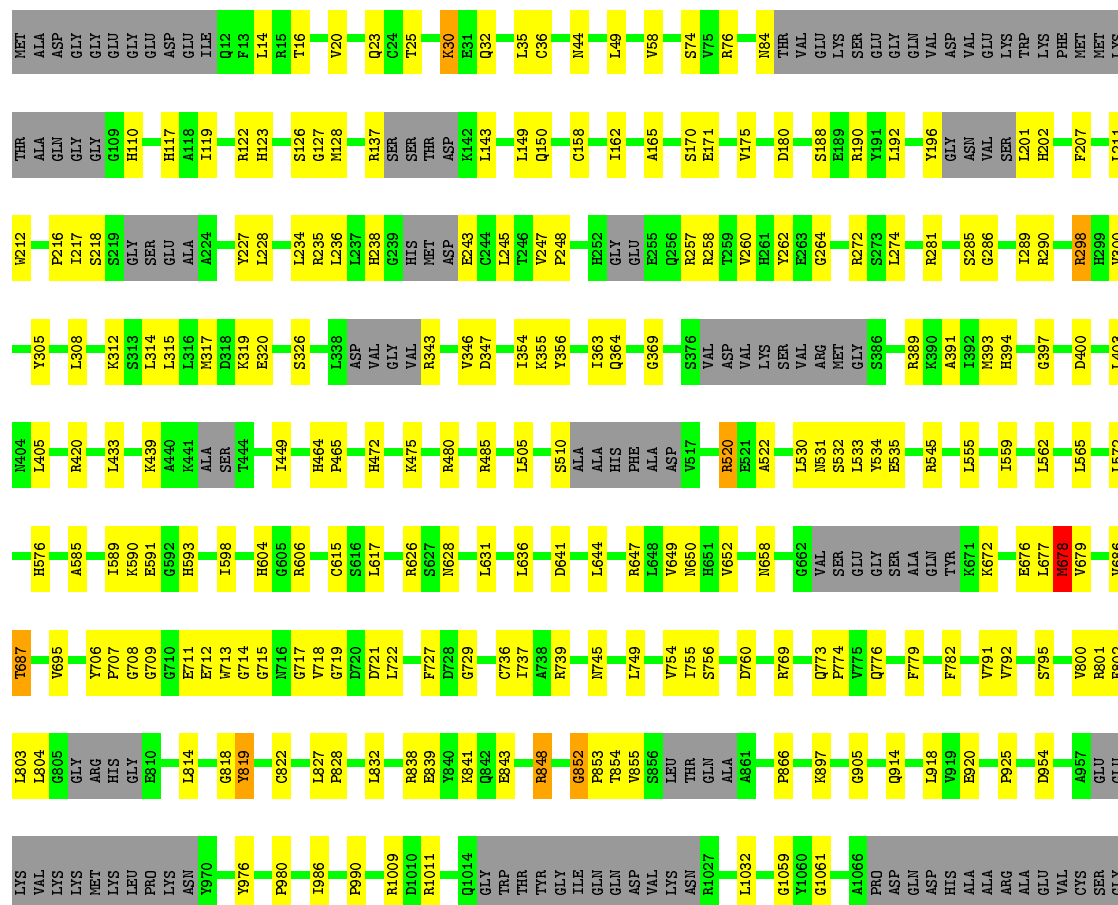






• Molecule 1: RyR2

Chain B: 54% 14% 31%





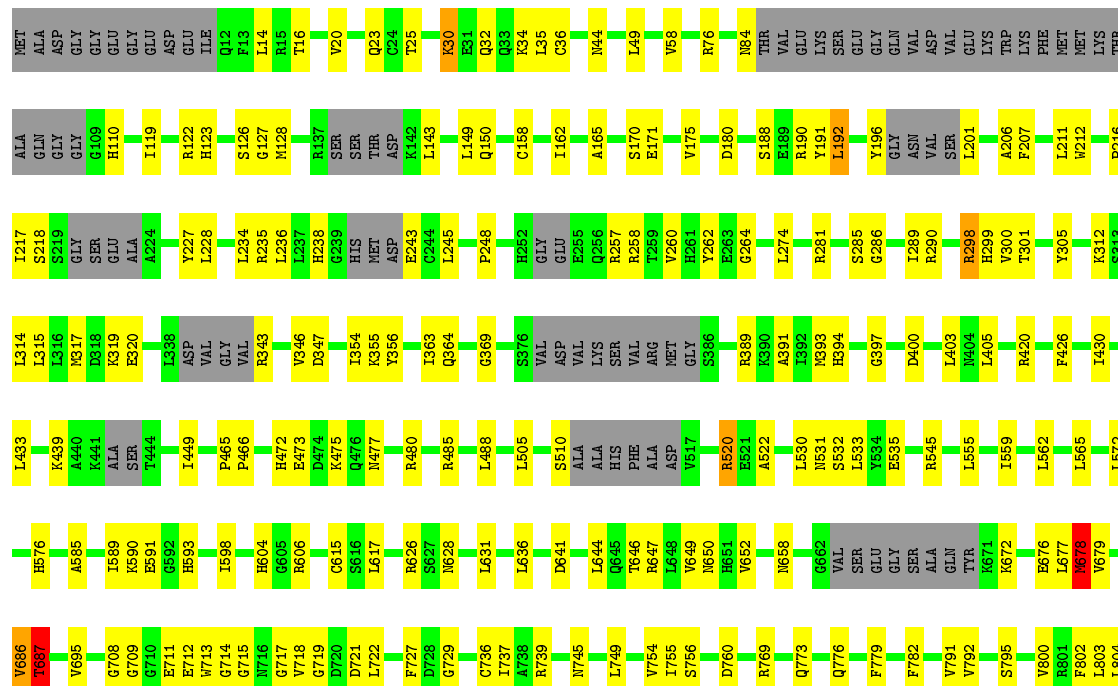






M2469	M2390	P2293	K2192	VAL	LYS	SER	F1763	L1651	A1568	G1470	SER	ASP	M1249	E1104	P980
T2391	T2391	D2301	F2204	GLU	GLU	GLU	S1764	K1652	G1569	K1475	THR	ALA	M1250	G1121	I986
F2392	F2392	R2306	C2205	ASP	PHE	ASP	S1770	F1653	L1570	V1476	SER	ASP	L1251	P1124	P990
L2396	L2396	R2304	R2206	SER	ARG	SER	ILE	H1654	V1579	I1480	SER	PHE	K1253	L1128	R1009
A2404	A2404	I2326	M2211	LYS	PRO	LEU	ASN	T1657	P1584	M1486	ARG	GLU	F1258	E1132	R1010
PRO	PRO	P2329	Q2212	GLN	GLN	GLY	GLU	V1664	P1584	CYS	THR	VAL	E1266	R1133	R1011
GLU	GLU	E2330	K2213	ALA	ALA	PRO	CYS	V1672	L1586	M1487	GLU	LEU	H1267	Q1014	Q1014
MET	MET	CYS	L2222	ILE	ILE	GLY	TYR	D1681	L1587	V1488	ASP	THR	R1273	A1136	GLY
L2489	L2489	PHE	S2226	ASN	ASN	GLU	S1778	V1689	H1588	C1489	VAL	ALA	D1274	F1137	THR
HIS	HIS	PRO	S2227	GLU	GLU	SER	S1779	I1689	V1590	A1490	ALA	HIS	GLY	D1138	THR
ALA	ALA	LEU	V2076	LEU	LEU	LYS	L1787	E1690	F1590	GLY	ASP	GLY	THR	R1144	GLY
ALA	ALA	ALA	E2077	ASN	ASN	GLY	M1691	M1691	H1593	GLU	ASP	HIS	THR	W1145	GLY
LYS	LYS	ARG	E2080	PHE	PHE	GLY	K1790	K1692	H1593	MET	ASP	VAL	ILE	D1160	GLN
GLY	GLY	GLY	L2081	LYS	LYS	LYS	V1799	P1695	R1598	SER	ASP	PRO	ASP	G1163	ASP
E2416	E2416	GLY	V2082	ASP	ASP	ARG	Q1800	R1699	M1599	PRO	THR	ASP	SER	C1164	VAL
ASP	ASP	GLY	R2083	ASP	ASP	PRO	E1801	Y1703	P1600	GLY	ASP	ARG	PRO	M1165	LYS
THR	THR	GLY	G2343	SER	SER	GLU	D1808	Y1703	M1601	GLY	THR	VAL	CYS	GLY	ASN
ALA	ALA	ASN	I2109	GLU	GLU	GLU	P1809	Y1703	Q1602	ARG	MET	ASP	LEU	L1027	R1027
SER	SER	GLY	L2121	CYS	CYS	L1894	V1810	L1706	K1605	M1501	GLN	ASP	LYS	E1170	GLY
ALA	ALA	SER	L2121	PRO	PRO	L1899	F1816	I1707	V1606	L1505	THR	LYS	T1286	H1171	THR
T2511	T2511	E2349	T2239	CYS	CYS	L1899	F1816	I1707	D1607	L1505	SER	GLU	T1286	T1172	ALA
PRO	PRO	ALA	P2240	PRO	PRO	L1899	F1816	I1707	V1607	G1508	THR	ALA	M1294	M1173	G1059
GLU	GLU	GLU	L2241	GLU	GLU	V1903	P1820	L1711	D1608	C1509	ALA	ALA	Y1060	M1174	Y1060
L2520	L2520	ASP	D2242	GLU	GLU	K1904	L1821	T1716	R1610	V1510	L1432	PRO	R1303	M1178	G1061
L2521	L2521	PRO	V2243	ILE	ILE	L1905	L1821	T1716	I1611	V1511	GLU	GLU	L1304	GLY	ALA
C2522	C2522	ARG	V2133	ARG	ARG	L1926	L1833	L1719	S1612	ASP	ALA	GLU	C1310	D1184	PRO
T2523	T2523	SER	E2283	ASP	ASP	V1927	F1834	L1726	E1613	ALA	GLY	ASN	G1310	D1185	ASN
ARG	ARG	GLY	L2254	GLN	GLN	I1726	H1835	V1727	L1618	ALA	GLN	GLN	ALA	G1186	GLN
S2438	S2438	ASP	A2255	LEU	LEU	H1836	N1836	V1727	W1617	SER	ALA	HIS	VAL	G1187	ASP
L2439	L2439	GLY	L2256	LEU	LEU	N1836	N1836	V1727	L1618	G1516	ALA	PRO	PHE	E1188	HIS
Q2442	Q2442	PRO	E2138	D1999	D1999	E1847	E1847	I1736	V1619	GLY	ALA	ASP	SER	L1190	ALA
MET	MET	SER	E2139	GLU	GLU	P1848	P1848	T1737	Q1620	M1523	ALA	TYR	LYS	ALA	ALA
THR	THR	PRO	E2140	GLU	GLU	S1849	S1849	L1738	C1621	GLY	ALA	ALA	THR	ALA	ALA
ILE	ILE	GLY	M2143	ASP	ASP	VAL	VAL	F1739	L1622	VAL	ALA	GLN	ALA	GLU	ARG
L2528	L2528	GLY	M2143	SER	SER	PHE	PHE	F1739	C1621	P1541	ALA	GLN	ALA	GLU	ALA
THR	THR	SER	M2163	TYR	TYR	LYS	LYS	P1740	Q1626	F1544	ALA	LYS	ALA	VAL	VAL
ARG	ARG	PRO	L2166	ASN	ASN	GLU	GLU	D1741	Q1626	Q1546	GLY	PRO	GLY	CYS	CYS
CYS	CYS	PRO	L2173	GLY	GLY	ALA	ALA	ASN	S1629	A1545	LEU	SER	ILE	S1206	SER
ALA	ALA	PRO	M2175	VAL	VAL	ALA	ALA	LYS	I1632	Q1554	GLY	ARG	GLY	L1207	GLY
P2534	P2534	THR	E2174	GLN	GLN	PRO	PRO	HIS	E1635	F1555	ALA	LYS	ALA	K1219	GLY
V2553	V2553	SER	V2175	ASP	ASP	GLU	GLU	G1747	N1636	E1556	GLN	ARG	LEU	T1228	GLU
TYR	TYR	GLY	G2181	LEU	LEU	GLU	GLU	G1747	R1637	LEU	ARG	PHE	PHE	T1228	GLU
ARG	ARG	MET	G2181	ASN	ASN	GLU	GLU	G1747	E1635	LEU	ARG	ARG	ARG	F1085	F1085
LEU	LEU	GLY	G2181	GLY	GLY	GLU	GLU	G1747	N1636	LEU	ARG	ARG	ARG	R1086	R1086
P2558	P2558	THR	G2181	GLY	GLY	GLU	GLU	G1747	R1637	LEU	ARG	ARG	ARG	I1087	I1087
F2568	F2568	GLY	G2181	GLY	GLY	GLU	GLU	G1747	E1635	LEU	ARG	ARG	ARG	F1088	F1088
ILE	ILE	GLY	G2181	GLY	GLY	GLU	GLU	G1747	R1637	LEU	ARG	ARG	ARG	R1089	R1089
S2576	S2576	CYS	G2181	GLY	GLY	GLU	GLU	G1747	E1635	LEU	ARG	ARG	ARG	A1090	A1090
C2582	C2582	GLY	G2181	GLY	GLY	GLU	GLU	G1747	R1637	LEU	ARG	ARG	ARG	E1091	E1091
GLY	GLY	GLY	G2181	GLY	GLY	GLU	GLU	G1747	E1635	LEU	ARG	ARG	ARG	Y1094	Y1094
GLN	GLN	GLY	G2181	GLY	GLY	GLU	GLU	G1747	R1637	LEU	ARG	ARG	ARG	Y1094	Y1094
LEU	LEU	GLY	G2181	GLY	GLY	GLU	GLU	G1747	E1635	LEU	ARG	ARG	ARG	Y1094	Y1094
R2582	R2582	THR	G2181	GLY	GLY	GLU	GLU	G1747	R1637	LEU	ARG	ARG	ARG	Y1094	Y1094
P2583	P2583	ASP	G2181	GLY	GLY	GLU	GLU	G1747	E1635	LEU	ARG	ARG	ARG	Y1094	Y1094

I4153	I4014	I3899	F3790	R3674	PRO	LEU	TYR	VAL	HIS	ASN	VAL	P3104	LYS	G2907	I02723	Q2587
R4158	I4015	Q3904	F3791	L3677	ARG	ASP	SER	GLU	LEU	ILE	ASP	F3118	VAL	PHE	D2736	R2591
I4161	F4017	N3906	L3794	L3688	LYS	ALA	THR	PHE	GLU	ILE	GLU	GLY	LEU	LYS	L2737	P2598
I4162	F4018	F3907	L3797	I3689	LYS	ILE	SER	TYR	VAL	TYR	SER	ASP	LEU	LEU	L2738	
K4163	F4020	A3910	S3800	I3690	ALA	TRP	ILE	TRP	GLY	ASN	ILE	ILE	ASP	GLU	I2742	R2601
P4164	I4022	I3911	C3801	M3696	TRP	GLN	ILE	SER	ASP	ASN	ARG	L3124	ASN	ASP	E2770	GLU
E4168		A3914	S3802	M3699	HIS	LYS	GLU	PHE	GLY	ILE	THR	S3144	PHE	THR	R2773	HIS
S4169	S4030	V3917	V3803	S3699	ASN	TYR	LEU	ASN	GLU	ILE	ALA	LYS	LYS	SER	I2776	K2605
K4170	I4031	F3915	L3804	C3700	LEU	LYS	LEU	ARG	ALA	ASP	MET	ILE	ASN	ILE		M2606
R4171	I4032	F3916	D3805	HIS	SER	LYS	ARG	PHE	GLU	GLU	PRO	ILE	HIS	GLU	P2607	
I4174	S4045	N3919	R3811	ASP	ASP	LYS	LEU	LYS	LEU	GLY	HIS	VAL	ARG	LYS	R2794	P2625
N4179	R4046	T3920	Q3812	GLU	GLU	PRO	LEU	ARG	ILE	TRP	VAL	T3149	LEU	ARG	G2796	G2626
		T3921	N3813	ASP	LYS	ASN	ILE	GLU	LEU	MET	GLU	A3166	MET	ALA	G2797	G2627
	A4052	F3923	K3814	ASP	ARG	ARG	GLY	GLN	ASP	LYS	VAL		VAL	ALA	THR	THR
K4184	F4056	I3924	ALA	ASP	ALA	THR	LEU	ASN	GLU	ARG	VAL	PHE	PRO	ILE	ASN	A2634
M4187		I3925	GLU	GLY	VAL	GLU	ASN	PHE	GLU	GLU	VAL	VAL	LEU	PHE	ALA	GLY
E4188	T4060	Q3926	GLY	GLU	VAL	THR	ILE	THR	THR	ALA	PRO	A3170	LEU	LEU	PHE	ASN
I4189			LEU	GLU	ALA	THR	THR	VAL	THR	VAL	MET		SER	GLN	TYR	PHE
F4190	E4063	N3932	GLY	GLU	CYS	SER	ALA	GLN	LEU	PHE	LEU	S3183	LEU	GLN	GLN	ALA
V4191		Q3933	MET	VAL	PHE	ASP	PRO	ASN	ALA	SER	CYS	ILE	THR	GLN	ARG	
M4192	I4067	L3936	VAL	LYS	ARG	PRO	GLY	GLU	ARG	GLN	THR	THR	THR	ILE	THR	A2634
F4193	I4068	T3940	THR	L3726	MET	GLU	ASP	ILE	ASP	PRO	THR	ASN	T3028	ARG	ARG	L2653
C4194	A4071	R3940	ALA	L3732	ALA	LYS	GLN	ASN	LEU	ILE	THR	THR	SER	THR	ILE	SER
E4195	E4072	L3941	GLY	H3733	LEU	ASP	LEU	ASN	THR	ASN	VAL	VAL	VAL	ASP	ILE	LYS
D4196	F4073	N3948	GLY	D3729	TYR	GLU	ILE	SER	PHE	LYS	SER	ARG	CYS	ALA	GLN	LYS
	D4074	F3952	GLY	R3730	ASN	ARG	ALA	PHE	TYR	VAL	TRP	ARG	LYS	ALA	THR	Y2658
E4200	T4078	N3955	LEU	R3731	LEU	VAL	ILE	ILE	PRO	LEU	LYS	GLU	CYS	ALA	SER	
I4207		M3955	GLN	H3732	PRO	VAL	ALA	THR	ARG	LEU	GLU	ALA	ALA	LEU	THR	P2668
SER		L3959	D3833	D3734	ASN	ALA	ARG	THR	LYS	LEU	LEU	ASN	SER	LEU	SER	P2678
GLU	V4085	L3959	D3833	D3735	VAL	ASN	ARG	THR	LYS	LEU	LEU	ASN	ALA	LEU	ASP	P2679
SER	F4086	L3959	D3833	D3736	VAL	ASN	PHE	THR	LYS	LEU	LEU	ASN	ALA	LEU	ASP	
ASP	R4087	Q3965	F3841	A3737	VAL	VAL	SER	LYS	VAL	ASN	ASN	LEU	LEU	GLU	THR	TYR
LEU	HIS	Q3965	F3841	A3737	LEU	LEU	SER	LYS	ASP	THR	THR	PRO	ARG	ASP	MET	MET
ASN		L3968	G3850	M3740	HIS	HIS	ASP	SER	TYR	ASN	ASN	ASN	GLY	GLY	GLU	SER
GLU	E4090	L3968	G3850	V3741	LEU	LEU	ASP	SER	ASN	ASN	VAL	VAL	T3082	SER	ASN	TYR
ARG		E3971	D3854	L3742	GLU	GLN	THR	ALA	ALA	PRO	ALA	GLU	HIS	ARG	TYR	VAL
ALA	I4102		D3854	S3748	ALA	GLN	ASP	ALA	LYS	LEU	MET	ASP	THR	SER	VAL	SER
ASN	T4114	L3975	Y3858	E3751	VAL	LYS	GLU	VAL	TRP	GLU	CYS	VAL	THR	LYS	SER	SER
LYS	R4115		Y3858	E3751	PRO	SER	VAL	SER	LEU	LYS	CYS	CYS	ASN	GLY	MET	MET
GLU	I4116	M3982	T3875	M3755	ASP	THR	ARG	ASP	LYS	LEU	THR	PRO	GLN	GLU	MET	MET
GLU	Q4117	L3983	T3875	M3755	GLU	CYS	ASP	GLN	LYS	LYS	ALA	ASN	PRO	HIS	GLU	LYS
SER			Y3878	M3755	GLU	MET	ILE	GLU	PRO	LYS	ALA	ILE	LYS	PHE	LYS	GLN
GLU	I4122	E3988	L3879	L3767	ASP	ARG	ILE	ARG	ASN	LYS	ASN	PRO	GLY	PRO	GLN	GLN
LYS	F4130	G3989	Y3879	I3768	GLU	ARG	ARG	LYS	PRO	ALA	THR	VAL	VAL	TYR	SER	SER
GLU		N3990	Y3882	G3769	GLY	ARG	SER	LYS	GLU	ALA	GLU	SER	VAL	GLU	MET	MET
LYS		V3991	Y3882	G3770	THR	TYR	ASN	LYS	ALA	MET	HIS	GLU	THR	GLN	MET	MET
PRO	I4134		Y3891	G3770	LYS	TYR	ILE	LYS	GLU	VAL	LYS	LEU	ILE	GLU	ASP	ASP
GLU		D4002	Y3892	L3779	LYS	TYR	ILE	LYS	VAL	VAL	ASN	GLY	GLY	GLU	SER	SER
GLU	E4138		Y3892	L3779	LYS	SER	HIS	ARG	ASP	VAL	ASN	THR	ILE	ILE	LYS	GLU
GLN	I4139	F4003	Y3893	E3780	GLU	LEU	LEU	LYS	LEU	GLY	THR	MET	ASN	LYS	GLU	GLY
GLY		L4004	Y3893	E3780	GLU	VAL	GLN	GLY	PHE	GLU	LEU	GLU	THR	PHE	PHE	N2701
PRO	Y4150		K3896	I3782	ASP	GLU	GLU	ASP	ARG	GLU	LEU	GLU	TYR	ASN	GLY	
			K3896	I3782	ASP	GLU	GLU	ASP	ARG	GLU	LEU	GLU	TYR	ASN	GLY	
			K3783	K3783	ARG	ARG	MET	ASP	MET	ASP	GLY	ILE	THR	LYS	ALA	







WORLDWIDE PDB
 PROTEIN DATA BANK

EMDataBank
 Unified Data Resource for 3DEM

C4949	T4950	I4747	G4629	SER	ASP	ARG	LYS	LYS	L4207	K4086
W4950	F4951	K4752	Q4630	VAL	GLY	GLU	VAL	GLN	SER	R4087
E4951	F4952	K4753	W4631	VAL	GLU	GLY	GLU	MET	GLU	PHE
F4952	F4953	T4753	G4640	GLU	LYS	GLU	GLY	LYS	SER	HIS
F4953	F4954	L4754	S4641	GLY	GLU	GLN	GLU	LYS	ASP	E4090
F4955	F4955	L4757	F4642	LYS	GLU	TYR	TYR	VAL	LEU	
T4956	T4956	L4758	P4643	GLU	LYS	LYS	LYS	LYS	ASN	L4102
V4957	V4957	L4758	N4643	LEU	ALA	LEU	LEU	LYS	GLU	
				PRO	ALA	ILE	ILE	MET	ARG	T4114
A4861	A4861	Q4767	W4646	LYS	GLU	PRO	PRO	THR	SER	R4115
I4862	I4862	D4647	D4647	THR	ASP	HIS	HIS	VAL	ALA	L4116
I4863	I4863	K4648	K4648	ARG	LYS	ASN	ASN	ASP	ASN	Q4117
Q4864	Q4864	L4770	F4649	SER	GLY	PRO	PRO	THR	LYS	
G4865	G4865	L4774	V4650	SER	LYS	ASN	GLN	ASP	GLU	L4122
L4966	L4966			GLU	GLN	ALA	ASP	VAL	GLU	
		Y4780	D4665	ASN	LYS	GLY	GLU	THR	SER	F4130
F4871	F4871	L4781		ALA	LEU	LEU	VAL	ALA	GLU	
R4875	R4875	Y4782	S4668	ASN	ARG	SER	ARG	PHE	LYS	L4134
		T4783		PHE	GLN	ASP	GLY	PHE	GLU	C4135
K4888	K4888	V4784	G4672	GLY	LEU	LEU	ASP	THR	LYS	R4136
			MET	SER	HIS	MET	GLY	SER	PRO	I4137
I4891	I4891	F4789	ASP	LEU	THR	SER	SER	TYR	GLU	E4138
C4892	C4892	F4790	LYS	ASP	HIS	SER	GLU	TRP	GLU	I4139
		R4791	ALA	SER	TYR	PRO	GLY	SER	GLN	
G4895	G4895		ALA	SER	GLY	ALA	GLU	VAL	GLY	Y4150
		Y4794	LEU	SER	GLY	PRO	ARG	PHE	PRO	
Y4898	Y4898	N4795	ASP	PRO	GLU	ILE	LYS	MET	ARG	I4153
K4796	K4796	K4796	PHE	ARG	PRO	GLU	VAL	THR	MET	
G4800	G4800		SER	ILE	GLU	LEU	LEU	GLY	GLY	R4158
			ASP	ILE	VAL	VAL	GLU	LEU	PHE	
D4804	D4804		ALA	ALA	PRO	GLN	GLY	HIS	PHE	W4161
E4807	E4807		ARG	V4858	GLU	GLU	THR	PHE	SER	E4162
T4808	T4808		GLU	H4859	SER	LYS	LEU	ALA	LEU	K4163
H4909	H4909	C4807	LYS	Y4860	ALA	PHE	PRO	ALA	VAL	P4164
			LYS		PHE	GLN	GLN	SER	THR	
H4914	H4914	M4810	LYS	TRP	TRP	GLU	GLU	VAL	VAL	K4170
N4915	N4915		PRO	H4880	LYS	GLN	ASP	SER	ARG	R4171
L4916	L4916	H4817	LYS		LYS	LYS	LEU	ARG	SER	
A4917	A4917	M4818	LYS	I4883	ILE	ALA	THR	GLY	ALA	I4174
Y4919	Y4919		ASP	Y4891	G4486	LYS	ASP	PHE	LEU	
L4920	L4920	G4821	SER	O4821	R4498	GLU	LEU	SER	LEU	N4179
F4921	F4921	V4822	SER	K4595	N4499	GLU	LYS	ARG	ALA	
		R4823	LEU		F4500	LYS	LEU	ILE	ARG	G4182
Y4925	Y4925	A4824	S4696	R4603		GLU	THR	ILE	ARG	E4183
		G4825			R4504	GLU	GLU	GLY	ASN	K4184
K4929	K4929	G4826	W4709	A4608		LYS	GLU	GLY	VAL	E4185
D4930	D4930	G4827	L4721	R4609	L4508	GLU	SER	LEU	VAL	K4186
E4931	E4931	I4828		K4610		GLU	ASP	LEU	THR	M4187
			Y4726	L4611	A4511	ASN	LEU	GLY	THR	E4188
Q4937	Q4937	I4832	W4727	E4612		LYS	LEU	GLY	MET	I4189
E4938	E4938	P4835		G4615	I4514	SER	SER	ARG	ARG	F4190
S4939	S4939		L4732	L4616	N4515	GLU	GLU	MET	MET	V4191
Y4940	Y4940	E4839	G4733	L4617		PRO	ILE	LEU	LEU	M4192
V4941	V4941	W4840	H4734	Y4617	L4518	GLU	PHE	GLU	SER	F4193
W4942	W4942	E4841	Y4735	E4620	L4519	LYS	GLY	LEU	LEU	C4194
				F4739	S4524	ALA	LEU	ALA	LYS	E4195
Y4945	Y4945	R4844	F4739	THR		GLU	ASP	LYS	SER	D4196
R4948	R4948	I4849	F4740	K4628	SER	GLU	LEU	LEU	LEU	
								ILE	LYS	E4200

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	133196	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.09	70/26752 (0.3%)	1.00	96/36151 (0.3%)
1	B	1.09	66/26752 (0.2%)	1.00	95/36151 (0.3%)
1	C	1.08	67/26752 (0.3%)	1.00	95/36151 (0.3%)
1	D	1.09	67/26752 (0.3%)	1.00	99/36151 (0.3%)
All	All	1.08	270/107008 (0.3%)	1.00	385/144604 (0.3%)

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	23
1	B	0	23
1	C	0	24
1	D	0	23
All	All	0	93

All (270) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3700	CYS	CB-SG	13.49	2.05	1.82
1	D	3700	CYS	CB-SG	13.43	2.05	1.82
1	A	3700	CYS	CB-SG	13.37	2.04	1.82
1	C	3700	CYS	CB-SG	13.08	2.04	1.82
1	B	3878	TYR	CG-CD1	-12.72	1.22	1.39
1	C	3878	TYR	CG-CD1	-12.50	1.22	1.39
1	A	3878	TYR	CG-CD1	-12.34	1.23	1.39
1	D	3878	TYR	CG-CD1	-12.33	1.23	1.39
1	C	4849	ILE	C-O	10.92	1.44	1.23
1	A	4849	ILE	C-O	10.87	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4849	ILE	C-O	10.86	1.44	1.23
1	B	4849	ILE	C-O	10.81	1.43	1.23
1	B	4646	TRP	CZ3-CH2	9.99	1.56	1.40
1	A	4646	TRP	CZ3-CH2	9.96	1.55	1.40
1	C	4646	TRP	CZ3-CH2	9.86	1.55	1.40
1	D	4646	TRP	CZ3-CH2	9.54	1.55	1.40
1	A	4940	TYR	CE1-CZ	-9.18	1.26	1.38
1	B	4940	TYR	CE1-CZ	-8.95	1.26	1.38
1	D	4940	TYR	CE1-CZ	-8.94	1.26	1.38
1	C	4940	TYR	CE1-CZ	-8.90	1.26	1.38
1	B	4953	PHE	CG-CD1	-8.71	1.25	1.38
1	A	4940	TYR	CG-CD2	-8.64	1.27	1.39
1	C	4940	TYR	CG-CD2	-8.63	1.27	1.39
1	A	4953	PHE	CG-CD1	-8.52	1.25	1.38
1	D	4940	TYR	CG-CD2	-8.52	1.28	1.39
1	B	4940	TYR	CG-CD2	-8.47	1.28	1.39
1	D	4919	TYR	CE1-CZ	-8.46	1.27	1.38
1	C	4919	TYR	CE1-CZ	-8.33	1.27	1.38
1	C	4953	PHE	CG-CD1	-8.32	1.26	1.38
1	D	4953	PHE	CG-CD1	-8.31	1.26	1.38
1	B	3858	TYR	CG-CD2	-8.30	1.28	1.39
1	D	887	GLU	CG-CD	8.25	1.64	1.51
1	C	3878	TYR	CE2-CZ	-8.15	1.27	1.38
1	A	3858	TYR	CG-CD2	-8.03	1.28	1.39
1	B	3878	TYR	CE2-CZ	-7.99	1.28	1.38
1	D	3858	TYR	CG-CD2	-7.95	1.28	1.39
1	D	4818	MET	CG-SD	7.94	2.01	1.81
1	A	3878	TYR	CE2-CZ	-7.93	1.28	1.38
1	D	3878	TYR	CE2-CZ	-7.90	1.28	1.38
1	C	3858	TYR	CG-CD2	-7.88	1.28	1.39
1	B	4646	TRP	CG-CD1	-7.88	1.25	1.36
1	A	4646	TRP	CG-CD1	-7.86	1.25	1.36
1	C	4818	MET	CG-SD	7.83	2.01	1.81
1	A	4818	MET	CG-SD	7.68	2.01	1.81
1	A	887	GLU	CG-CD	7.60	1.63	1.51
1	D	4646	TRP	CG-CD1	-7.55	1.26	1.36
1	B	4953	PHE	CG-CD2	-7.52	1.27	1.38
1	A	3699	SER	CB-OG	-7.51	1.32	1.42
1	B	3699	SER	CB-OG	-7.51	1.32	1.42
1	C	4646	TRP	CG-CD1	-7.51	1.26	1.36
1	A	4612	GLU	CD-OE2	7.50	1.33	1.25
1	B	4818	MET	CG-SD	7.50	2.00	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4919	TYR	CE1-CZ	-7.48	1.28	1.38
1	B	4919	TYR	CE1-CZ	-7.44	1.28	1.38
1	A	4953	PHE	CG-CD2	-7.43	1.27	1.38
1	C	4953	PHE	CG-CD2	-7.41	1.27	1.38
1	C	4853	PHE	CD1-CE1	7.36	1.53	1.39
1	D	3699	SER	CB-OG	-7.36	1.32	1.42
1	D	4953	PHE	CG-CD2	-7.32	1.27	1.38
1	C	4612	GLU	CD-OE2	7.31	1.33	1.25
1	C	3699	SER	CB-OG	-7.31	1.32	1.42
1	B	4612	GLU	CD-OE2	7.28	1.33	1.25
1	D	4853	PHE	CD1-CE1	7.28	1.53	1.39
1	A	4952	PHE	CG-CD1	-7.20	1.27	1.38
1	C	4161	TRP	CG-CD2	-7.14	1.31	1.43
1	B	4161	TRP	CG-CD2	-7.12	1.31	1.43
1	C	4945	TYR	CE2-CZ	-7.12	1.29	1.38
1	B	4952	PHE	CG-CD1	-7.11	1.28	1.38
1	D	4161	TRP	CG-CD2	-7.09	1.31	1.43
1	D	4952	PHE	CG-CD1	-7.08	1.28	1.38
1	A	4161	TRP	CG-CD2	-7.04	1.31	1.43
1	D	4612	GLU	CD-OE2	7.04	1.33	1.25
1	B	4709	TRP	CE3-CZ3	-7.01	1.26	1.38
1	C	3841	PHE	CG-CD2	-7.00	1.28	1.38
1	A	3924	TYR	CE1-CZ	-6.99	1.29	1.38
1	B	4945	TYR	CE2-CZ	-6.98	1.29	1.38
1	B	4789	PHE	CG-CD2	6.95	1.49	1.38
1	A	4853	PHE	CD1-CE1	6.91	1.53	1.39
1	C	4709	TRP	CE3-CZ3	-6.88	1.26	1.38
1	A	4945	TYR	CE2-CZ	-6.87	1.29	1.38
1	C	4952	PHE	CG-CD1	-6.85	1.28	1.38
1	D	4945	TYR	CE2-CZ	-6.85	1.29	1.38
1	D	3924	TYR	CE1-CZ	-6.82	1.29	1.38
1	A	4709	TRP	CE3-CZ3	-6.81	1.26	1.38
1	B	4853	PHE	CD1-CE1	6.79	1.52	1.39
1	B	3841	PHE	CG-CD2	-6.79	1.28	1.38
1	D	3841	PHE	CG-CD2	-6.76	1.28	1.38
1	B	4952	PHE	CE2-CZ	-6.75	1.24	1.37
1	D	4709	TRP	CE3-CZ3	-6.72	1.27	1.38
1	A	4952	PHE	CE2-CZ	-6.70	1.24	1.37
1	A	4953	PHE	CE1-CZ	-6.68	1.24	1.37
1	A	3841	PHE	CG-CD2	-6.67	1.28	1.38
1	B	1778	TYR	CB-CG	-6.67	1.41	1.51
1	C	4853	PHE	CD2-CE2	6.66	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4853	PHE	CD2-CE2	6.63	1.52	1.39
1	A	1778	TYR	CB-CG	-6.63	1.41	1.51
1	A	4789	PHE	CG-CD2	6.62	1.48	1.38
1	D	4952	PHE	CG-CD2	-6.60	1.28	1.38
1	A	4925	TYR	CD1-CE1	-6.55	1.29	1.39
1	C	4952	PHE	CE2-CZ	-6.50	1.25	1.37
1	C	4150	TYR	C-O	-6.46	1.11	1.23
1	B	4150	TYR	C-O	-6.46	1.11	1.23
1	D	4150	TYR	C-O	-6.46	1.11	1.23
1	B	4952	PHE	CG-CD2	-6.44	1.29	1.38
1	B	2192	LYS	N-CA	6.42	1.59	1.46
1	B	3924	TYR	CE1-CZ	-6.42	1.30	1.38
1	A	4150	TYR	C-O	-6.42	1.11	1.23
1	B	4591	TYR	CG-CD1	-6.40	1.30	1.39
1	C	3924	TYR	CE1-CZ	-6.40	1.30	1.38
1	D	4952	PHE	CE2-CZ	-6.40	1.25	1.37
1	C	4789	PHE	CG-CD2	6.36	1.48	1.38
1	A	4952	PHE	CG-CD2	-6.34	1.29	1.38
1	B	4138	GLU	CD-OE1	-6.34	1.18	1.25
1	A	2192	LYS	N-CA	6.32	1.58	1.46
1	D	4925	TYR	CD1-CE1	-6.31	1.29	1.39
1	D	4789	PHE	CG-CD2	6.30	1.48	1.38
1	C	4138	GLU	CD-OE1	-6.29	1.18	1.25
1	C	4925	TYR	CD1-CE1	-6.28	1.29	1.39
1	D	4138	GLU	CD-OE1	-6.27	1.18	1.25
1	A	4853	PHE	CD2-CE2	6.27	1.51	1.39
1	C	4952	PHE	CG-CD2	-6.24	1.29	1.38
1	C	4591	TYR	CG-CD1	-6.23	1.31	1.39
1	D	1778	TYR	CB-CG	-6.22	1.42	1.51
1	C	1778	TYR	CB-CG	-6.21	1.42	1.51
1	B	4853	PHE	CD2-CE2	6.20	1.51	1.39
1	B	4925	TYR	CD1-CE1	-6.20	1.30	1.39
1	A	4138	GLU	CD-OE1	-6.20	1.18	1.25
1	C	4839	GLU	CG-CD	6.19	1.61	1.51
1	A	4591	TYR	CG-CD1	-6.16	1.31	1.39
1	B	615	CYS	CB-SG	-6.15	1.71	1.82
1	D	2192	LYS	N-CA	6.15	1.58	1.46
1	C	2192	LYS	N-CA	6.12	1.58	1.46
1	A	3893	TYR	CE1-CZ	-6.11	1.30	1.38
1	D	4195	GLU	CG-CD	6.10	1.61	1.51
1	A	4925	TYR	CD2-CE2	-6.07	1.30	1.39
1	B	2080	GLU	CG-CD	6.04	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4953	PHE	CE1-CZ	-6.04	1.25	1.37
1	A	3755	MET	N-CA	-6.04	1.34	1.46
1	C	4945	TYR	CG-CD1	-6.04	1.31	1.39
1	A	615	CYS	CB-SG	-6.02	1.72	1.82
1	D	4591	TYR	CG-CD1	-6.01	1.31	1.39
1	B	4898	TYR	CG-CD2	-5.99	1.31	1.39
1	C	3850	GLY	N-CA	-5.99	1.37	1.46
1	D	4925	TYR	CD2-CE2	-5.99	1.30	1.39
1	B	3850	GLY	N-CA	-5.99	1.37	1.46
1	A	4195	GLU	CG-CD	5.95	1.60	1.51
1	D	4735	TYR	CE1-CZ	5.92	1.46	1.38
1	C	4925	TYR	CD2-CE2	-5.91	1.30	1.39
1	D	4945	TYR	CG-CD1	-5.91	1.31	1.39
1	B	4735	TYR	CE1-CZ	5.90	1.46	1.38
1	C	4195	GLU	CG-CD	5.89	1.60	1.51
1	B	4938	GLU	CD-OE2	-5.89	1.19	1.25
1	A	4898	TYR	CG-CD2	-5.88	1.31	1.39
1	B	4945	TYR	CG-CD1	-5.88	1.31	1.39
1	A	4938	GLU	CD-OE2	-5.88	1.19	1.25
1	B	4925	TYR	CD2-CE2	-5.87	1.30	1.39
1	C	615	CYS	CB-SG	-5.84	1.72	1.81
1	A	4735	TYR	CE1-CZ	5.83	1.46	1.38
1	A	3850	GLY	N-CA	-5.83	1.37	1.46
1	D	615	CYS	CB-SG	-5.83	1.72	1.81
1	B	3755	MET	N-CA	-5.81	1.34	1.46
1	D	3850	GLY	N-CA	-5.80	1.37	1.46
1	A	4945	TYR	CG-CD1	-5.78	1.31	1.39
1	C	2080	GLU	CG-CD	5.77	1.60	1.51
1	C	4735	TYR	CE1-CZ	5.77	1.46	1.38
1	D	3755	MET	N-CA	-5.77	1.34	1.46
1	D	4953	PHE	CE1-CZ	-5.76	1.26	1.37
1	C	3988	GLU	CD-OE2	-5.74	1.19	1.25
1	C	4919	TYR	CG-CD2	-5.74	1.31	1.39
1	C	4953	PHE	CE1-CZ	-5.73	1.26	1.37
1	B	4195	GLU	CG-CD	5.72	1.60	1.51
1	B	4853	PHE	N-CA	5.71	1.57	1.46
1	C	4726	TYR	CE1-CZ	-5.70	1.31	1.38
1	B	3988	GLU	CD-OE2	-5.70	1.19	1.25
1	C	4938	GLU	CD-OE2	-5.70	1.19	1.25
1	A	4853	PHE	N-CA	5.69	1.57	1.46
1	D	3893	TYR	CE1-CZ	-5.69	1.31	1.38
1	D	4919	TYR	CG-CD2	-5.67	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4938	GLU	CD-OE2	-5.67	1.19	1.25
1	C	4865	GLY	CA-C	-5.66	1.42	1.51
1	D	4898	TYR	CG-CD2	-5.66	1.31	1.39
1	B	4726	TYR	CE1-CZ	-5.65	1.31	1.38
1	B	4790	PHE	CG-CD2	-5.63	1.30	1.38
1	C	4853	PHE	N-CA	5.62	1.57	1.46
1	C	3755	MET	N-CA	-5.60	1.35	1.46
1	C	4898	TYR	CG-CD2	-5.59	1.31	1.39
1	A	3854	ASP	CG-OD1	-5.58	1.12	1.25
1	B	4865	GLY	CA-C	-5.58	1.43	1.51
1	C	2253	GLU	CG-CD	5.57	1.60	1.51
1	D	4865	GLY	CA-C	-5.57	1.43	1.51
1	D	2080	GLU	CB-CG	5.57	1.62	1.52
1	B	4839	GLU	CG-CD	5.56	1.60	1.51
1	B	4646	TRP	CE3-CZ3	-5.55	1.29	1.38
1	B	3893	TYR	CE1-CZ	-5.54	1.31	1.38
1	C	4950	TRP	CD2-CE3	-5.53	1.32	1.40
1	D	3907	PHE	CG-CD2	-5.53	1.30	1.38
1	B	4950	TRP	CD2-CE3	-5.52	1.32	1.40
1	C	4591	TYR	CE2-CZ	-5.51	1.31	1.38
1	C	3907	PHE	CG-CD2	-5.51	1.30	1.38
1	D	4591	TYR	CE2-CZ	-5.51	1.31	1.38
1	D	3988	GLU	CD-OE2	-5.51	1.19	1.25
1	D	4790	PHE	CG-CD2	-5.50	1.30	1.38
1	B	3854	ASP	CG-OD1	-5.50	1.12	1.25
1	A	4790	PHE	CG-CD2	-5.50	1.30	1.38
1	D	2253	GLU	CG-CD	5.49	1.60	1.51
1	D	4853	PHE	N-CA	5.49	1.57	1.46
1	C	4790	PHE	CG-CD2	-5.48	1.30	1.38
1	C	3854	ASP	CG-OD1	-5.48	1.12	1.25
1	A	4839	GLU	CG-CD	5.47	1.60	1.51
1	B	4919	TYR	CG-CD1	-5.47	1.32	1.39
1	D	4950	TRP	CD2-CE3	-5.46	1.32	1.40
1	A	2080	GLU	CB-CG	5.46	1.62	1.52
1	C	3770	GLY	C-O	-5.46	1.15	1.23
1	A	4865	GLY	CA-C	-5.45	1.43	1.51
1	C	3811	ARG	CZ-NH1	5.44	1.40	1.33
1	A	4646	TRP	CE3-CZ3	-5.41	1.29	1.38
1	C	4753	THR	C-O	-5.40	1.13	1.23
1	A	4591	TYR	CE2-CZ	-5.39	1.31	1.38
1	D	4839	GLU	CG-CD	5.39	1.60	1.51
1	D	4726	TYR	CE1-CZ	-5.38	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4950	TRP	CD2-CE3	-5.38	1.32	1.40
1	C	4919	TYR	CG-CD1	-5.37	1.32	1.39
1	A	3791	PHE	CG-CD1	-5.36	1.30	1.38
1	C	4862	ILE	CA-CB	-5.35	1.42	1.54
1	B	4591	TYR	CE2-CZ	-5.35	1.31	1.38
1	D	3854	ASP	CG-OD1	-5.35	1.13	1.25
1	B	3790	PHE	CG-CD2	-5.35	1.30	1.38
1	A	3907	PHE	CG-CD2	-5.35	1.30	1.38
1	B	4919	TYR	CG-CD2	-5.35	1.32	1.39
1	A	4862	ILE	CA-CB	-5.33	1.42	1.54
1	C	2077	GLU	CG-CD	5.33	1.59	1.51
1	D	4862	ILE	CA-CB	-5.33	1.42	1.54
1	A	2077	GLU	CG-CD	5.32	1.59	1.51
1	A	3988	GLU	CD-OE2	-5.31	1.19	1.25
1	D	4753	THR	C-O	-5.31	1.13	1.23
1	D	3770	GLY	C-O	-5.30	1.15	1.23
1	D	2077	GLU	CG-CD	5.29	1.59	1.51
1	B	2253	GLU	CG-CD	5.28	1.59	1.51
1	B	3907	PHE	CG-CD2	-5.28	1.30	1.38
1	D	3811	ARG	CZ-NH1	5.26	1.39	1.33
1	C	3893	TYR	CE1-CZ	-5.26	1.31	1.38
1	B	3811	ARG	CZ-NH1	5.25	1.39	1.33
1	B	4753	THR	C-O	-5.25	1.13	1.23
1	A	3790	PHE	CG-CD2	-5.24	1.30	1.38
1	C	3790	PHE	CG-CD2	-5.24	1.30	1.38
1	A	4753	THR	C-O	-5.23	1.13	1.23
1	D	2080	GLU	CG-CD	5.22	1.59	1.51
1	A	3811	ARG	CZ-NH1	5.21	1.39	1.33
1	B	4862	ILE	CA-CB	-5.21	1.42	1.54
1	B	3770	GLY	C-O	-5.21	1.15	1.23
1	A	3770	GLY	C-O	-5.18	1.15	1.23
1	B	2077	GLU	CG-CD	5.18	1.59	1.51
1	C	3791	PHE	CG-CD1	-5.12	1.31	1.38
1	C	4925	TYR	CE2-CZ	-5.11	1.31	1.38
1	A	2253	GLU	CG-CD	5.11	1.59	1.51
1	D	3791	PHE	CG-CD1	-5.09	1.31	1.38
1	A	4919	TYR	CG-CD2	-5.08	1.32	1.39
1	A	4726	TYR	CE1-CZ	-5.07	1.31	1.38
1	B	4754	LEU	N-CA	-5.07	1.36	1.46
1	D	4921	PHE	CG-CD1	-5.07	1.31	1.38
1	D	4136	ARG	C-O	-5.07	1.13	1.23
1	C	534	TYR	CE1-CZ	-5.05	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3753	GLY	N-CA	-5.05	1.38	1.46
1	A	4925	TYR	CE2-CZ	-5.05	1.31	1.38
1	C	4942	TRP	CG-CD2	-5.04	1.35	1.43
1	B	534	TYR	CE1-CZ	-5.03	1.32	1.38
1	A	534	TYR	CE1-CZ	-5.02	1.32	1.38
1	A	4136	ARG	C-O	-5.02	1.13	1.23
1	D	4925	TYR	CE2-CZ	-5.02	1.32	1.38
1	A	4919	TYR	CG-CD1	-5.01	1.32	1.39

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4948	ARG	NE-CZ-NH2	13.56	127.08	120.30
1	D	4948	ARG	NE-CZ-NH2	13.25	126.92	120.30
1	B	4948	ARG	NE-CZ-NH2	13.09	126.84	120.30
1	C	4948	ARG	NE-CZ-NH2	12.28	126.44	120.30
1	A	1089	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	B	1089	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	4818	MET	CG-SD-CE	9.16	114.86	100.20
1	B	4853	PHE	N-CA-CB	9.15	127.06	110.60
1	D	4853	PHE	N-CA-CB	9.12	127.01	110.60
1	A	4853	PHE	N-CA-CB	9.10	126.99	110.60
1	D	1089	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	C	4853	PHE	N-CA-CB	9.02	126.84	110.60
1	A	3854	ASP	CB-CG-OD2	8.98	126.38	118.30
1	D	4948	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	C	1089	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	D	4818	MET	CG-SD-CE	8.78	114.25	100.20
1	B	4818	MET	CG-SD-CE	8.76	114.21	100.20
1	C	4818	MET	CG-SD-CE	8.76	114.21	100.20
1	C	3854	ASP	CB-CG-OD2	8.74	126.17	118.30
1	B	3854	ASP	CB-CG-OD2	8.73	126.15	118.30
1	D	3854	ASP	CB-CG-OD2	8.73	126.15	118.30
1	A	4948	ARG	NE-CZ-NH1	-8.69	115.96	120.30
1	D	4818	MET	CA-CB-CG	8.49	127.73	113.30
1	C	4818	MET	CA-CB-CG	8.32	127.44	113.30
1	B	4727	MET	CG-SD-CE	8.24	113.39	100.20
1	C	4727	MET	CG-SD-CE	8.23	113.36	100.20
1	C	4948	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	D	2239	THR	N-CA-CB	-8.13	94.85	110.30
1	D	2495	PRO	N-CA-CB	8.12	113.04	103.30
1	A	4818	MET	CA-CB-CG	8.12	127.10	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4727	MET	CG-SD-CE	8.09	113.14	100.20
1	A	2495	PRO	N-CA-CB	8.08	112.99	103.30
1	D	4875	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	C	2495	PRO	N-CA-CB	8.05	112.96	103.30
1	B	2495	PRO	N-CA-CB	8.05	112.96	103.30
1	B	3878	TYR	CB-CG-CD2	7.95	125.77	121.00
1	A	347	ASP	CB-CG-OD1	7.93	125.44	118.30
1	B	4948	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	B	4818	MET	CA-CB-CG	7.86	126.65	113.30
1	C	2239	THR	N-CA-CB	-7.85	95.38	110.30
1	C	3878	TYR	CB-CG-CD2	7.84	125.70	121.00
1	A	2239	THR	N-CA-CB	-7.79	95.49	110.30
1	D	3878	TYR	CB-CG-CD2	7.78	125.67	121.00
1	A	3878	TYR	CB-CG-CD2	7.77	125.66	121.00
1	A	4727	MET	CG-SD-CE	7.74	112.58	100.20
1	B	1758	ARG	NE-CZ-NH1	-7.69	116.46	120.30
1	D	1758	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	D	347	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	2583	PRO	N-CA-CB	7.52	112.33	103.30
1	B	4781	LEU	CB-CG-CD1	7.44	123.65	111.00
1	A	2583	PRO	N-CA-CB	7.44	112.22	103.30
1	A	1758	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	C	1758	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	C	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	485	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	C	4781	LEU	CB-CG-CD1	7.31	123.43	111.00
1	B	347	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	3896	LYS	CD-CE-NZ	7.28	128.45	111.70
1	C	2583	PRO	N-CA-CB	7.27	112.02	103.30
1	C	2607	PRO	N-CA-CB	7.24	111.99	103.30
1	C	4875	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	D	2598	PRO	N-CA-CB	7.21	111.95	103.30
1	B	2239	THR	N-CA-CB	-7.19	96.65	110.30
1	A	2607	PRO	N-CA-CB	7.18	111.92	103.30
1	B	2598	PRO	N-CA-CB	7.17	111.90	103.30
1	D	3896	LYS	CD-CE-NZ	7.17	128.18	111.70
1	B	2607	PRO	N-CA-CB	7.17	111.90	103.30
1	D	2583	PRO	N-CA-CB	7.16	111.89	103.30
1	D	2607	PRO	N-CA-CB	7.14	111.86	103.30
1	A	4781	LEU	CB-CG-CD1	7.13	123.13	111.00
1	A	2598	PRO	N-CA-CB	7.12	111.84	103.30
1	C	2598	PRO	N-CA-CB	7.11	111.84	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3896	LYS	CD-CE-NZ	7.08	128.00	111.70
1	C	3896	LYS	CD-CE-NZ	6.97	127.73	111.70
1	A	4875	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	4875	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	D	4952	PHE	CB-CG-CD2	-6.91	115.96	120.80
1	A	2625	PRO	N-CA-CB	6.90	111.58	103.30
1	B	2625	PRO	N-CA-CB	6.90	111.58	103.30
1	D	2173	MET	CG-SD-CE	-6.89	89.17	100.20
1	B	4498	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	3882	VAL	CG1-CB-CG2	-6.88	99.90	110.90
1	D	2625	PRO	N-CA-CB	6.86	111.53	103.30
1	B	3882	VAL	CG1-CB-CG2	-6.86	99.93	110.90
1	C	545	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	3948	PHE	CB-CG-CD2	-6.81	116.03	120.80
1	B	2736	ASP	CB-CG-OD2	6.79	124.41	118.30
1	C	3948	PHE	CB-CG-CD2	-6.79	116.05	120.80
1	D	545	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	3104	PRO	N-CA-CB	6.76	111.41	103.30
1	D	4781	LEU	CB-CG-CD1	6.76	122.49	111.00
1	A	3104	PRO	N-CA-CB	6.75	111.41	103.30
1	A	3882	VAL	CG1-CB-CG2	-6.75	100.10	110.90
1	C	2625	PRO	N-CA-CB	6.75	111.40	103.30
1	A	2173	MET	CG-SD-CE	-6.73	89.43	100.20
1	D	3882	VAL	CG1-CB-CG2	-6.72	100.15	110.90
1	A	4739	PHE	CB-CG-CD2	6.71	125.50	120.80
1	D	4498	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	B	4789	PHE	CB-CG-CD1	6.69	125.48	120.80
1	C	4139	ILE	CG1-CB-CG2	-6.67	96.73	111.40
1	D	4139	ILE	CG1-CB-CG2	-6.67	96.73	111.40
1	B	3858	TYR	CB-CG-CD1	6.67	125.00	121.00
1	A	545	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	4498	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	485	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	2173	MET	CG-SD-CE	-6.64	89.58	100.20
1	A	4941	VAL	CG1-CB-CG2	-6.63	100.29	110.90
1	C	2736	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	4498	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	4139	ILE	CG1-CB-CG2	-6.62	96.83	111.40
1	C	1610	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	721	ASP	CB-CG-OD1	6.62	124.26	118.30
1	C	3104	PRO	N-CA-CB	6.61	111.23	103.30
1	C	4941	VAL	CG1-CB-CG2	-6.61	100.33	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2668	PRO	N-CA-CB	6.61	111.23	103.30
1	C	485	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	4952	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	D	2668	PRO	N-CA-CB	6.59	111.21	103.30
1	A	3948	PHE	CB-CG-CD2	-6.58	116.19	120.80
1	D	2736	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	4739	PHE	CB-CG-CD2	6.57	125.40	120.80
1	B	4941	VAL	CG1-CB-CG2	-6.57	100.39	110.90
1	C	4789	PHE	CB-CG-CD1	6.56	125.39	120.80
1	C	2173	MET	CG-SD-CE	-6.55	89.72	100.20
1	A	2668	PRO	N-CA-CB	6.55	111.16	103.30
1	A	4139	ILE	CG1-CB-CG2	-6.55	97.00	111.40
1	A	4789	PHE	CB-CG-CD1	6.55	125.38	120.80
1	D	3104	PRO	N-CA-CB	6.54	111.15	103.30
1	C	721	ASP	CB-CG-OD1	6.53	124.18	118.30
1	D	485	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	C	4952	PHE	CB-CG-CD2	-6.52	116.23	120.80
1	A	2736	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	545	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	4941	VAL	CG1-CB-CG2	-6.49	100.52	110.90
1	D	3700	CYS	N-CA-CB	-6.48	98.94	110.60
1	A	3858	TYR	CB-CG-CD1	6.45	124.87	121.00
1	D	4739	PHE	CB-CG-CD2	6.45	125.31	120.80
1	B	2668	PRO	N-CA-CB	6.45	111.03	103.30
1	D	3948	PHE	CB-CG-CD2	-6.45	116.29	120.80
1	A	4916	LEU	CB-CG-CD1	-6.42	100.08	111.00
1	B	2396	LEU	CB-CG-CD2	6.41	121.90	111.00
1	B	4952	PHE	CB-CG-CD2	-6.40	116.32	120.80
1	A	2678	PRO	N-CA-CB	6.40	110.98	103.30
1	D	2679	PRO	N-CA-CB	6.40	110.98	103.30
1	C	3690	MET	CG-SD-CE	-6.38	90.00	100.20
1	D	4789	PHE	CB-CG-CD1	6.37	125.26	120.80
1	B	3982	MET	CG-SD-CE	-6.37	90.02	100.20
1	D	1610	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	D	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	B	2678	PRO	N-CA-CB	6.35	110.92	103.30
1	A	4774	LEU	CB-CG-CD2	6.35	121.80	111.00
1	D	2990	PRO	N-CA-CB	6.34	110.91	103.30
1	C	2679	PRO	N-CA-CB	6.33	110.90	103.30
1	A	2679	PRO	N-CA-CB	6.31	110.87	103.30
1	A	2990	PRO	N-CA-CB	6.30	110.86	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4758	LEU	CB-CG-CD2	6.30	121.72	111.00
1	C	2990	PRO	N-CA-CB	6.30	110.86	103.30
1	C	3700	CYS	N-CA-CB	-6.29	99.29	110.60
1	C	4739	PHE	CB-CG-CD2	6.28	125.19	120.80
1	B	3700	CYS	N-CA-CB	-6.27	99.31	110.60
1	C	3858	TYR	CB-CG-CD1	6.27	124.76	121.00
1	D	4871	PHE	CB-CG-CD1	-6.25	116.42	120.80
1	A	3982	MET	CG-SD-CE	-6.25	90.20	100.20
1	C	4871	PHE	CB-CG-CD1	-6.25	116.42	120.80
1	B	2990	PRO	N-CA-CB	6.24	110.79	103.30
1	A	721	ASP	CB-CG-OD1	6.22	123.89	118.30
1	B	3690	MET	CG-SD-CE	-6.21	90.26	100.20
1	D	3858	TYR	CB-CG-CD1	6.21	124.73	121.00
1	B	2139	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	C	2139	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	A	4871	PHE	CB-CG-CD1	-6.21	116.46	120.80
1	D	3982	MET	CG-SD-CE	-6.20	90.28	100.20
1	B	2679	PRO	N-CA-CB	6.20	110.73	103.30
1	B	4871	PHE	CB-CG-CD1	-6.18	116.47	120.80
1	C	3982	MET	CG-SD-CE	-6.18	90.31	100.20
1	D	3690	MET	CG-SD-CE	-6.18	90.31	100.20
1	D	4916	LEU	CB-CG-CD1	-6.15	100.54	111.00
1	A	1610	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	3700	CYS	N-CA-CB	-6.13	99.56	110.60
1	B	1457	PHE	CB-CG-CD1	-6.13	116.51	120.80
1	C	848	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	1610	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	D	4195	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	A	4603	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	848	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	4758	LEU	CB-CG-CD2	6.00	121.19	111.00
1	B	4758	LEU	CB-CG-CD2	5.99	121.19	111.00
1	A	2396	LEU	CB-CG-CD2	5.98	121.16	111.00
1	A	4940	TYR	CB-CG-CD2	5.97	124.58	121.00
1	B	721	ASP	CB-CG-OD1	5.95	123.66	118.30
1	C	1457	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	C	3700	CYS	CB-CA-C	5.92	122.25	110.40
1	A	4854	PHE	CB-CG-CD2	-5.92	116.66	120.80
1	B	1303	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	4195	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	1303	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	C	687	THR	CA-CB-CG2	-5.88	104.16	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3690	MET	CG-SD-CE	-5.87	90.81	100.20
1	A	520	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	4102	LEU	CA-CB-CG	5.85	128.75	115.30
1	D	687	THR	CA-CB-CG2	-5.84	104.22	112.40
1	B	3700	CYS	CB-CA-C	5.83	122.07	110.40
1	B	4774	LEU	CB-CG-CD2	5.82	120.90	111.00
1	B	4940	TYR	CB-CG-CD2	5.82	124.49	121.00
1	D	3700	CYS	CB-CA-C	5.82	122.03	110.40
1	D	4102	LEU	CA-CB-CG	5.81	128.67	115.30
1	D	2140	GLU	OE1-CD-OE2	-5.81	116.33	123.30
1	D	4854	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	B	4102	LEU	CA-CB-CG	5.80	128.65	115.30
1	B	520	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	687	THR	CA-CB-CG2	-5.79	104.29	112.40
1	B	4195	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	D	4758	LEU	CB-CG-CD2	5.79	120.85	111.00
1	A	3700	CYS	CB-CA-C	5.79	121.98	110.40
1	B	4721	LEU	CA-CB-CG	5.78	128.60	115.30
1	C	1089	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	4721	LEU	CA-CB-CG	5.77	128.56	115.30
1	A	4735	TYR	CB-CG-CD1	5.76	124.46	121.00
1	B	4854	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	D	4940	TYR	CB-CG-CD2	5.75	124.45	121.00
1	C	3811	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	D	4774	LEU	CB-CG-CD2	5.75	120.78	111.00
1	A	687	THR	CA-CB-CG2	-5.75	104.35	112.40
1	D	4721	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	4102	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	4721	LEU	CA-CB-CG	5.74	128.49	115.30
1	B	4916	LEU	CB-CG-CD1	-5.73	101.25	111.00
1	B	4735	TYR	CB-CG-CD1	5.71	124.43	121.00
1	A	4822	VAL	CA-CB-CG1	5.71	119.47	110.90
1	A	2083	ARG	CG-CD-NE	-5.70	99.83	111.80
1	D	4822	VAL	CA-CB-CG1	5.69	119.44	110.90
1	C	520	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	1457	PHE	CB-CG-CD1	-5.68	116.83	120.80
1	B	3726	LEU	CA-CB-CG	5.68	128.36	115.30
1	C	4940	TYR	CB-CG-CD2	5.67	124.40	121.00
1	C	4822	VAL	CA-CB-CG1	5.65	119.37	110.90
1	A	4087	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	2396	LEU	CB-CG-CD2	5.64	120.59	111.00
1	B	4822	VAL	CA-CB-CG1	5.64	119.36	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4195	GLU	OE1-CD-OE2	-5.64	116.54	123.30
1	B	678	MET	CB-CG-SD	5.63	129.29	112.40
1	B	4757	ILE	CG1-CB-CG2	-5.63	99.02	111.40
1	C	678	MET	CB-CG-SD	5.63	129.28	112.40
1	D	4087	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	4757	ILE	CG1-CB-CG2	-5.62	99.04	111.40
1	D	4603	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	4844	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	4854	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	D	2083	ARG	CG-CD-NE	-5.58	100.09	111.80
1	B	1089	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	3642	ILE	CG1-CB-CG2	-5.57	99.14	111.40
1	C	814	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	678	MET	CB-CG-SD	5.56	129.08	112.40
1	C	1303	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	4603	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	678	MET	CB-CG-SD	5.56	129.07	112.40
1	B	1652	LYS	CD-CE-NZ	5.55	124.46	111.70
1	C	2140	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	B	3940	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	1089	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	2139	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	D	2396	LEU	CB-CG-CD2	5.53	120.40	111.00
1	B	3811	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	2083	ARG	CG-CD-NE	-5.51	100.22	111.80
1	C	4916	LEU	CB-CG-CD1	-5.51	101.64	111.00
1	D	1089	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	3642	ILE	CG1-CB-CG2	-5.49	99.33	111.40
1	D	4757	ILE	CG1-CB-CG2	-5.49	99.33	111.40
1	D	814	LEU	CA-CB-CG	5.48	127.91	115.30
1	D	3726	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	4732	LEU	CB-CG-CD2	5.48	120.31	111.00
1	C	3726	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	3726	LEU	CA-CB-CG	5.48	127.90	115.30
1	D	4735	TYR	CB-CG-CD1	5.47	124.28	121.00
1	D	1303	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	4087	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	4087	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	814	LEU	CA-CB-CG	5.43	127.78	115.30
1	B	814	LEU	CA-CB-CG	5.42	127.77	115.30
1	C	2083	ARG	CG-CD-NE	-5.42	100.42	111.80
1	D	4732	LEU	CB-CG-CD2	5.42	120.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1652	LYS	CD-CE-NZ	5.41	124.15	111.70
1	A	1457	PHE	CB-CG-CD1	-5.41	117.02	120.80
1	B	4115	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	1905	LEU	CB-CG-CD1	5.40	120.18	111.00
1	B	3878	TYR	OH-CZ-CE2	5.39	134.66	120.10
1	B	4732	LEU	CB-CG-CD2	5.39	120.17	111.00
1	A	3878	TYR	OH-CZ-CE2	5.37	134.60	120.10
1	A	2140	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	D	3878	TYR	OH-CZ-CE2	5.37	134.59	120.10
1	A	1905	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	1778	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	A	4735	TYR	CG-CD2-CE2	5.34	125.57	121.30
1	D	1905	LEU	CA-CB-CG	5.34	127.57	115.30
1	A	30	LYS	CA-CB-CG	5.33	125.12	113.40
1	D	1112	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	801	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	4732	LEU	CB-CG-CD2	5.31	120.02	111.00
1	D	520	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	4727	MET	CB-CG-SD	5.29	128.28	112.40
1	A	1652	LYS	CD-CE-NZ	5.29	123.87	111.70
1	C	1944	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	D	4189	LEU	CB-CG-CD1	5.29	119.99	111.00
1	A	3940	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	3940	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	678	MET	CG-SD-CE	5.28	108.65	100.20
1	D	30	LYS	CA-CB-CG	5.28	125.01	113.40
1	A	1644	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	30	LYS	CA-CB-CG	5.28	125.00	113.40
1	D	1644	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	848	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	3642	ILE	CG1-CB-CG2	-5.27	99.80	111.40
1	C	2534	PRO	N-CA-CB	5.26	109.62	103.30
1	A	3642	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	B	678	MET	CG-SD-CE	5.25	108.60	100.20
1	A	1112	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	D	4862	ILE	CA-CB-CG1	-5.23	101.05	111.00
1	B	801	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	678	MET	CG-SD-CE	5.23	108.57	100.20
1	C	3878	TYR	OH-CZ-CE2	5.23	134.22	120.10
1	D	3940	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	678	MET	CG-SD-CE	5.23	108.56	100.20
1	C	4844	ARG	NE-CZ-NH2	5.23	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1942	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	848	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	1644	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	1905	LEU	CB-CG-CD1	5.22	119.87	111.00
1	B	1185	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	4853	PHE	CE1-CZ-CE2	-5.21	110.61	120.00
1	C	1905	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	4757	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	B	4735	TYR	CG-CD2-CE2	5.21	125.47	121.30
1	B	1644	LEU	CA-CB-CG	5.20	127.27	115.30
1	C	4115	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	C	1905	LEU	CB-CG-CD1	5.20	119.84	111.00
1	D	3811	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	2173	MET	CB-CG-SD	5.20	127.99	112.40
1	A	4862	ILE	CA-CB-CG1	-5.19	101.13	111.00
1	D	2534	PRO	N-CA-CB	5.19	109.53	103.30
1	C	30	LYS	CA-CB-CG	5.19	124.82	113.40
1	D	4134	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	4774	LEU	CB-CG-CD2	5.19	119.82	111.00
1	A	1303	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	4134	LEU	CA-CB-CG	5.18	127.20	115.30
1	C	4853	PHE	CE1-CZ-CE2	-5.16	110.71	120.00
1	A	4115	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	1303	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	4189	LEU	CB-CG-CD1	5.14	119.74	111.00
1	D	4115	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	2534	PRO	N-CA-CB	5.13	109.46	103.30
1	B	1905	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	2534	PRO	N-CA-CB	5.12	109.45	103.30
1	B	4134	LEU	CA-CB-CG	5.12	127.08	115.30
1	D	1652	LYS	CD-CE-NZ	5.11	123.45	111.70
1	D	4004	LEU	CB-CG-CD2	5.11	119.69	111.00
1	D	4174	ILE	CG1-CB-CG2	-5.11	100.16	111.40
1	C	4189	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	887	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	C	1778	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	D	2432	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	D	2203	TYR	CB-CG-CD2	-5.09	117.94	121.00
1	D	1778	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	A	2173	MET	CB-CG-SD	5.08	127.65	112.40
1	C	4134	LEU	CA-CB-CG	5.08	126.99	115.30
1	D	2139	GLU	OE1-CD-OE2	-5.08	117.20	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4174	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	B	4603	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	4735	TYR	CG-CD2-CE2	5.07	125.36	121.30
1	A	3700	CYS	CA-CB-SG	5.07	123.12	114.00
1	C	4004	LEU	CB-CG-CD2	5.06	119.61	111.00
1	A	4518	LEU	CB-CG-CD2	5.06	119.60	111.00
1	A	4174	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	B	2173	MET	CB-CG-SD	5.05	127.56	112.40
1	D	4518	LEU	CB-CG-CD2	5.05	119.58	111.00
1	B	4518	LEU	CB-CG-CD2	5.04	119.57	111.00
1	C	2392	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	C	4518	LEU	CB-CG-CD2	5.04	119.56	111.00
1	D	4853	PHE	CB-CG-CD1	5.04	124.33	120.80
1	A	2203	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	C	4853	PHE	CB-CG-CD1	5.03	124.32	120.80
1	D	4561	VAL	CG1-CB-CG2	5.03	118.94	110.90
1	B	2140	GLU	OE1-CD-OE2	-5.01	117.29	123.30
1	B	4174	ILE	CG1-CB-CG2	-5.01	100.38	111.40
1	A	1905	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1475	LYS	Peptide
1	A	1579	VAL	Peptide
1	A	1635	GLU	Peptide
1	A	1736	ILE	Peptide
1	A	1755	THR	Peptide
1	A	1808	ASP	Peptide
1	A	1835	HIS	Peptide
1	A	1847	GLU	Peptide
1	A	2075	VAL	Peptide
1	A	2329	PRO	Mainchain,Peptide
1	A	3800	SER	Peptide
1	A	4163	LYS	Peptide
1	A	4952	PHE	Sidechain
1	A	641	ASP	Peptide
1	A	686	VAL	Peptide
1	A	791	VAL	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	827	LEU	Peptide
1	A	838	ARG	Peptide
1	A	852	GLY	Mainchain,Peptide
1	B	1475	LYS	Peptide
1	B	1579	VAL	Peptide
1	B	1635	GLU	Peptide
1	B	1736	ILE	Peptide
1	B	1755	THR	Peptide
1	B	1808	ASP	Peptide
1	B	1835	HIS	Peptide
1	B	1847	GLU	Peptide
1	B	2075	VAL	Peptide
1	B	2329	PRO	Mainchain,Peptide
1	B	3800	SER	Peptide
1	B	4163	LYS	Peptide
1	B	4952	PHE	Sidechain
1	B	641	ASP	Peptide
1	B	686	VAL	Peptide
1	B	791	VAL	Peptide
1	B	818	GLY	Peptide
1	B	819	TYR	Peptide
1	B	827	LEU	Peptide
1	B	838	ARG	Peptide
1	B	852	GLY	Mainchain,Peptide
1	C	1475	LYS	Peptide
1	C	1579	VAL	Peptide
1	C	1635	GLU	Peptide
1	C	1736	ILE	Peptide
1	C	1755	THR	Peptide
1	C	1756	SER	Peptide
1	C	1808	ASP	Peptide
1	C	1835	HIS	Peptide
1	C	1847	GLU	Peptide
1	C	2075	VAL	Peptide
1	C	2329	PRO	Mainchain,Peptide
1	C	3800	SER	Peptide
1	C	4163	LYS	Peptide
1	C	4952	PHE	Sidechain
1	C	641	ASP	Peptide
1	C	686	VAL	Peptide
1	C	791	VAL	Peptide
1	C	818	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	819	TYR	Peptide
1	C	827	LEU	Peptide
1	C	838	ARG	Peptide
1	C	852	GLY	Mainchain,Peptide
1	D	1475	LYS	Peptide
1	D	1579	VAL	Peptide
1	D	1635	GLU	Peptide
1	D	1736	ILE	Peptide
1	D	1755	THR	Peptide
1	D	1808	ASP	Peptide
1	D	1835	HIS	Peptide
1	D	1847	GLU	Peptide
1	D	2075	VAL	Peptide
1	D	2329	PRO	Mainchain,Peptide
1	D	3800	SER	Peptide
1	D	4163	LYS	Peptide
1	D	4952	PHE	Sidechain
1	D	641	ASP	Peptide
1	D	686	VAL	Peptide
1	D	791	VAL	Peptide
1	D	818	GLY	Peptide
1	D	819	TYR	Peptide
1	D	827	LEU	Peptide
1	D	838	ARG	Peptide
1	D	852	GLY	Mainchain,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	26267	0	24896	381	0
1	B	26267	0	24897	372	0
1	C	26267	0	24897	370	0
1	D	26267	0	24896	377	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	105072	0	99586	1447	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 7.

All (1447) 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)
1:D:4818:MET:SD	1:D:4818:MET:CG	2.01	1.49
1:C:4818:MET:CG	1:C:4818:MET:SD	2.01	1.48
1:C:3700:CYS:SG	1:C:3700:CYS:CB	2.04	1.45
1:D:3700:CYS:SG	1:D:3700:CYS:CB	2.05	1.43
1:B:3700:CYS:CB	1:B:3700:CYS:SG	2.05	1.43
1:A:3700:CYS:SG	1:A:3700:CYS:CB	2.05	1.43
1:A:4171:ARG:NH1	1:A:4752:LYS:HD3	1.63	1.12
1:D:4171:ARG:NH1	1:D:4752:LYS:HE3	1.76	1.00
1:A:4171:ARG:HH12	1:A:4752:LYS:HD3	1.28	0.94
1:A:4767:GLN:HE22	1:B:4753:THR:HB	1.29	0.94
1:B:4767:GLN:HE22	1:C:4753:THR:HB	1.31	0.93
1:A:4767:GLN:NE2	1:B:4753:THR:HB	1.84	0.93
1:C:4767:GLN:HE22	1:D:4753:THR:HB	1.32	0.93
1:D:4171:ARG:HH11	1:D:4752:LYS:HE3	1.30	0.93
1:B:4767:GLN:NE2	1:C:4753:THR:HB	1.84	0.92
1:A:4753:THR:HB	1:D:4767:GLN:HE22	1.32	0.92
1:A:4753:THR:HB	1:D:4767:GLN:NE2	1.85	0.91
1:C:4767:GLN:NE2	1:D:4753:THR:HB	1.85	0.91
1:A:76:ARG:HD2	1:B:3891:TRP:HB3	1.54	0.89
1:C:76:ARG:HD2	1:D:3891:TRP:HB3	1.54	0.89
1:A:3891:TRP:HB3	1:D:76:ARG:HD2	1.52	0.88
1:B:76:ARG:HD2	1:C:3891:TRP:HB3	1.53	0.87
1:A:4754:LEU:HD11	1:D:4770:LEU:HB3	1.66	0.78
1:C:4770:LEU:HB3	1:D:4754:LEU:HD11	1.67	0.77
1:B:4791:ARG:HH12	1:C:4559:HIS:CE1	2.04	0.76
1:C:4791:ARG:HH12	1:D:4559:HIS:CE1	2.04	0.75
1:A:4791:ARG:HH12	1:B:4559:HIS:CE1	2.04	0.75
1:B:4770:LEU:HB3	1:C:4754:LEU:HD11	1.68	0.75
1:C:4171:ARG:HH21	1:C:4171:ARG:HG3	1.50	0.74
1:A:4770:LEU:HB3	1:B:4754:LEU:HD11	1.69	0.74
1:A:4559:HIS:CE1	1:D:4791:ARG:HH12	2.05	0.73
1:A:4171:ARG:NH1	1:A:4752:LYS:CD	2.49	0.71
1:D:2349:GLU:HG2	1:D:2439:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2349:GLU:HG2	1:C:2439:ILE:HD11	1.72	0.71
1:C:1011:ARG:HB3	1:C:1032:LEU:HD21	1.73	0.71
1:D:1011:ARG:HB3	1:D:1032:LEU:HD21	1.72	0.70
1:A:2349:GLU:HG2	1:A:2439:ILE:HD11	1.72	0.70
1:B:2349:GLU:HG2	1:B:2439:ILE:HD11	1.72	0.70
1:B:4832:ILE:HG21	1:B:4844:ARG:HH21	1.57	0.69
1:A:4832:ILE:HG21	1:A:4844:ARG:HH21	1.58	0.69
1:B:1011:ARG:HB3	1:B:1032:LEU:HD21	1.74	0.69
1:B:986:ILE:HD12	1:B:1059:GLY:HA2	1.74	0.69
1:B:1645:THR:HG22	1:B:1695:PRO:HG3	1.73	0.69
1:C:4817:HIS:HE1	1:C:4828:ILE:HD12	1.57	0.68
1:C:4832:ILE:HG21	1:C:4844:ARG:HH21	1.58	0.68
1:A:1011:ARG:HB3	1:A:1032:LEU:HD21	1.75	0.68
1:B:4817:HIS:HE1	1:B:4828:ILE:HD12	1.57	0.68
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	1.73	0.68
1:A:4817:HIS:HE1	1:A:4828:ILE:HD12	1.57	0.68
1:A:4642:PRO:HG2	1:A:4648:LYS:HD2	1.76	0.68
1:B:4642:PRO:HG2	1:B:4648:LYS:HD2	1.76	0.68
1:D:4832:ILE:HG21	1:D:4844:ARG:HH21	1.57	0.68
1:B:4511:ALA:HA	1:B:4514:ILE:HD12	1.77	0.67
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.75	0.67
1:A:4511:ALA:HA	1:A:4514:ILE:HD12	1.77	0.67
1:C:1620:GLN:HE21	1:C:1622:LEU:HD21	1.60	0.67
1:D:4817:HIS:HE1	1:D:4828:ILE:HD12	1.58	0.67
1:A:143:LEU:HD23	1:B:2426:SER:HB3	1.77	0.67
1:B:2463:PRO:HB2	1:B:2519:ARG:HD2	1.76	0.67
1:D:644:LEU:HB2	1:D:1654:HIS:HD2	1.60	0.67
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.75	0.66
1:C:4642:PRO:HG2	1:C:4648:LYS:HD2	1.77	0.66
1:D:2463:PRO:HB2	1:D:2519:ARG:HD2	1.77	0.66
1:B:1620:GLN:HE21	1:B:1622:LEU:HD21	1.60	0.66
1:D:4642:PRO:HG2	1:D:4648:LYS:HD2	1.77	0.66
1:C:644:LEU:HB2	1:C:1654:HIS:HD2	1.60	0.66
1:D:4511:ALA:HA	1:D:4514:ILE:HD12	1.78	0.66
1:A:1620:GLN:HE21	1:A:1622:LEU:HD21	1.60	0.66
1:A:986:ILE:HD12	1:A:1059:GLY:HA2	1.78	0.65
1:C:4511:ALA:HA	1:C:4514:ILE:HD12	1.78	0.65
1:D:3802:SER:OG	1:D:3833:ASP:O	2.14	0.65
1:D:1620:GLN:HE21	1:D:1622:LEU:HD21	1.60	0.65
1:B:1304:LEU:HB3	1:B:1541:PRO:HG2	1.79	0.65
1:B:1258:PHE:HB2	1:B:1593:HIS:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3802:SER:OG	1:B:3833:ASP:O	2.15	0.65
1:A:2463:PRO:HB2	1:A:2519:ARG:HD2	1.76	0.65
1:A:3802:SER:OG	1:A:3833:ASP:O	2.14	0.65
1:B:644:LEU:HB2	1:B:1654:HIS:HD2	1.60	0.65
1:C:2463:PRO:HB2	1:C:2519:ARG:HD2	1.77	0.64
1:C:143:LEU:HD23	1:D:2426:SER:HB3	1.79	0.64
1:A:1304:LEU:HB3	1:A:1541:PRO:HG2	1.79	0.64
1:A:644:LEU:HB2	1:A:1654:HIS:HD2	1.61	0.64
1:A:4171:ARG:HH11	1:A:4752:LYS:HD3	1.59	0.64
1:D:1602:GLN:HE22	1:D:1642:LEU:HB3	1.63	0.64
1:B:3911:ILE:HG21	1:B:3971:GLU:HB3	1.80	0.64
1:C:986:ILE:HD12	1:C:1059:GLY:HA2	1.79	0.63
1:D:1258:PHE:HB2	1:D:1593:HIS:HB3	1.80	0.63
1:A:1602:GLN:HE22	1:A:1642:LEU:HB3	1.63	0.63
1:B:143:LEU:HD23	1:C:2426:SER:HB3	1.80	0.63
1:D:986:ILE:HD12	1:D:1059:GLY:HA2	1.79	0.63
1:A:1258:PHE:HB2	1:A:1593:HIS:HB3	1.80	0.63
1:C:1258:PHE:HB2	1:C:1593:HIS:HB3	1.79	0.63
1:C:4002:ASP:HA	1:C:4115:ARG:HH22	1.63	0.63
1:C:647:ARG:NH1	1:C:1681:ASP:OD2	2.32	0.63
1:D:1286:THR:HA	1:D:1586:LEU:HD11	1.80	0.63
1:D:1304:LEU:HB3	1:D:1541:PRO:HG2	1.80	0.63
1:C:1304:LEU:HB3	1:C:1541:PRO:HG2	1.79	0.62
1:C:1602:GLN:HE22	1:C:1642:LEU:HB3	1.63	0.62
1:A:3911:ILE:HG21	1:A:3971:GLU:HB3	1.81	0.62
1:A:3925:ILE:HG23	1:A:3933:GLN:HG2	1.82	0.62
1:B:1602:GLN:HE22	1:B:1642:LEU:HB3	1.63	0.62
1:A:1286:THR:HA	1:A:1586:LEU:HD11	1.80	0.62
1:A:4002:ASP:HA	1:A:4115:ARG:HH22	1.64	0.62
1:C:2256:LEU:O	1:C:3811:ARG:NH1	2.32	0.62
1:A:238:HIS:HE1	1:A:400:ASP:HB3	1.65	0.62
1:B:1286:THR:HA	1:B:1586:LEU:HD11	1.80	0.62
1:D:1605:LYS:HD3	1:D:1606:VAL:HG23	1.81	0.62
1:D:647:ARG:NH1	1:D:1681:ASP:OD2	2.33	0.62
1:D:3925:ILE:HG23	1:D:3933:GLN:HG2	1.82	0.62
1:B:2256:LEU:O	1:B:3811:ARG:NH1	2.32	0.62
1:D:228:LEU:HB3	1:D:289:ILE:HD12	1.82	0.62
1:A:647:ARG:NH1	1:A:1681:ASP:OD2	2.33	0.62
1:A:228:LEU:HB3	1:A:289:ILE:HD12	1.82	0.62
1:A:708:GLY:HA2	1:A:714:GLY:HA3	1.82	0.62
1:C:228:LEU:HB3	1:C:289:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3911:ILE:HG21	1:C:3971:GLU:HB3	1.82	0.62
1:B:647:ARG:NH1	1:B:1681:ASP:OD2	2.32	0.61
1:B:228:LEU:HB3	1:B:289:ILE:HD12	1.82	0.61
1:C:3802:SER:OG	1:C:3833:ASP:O	2.15	0.61
1:D:238:HIS:HE1	1:D:400:ASP:HB3	1.65	0.61
1:A:1605:LYS:HD3	1:A:1606:VAL:HG23	1.82	0.61
1:B:4002:ASP:HA	1:B:4115:ARG:HH22	1.64	0.61
1:C:1286:THR:HA	1:C:1586:LEU:HD11	1.80	0.61
1:C:1605:LYS:HD3	1:C:1606:VAL:HG23	1.81	0.61
1:A:2426:SER:HB3	1:D:143:LEU:HD23	1.81	0.61
1:D:4002:ASP:HA	1:D:4115:ARG:HH22	1.63	0.61
1:A:2256:LEU:O	1:A:3811:ARG:NH1	2.32	0.61
1:B:3925:ILE:HG23	1:B:3933:GLN:HG2	1.83	0.61
1:C:238:HIS:HE1	1:C:400:ASP:HB3	1.66	0.61
1:B:238:HIS:HE1	1:B:400:ASP:HB3	1.66	0.61
1:B:708:GLY:HA2	1:B:714:GLY:HA3	1.82	0.61
1:C:192:LEU:O	1:C:212:TRP:NE1	2.33	0.61
1:D:3922:THR:O	1:D:3926:GLN:N	2.34	0.61
1:B:1605:LYS:HD3	1:B:1606:VAL:HG23	1.82	0.61
1:C:3922:THR:O	1:C:3926:GLN:N	2.34	0.61
1:C:3925:ILE:HG23	1:C:3933:GLN:HG2	1.83	0.61
1:D:192:LEU:O	1:D:212:TRP:NE1	2.33	0.61
1:A:4170:LYS:HE2	1:A:4916:LEU:HD23	1.82	0.60
1:B:1445:TRP:HE1	1:B:1508:GLY:HA3	1.66	0.60
1:D:3911:ILE:HG21	1:D:3971:GLU:HB3	1.82	0.60
1:D:644:LEU:HD22	1:D:1632:ILE:HG22	1.83	0.60
1:D:2256:LEU:O	1:D:3811:ARG:NH1	2.32	0.60
1:A:4085:VAL:HG12	1:A:4090:GLU:HG3	1.84	0.60
1:C:3914:ALA:HB3	1:C:3975:LEU:HD11	1.82	0.60
1:C:4171:ARG:CG	1:C:4171:ARG:HH21	2.14	0.60
1:D:3914:ALA:HB3	1:D:3975:LEU:HD11	1.83	0.60
1:D:708:GLY:HA2	1:D:714:GLY:HA3	1.83	0.60
1:A:644:LEU:HD22	1:A:1632:ILE:HG22	1.83	0.60
1:A:192:LEU:O	1:A:212:TRP:NE1	2.33	0.60
1:A:3914:ALA:HB3	1:A:3975:LEU:HD11	1.84	0.60
1:C:708:GLY:HA2	1:C:714:GLY:HA3	1.83	0.60
1:A:4170:LYS:HE2	1:A:4916:LEU:CD2	2.32	0.60
1:B:300:VAL:HG13	1:B:420:ARG:HH21	1.67	0.60
1:C:300:VAL:HG13	1:C:420:ARG:HH21	1.66	0.60
1:D:4085:VAL:HG12	1:D:4090:GLU:HG3	1.84	0.60
1:C:4085:VAL:HG12	1:C:4090:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.67	0.59
1:C:779:PHE:HB3	1:C:782:PHE:HE2	1.67	0.59
1:A:1445:TRP:HE1	1:A:1508:GLY:HA3	1.67	0.59
1:B:3914:ALA:HB3	1:B:3975:LEU:HD11	1.84	0.59
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.67	0.59
1:B:1444:GLY:HA2	1:B:1487:MET:HB2	1.83	0.59
1:B:779:PHE:HB3	1:B:782:PHE:HE2	1.67	0.59
1:B:192:LEU:O	1:B:212:TRP:NE1	2.33	0.59
1:C:711:GLU:HG3	1:C:1449:ASP:HB3	1.85	0.59
1:C:644:LEU:HD22	1:C:1632:ILE:HG22	1.83	0.59
1:D:1272:ARG:NH1	1:D:1587:HIS:O	2.36	0.59
1:A:1444:GLY:HA2	1:A:1487:MET:HB2	1.83	0.59
1:A:779:PHE:HB3	1:A:782:PHE:HE2	1.67	0.59
1:D:779:PHE:HB3	1:D:782:PHE:HE2	1.67	0.59
1:D:1762:GLN:O	1:D:1779:SER:OG	2.21	0.59
1:A:650:ASN:HA	1:A:1626:GLN:HG2	1.85	0.59
1:C:4170:LYS:HE3	1:C:4916:LEU:HD23	1.85	0.59
1:D:2204:PHE:O	1:D:2211:ASN:ND2	2.36	0.59
1:D:300:VAL:HG13	1:D:420:ARG:HH21	1.67	0.59
1:A:300:VAL:HG13	1:A:420:ARG:HH21	1.67	0.59
1:B:644:LEU:HD22	1:B:1632:ILE:HG22	1.84	0.59
1:C:1445:TRP:HE1	1:C:1508:GLY:HA3	1.67	0.59
1:C:227:TYR:HE1	1:C:355:LYS:HG2	1.68	0.59
1:A:677:LEU:HB2	1:A:755:ILE:HB	1.85	0.59
1:C:1272:ARG:NH1	1:C:1587:HIS:O	2.36	0.58
1:C:1762:GLN:O	1:C:1779:SER:OG	2.21	0.58
1:C:2204:PHE:O	1:C:2211:ASN:ND2	2.36	0.58
1:A:1272:ARG:NH1	1:A:1587:HIS:O	2.36	0.58
1:B:3922:THR:O	1:B:3926:GLN:N	2.34	0.58
1:A:35:LEU:HD13	1:A:49:LEU:HD22	1.85	0.58
1:D:1444:GLY:HA2	1:D:1487:MET:HB2	1.84	0.58
1:D:1445:TRP:HE1	1:D:1508:GLY:HA3	1.68	0.58
1:B:711:GLU:HG3	1:B:1449:ASP:HB3	1.85	0.58
1:A:2204:PHE:O	1:A:2211:ASN:ND2	2.36	0.58
1:A:711:GLU:HG3	1:A:1449:ASP:HB3	1.84	0.58
1:A:1086:ARG:HB2	1:A:1207:LEU:HB2	1.86	0.58
1:B:4085:VAL:HG12	1:B:4090:GLU:HG3	1.84	0.58
1:C:1444:GLY:HA2	1:C:1487:MET:HB2	1.84	0.58
1:C:677:LEU:HB2	1:C:755:ILE:HB	1.86	0.58
1:B:58:VAL:HG22	1:B:320:GLU:HA	1.86	0.58
1:D:650:ASN:HA	1:D:1626:GLN:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.68	0.58
1:D:1726:ILE:HD11	1:D:2121:LEU:HD11	1.86	0.58
1:B:2204:PHE:O	1:B:2211:ASN:ND2	2.37	0.58
1:A:1762:GLN:O	1:A:1779:SER:OG	2.22	0.58
1:C:3879:LEU:HD12	1:C:3917:VAL:HG13	1.86	0.58
1:D:35:LEU:HD13	1:D:49:LEU:HD22	1.85	0.58
1:B:3879:LEU:HD12	1:B:3917:VAL:HG13	1.85	0.57
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.69	0.57
1:C:58:VAL:HG22	1:C:320:GLU:HA	1.86	0.57
1:B:1086:ARG:HB2	1:B:1207:LEU:HB2	1.85	0.57
1:D:227:TYR:HE1	1:D:355:LYS:HG2	1.68	0.57
1:D:711:GLU:HG3	1:D:1449:ASP:HB3	1.84	0.57
1:B:1272:ARG:NH1	1:B:1587:HIS:O	2.36	0.57
1:C:35:LEU:HD13	1:C:49:LEU:HD22	1.86	0.57
1:A:1726:ILE:HD11	1:A:2121:LEU:HD11	1.87	0.57
1:C:4617:TYR:OH	1:C:4629:GLY:O	2.23	0.57
1:A:3922:THR:O	1:A:3926:GLN:N	2.34	0.57
1:C:1086:ARG:HB2	1:C:1207:LEU:HB2	1.86	0.57
1:B:672:LYS:HA	1:B:760:ASP:HA	1.87	0.57
1:B:897:LYS:HD3	1:B:918:LEU:HD21	1.86	0.57
1:C:897:LYS:HD3	1:C:918:LEU:HD21	1.86	0.57
1:D:58:VAL:HG22	1:D:320:GLU:HA	1.86	0.57
1:A:58:VAL:HG22	1:A:320:GLU:HA	1.87	0.57
1:B:650:ASN:HA	1:B:1626:GLN:HG2	1.85	0.57
1:B:677:LEU:HB2	1:B:755:ILE:HB	1.85	0.57
1:A:3879:LEU:HD12	1:A:3917:VAL:HG13	1.87	0.57
1:B:227:TYR:HE1	1:B:355:LYS:HG2	1.70	0.57
1:B:4617:TYR:OH	1:B:4629:GLY:O	2.23	0.57
1:C:672:LYS:HA	1:C:760:ASP:HA	1.87	0.57
1:D:672:LYS:HA	1:D:760:ASP:HA	1.87	0.57
1:A:672:LYS:HA	1:A:760:ASP:HA	1.87	0.56
1:B:3914:ALA:HA	1:B:3917:VAL:HG12	1.87	0.56
1:D:1086:ARG:HB2	1:D:1207:LEU:HB2	1.86	0.56
1:C:650:ASN:HA	1:C:1626:GLN:HG2	1.86	0.56
1:D:4800:GLY:HA2	1:D:4804:ASP:HB3	1.87	0.56
1:A:2737:LYS:HB3	1:A:2742:TRP:HB2	1.88	0.56
1:D:677:LEU:HB2	1:D:755:ILE:HB	1.86	0.56
1:B:756:SER:HB3	1:B:769:ARG:HB2	1.87	0.56
1:C:1726:ILE:HD11	1:C:2121:LEU:HD11	1.87	0.56
1:C:4045:SER:HA	1:C:4078:THR:HA	1.87	0.56
1:D:2071:ALA:HA	1:D:2076:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ARG:NH1	1:D:317:MET:SD	2.79	0.56
1:B:1762:GLN:O	1:B:1779:SER:OG	2.22	0.56
1:B:2737:LYS:HB3	1:B:2742:TRP:HB2	1.88	0.56
1:C:4888:LYS:HA	1:C:4895:GLY:HA2	1.88	0.56
1:C:905:GLY:HA3	1:C:914:GLN:HB3	1.88	0.56
1:D:4617:TYR:OH	1:D:4629:GLY:O	2.23	0.56
1:A:364:GLN:HE21	1:A:369:GLY:HA2	1.71	0.56
1:B:905:GLY:HA3	1:B:914:GLN:HB3	1.87	0.56
1:D:897:LYS:HD3	1:D:918:LEU:HD21	1.87	0.56
1:B:258:ARG:NH1	1:B:317:MET:SD	2.78	0.56
1:B:35:LEU:HD13	1:B:49:LEU:HD22	1.87	0.56
1:B:4888:LYS:HA	1:B:4895:GLY:HA2	1.87	0.56
1:A:258:ARG:NH1	1:A:317:MET:SD	2.79	0.56
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.88	0.56
1:A:905:GLY:HA3	1:A:914:GLN:HB3	1.88	0.56
1:A:897:LYS:HD3	1:A:918:LEU:HD21	1.87	0.56
1:B:3804:LEU:HD13	1:B:3910:ALA:HB2	1.88	0.56
1:C:258:ARG:NH1	1:C:317:MET:SD	2.78	0.56
1:C:4800:GLY:HA2	1:C:4804:ASP:HB3	1.88	0.56
1:D:3879:LEU:HD12	1:D:3917:VAL:HG13	1.87	0.56
1:D:4045:SER:HA	1:D:4078:THR:HA	1.87	0.56
1:D:905:GLY:HA3	1:D:914:GLN:HB3	1.88	0.56
1:B:364:GLN:HE21	1:B:369:GLY:HA2	1.71	0.56
1:C:4835:PRO:HB2	1:C:4841:GLU:HG3	1.87	0.56
1:D:364:GLN:HE21	1:D:369:GLY:HA2	1.71	0.56
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.88	0.55
1:A:228:LEU:HD12	1:A:354:ILE:HB	1.89	0.55
1:A:227:TYR:HE1	1:A:355:LYS:HG2	1.70	0.55
1:A:4045:SER:HA	1:A:4078:THR:HA	1.87	0.55
1:A:4617:TYR:OH	1:A:4629:GLY:O	2.23	0.55
1:C:1137:PHE:HA	1:C:1144:ARG:HA	1.89	0.55
1:C:2737:LYS:HB3	1:C:2742:TRP:HB2	1.88	0.55
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.88	0.55
1:D:756:SER:HB3	1:D:769:ARG:HB2	1.87	0.55
1:A:756:SER:HB3	1:A:769:ARG:HB2	1.87	0.55
1:B:4780:TYR:HA	1:B:4783:THR:HG22	1.89	0.55
1:C:756:SER:HB3	1:C:769:ARG:HB2	1.88	0.55
1:C:4791:ARG:HH12	1:D:4559:HIS:HE1	1.53	0.55
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	1.88	0.55
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.88	0.55
1:B:4045:SER:HA	1:B:4078:THR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3914:ALA:HA	1:D:3917:VAL:HG12	1.88	0.55
1:C:364:GLN:HE21	1:C:369:GLY:HA2	1.71	0.55
1:D:4817:HIS:CE1	1:D:4828:ILE:HD12	2.40	0.55
1:A:1245:ARG:HE	1:A:1692:LYS:HG2	1.72	0.55
1:D:776:GLN:HB3	1:D:1470:GLY:HA3	1.89	0.55
1:D:2737:LYS:HB3	1:D:2742:TRP:HB2	1.88	0.55
1:A:2404:ALA:HB3	1:A:2475:ARG:HH21	1.72	0.54
1:A:4888:LYS:HA	1:A:4895:GLY:HA2	1.89	0.54
1:B:1726:ILE:HD11	1:B:2121:LEU:HD11	1.88	0.54
1:B:4835:PRO:HB2	1:B:4841:GLU:HG3	1.88	0.54
1:C:4817:HIS:CE1	1:C:4828:ILE:HD12	2.40	0.54
1:C:4915:ASN:O	1:C:4917:ALA:N	2.41	0.54
1:A:1607:ASP:HB3	1:A:1608:VAL:HG23	1.89	0.54
1:B:4817:HIS:CE1	1:B:4828:ILE:HD12	2.39	0.54
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.88	0.54
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.88	0.54
1:B:1137:PHE:HA	1:B:1144:ARG:HA	1.89	0.54
1:B:1245:ARG:HE	1:B:1692:LYS:HG2	1.72	0.54
1:B:4915:ASN:O	1:B:4917:ALA:N	2.40	0.54
1:C:3914:ALA:HA	1:C:3917:VAL:HG12	1.88	0.54
1:A:123:HIS:HD2	1:A:126:SER:H	1.55	0.54
1:A:1601:ASN:ND2	1:A:1643:GLU:OE2	2.41	0.54
1:A:3914:ALA:HA	1:A:3917:VAL:HG12	1.88	0.54
1:A:4754:LEU:CD1	1:D:4770:LEU:HB3	2.36	0.54
1:A:4791:ARG:HH12	1:B:4559:HIS:HE1	1.54	0.54
1:B:1607:ASP:HB3	1:B:1608:VAL:HG23	1.88	0.54
1:C:4780:TYR:HA	1:C:4783:THR:HG22	1.89	0.54
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.89	0.54
1:D:4835:PRO:HB2	1:D:4841:GLU:HG3	1.89	0.54
1:A:4817:HIS:CE1	1:A:4828:ILE:HD12	2.40	0.54
1:B:123:HIS:HD2	1:B:126:SER:H	1.56	0.54
1:B:1510:VAL:HG12	1:B:1511:VAL:HG23	1.90	0.54
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.90	0.54
1:A:4915:ASN:O	1:A:4917:ALA:N	2.41	0.54
1:C:1252:SER:HB2	1:C:1598:ARG:HB2	1.90	0.54
1:C:1607:ASP:HB3	1:C:1608:VAL:HG23	1.89	0.54
1:C:2071:ALA:HA	1:C:2076:ILE:HD11	1.88	0.54
1:B:228:LEU:HD12	1:B:354:ILE:HB	1.90	0.54
1:C:2404:ALA:HB3	1:C:2475:ARG:HH21	1.73	0.54
1:A:3670:LEU:HD22	1:A:3674:ARG:HH21	1.73	0.54
1:B:281:ARG:NH1	1:B:346:VAL:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1601:ASN:ND2	1:C:1643:GLU:OE2	2.41	0.54
1:C:2489:LEU:O	1:C:2492:GLY:N	2.41	0.54
1:C:652:VAL:HG11	1:C:715:GLY:HA2	1.90	0.54
1:D:228:LEU:HD12	1:D:354:ILE:HB	1.89	0.54
1:D:4915:ASN:O	1:D:4917:ALA:N	2.41	0.54
1:A:4835:PRO:HB2	1:A:4841:GLU:HG3	1.89	0.54
1:B:1601:ASN:ND2	1:B:1643:GLU:OE2	2.41	0.54
1:B:4800:GLY:HA2	1:B:4804:ASP:HB3	1.90	0.54
1:D:2404:ALA:HB3	1:D:2475:ARG:HH21	1.73	0.54
1:A:2489:LEU:O	1:A:2492:GLY:N	2.41	0.54
1:A:4823:ARG:NH1	1:D:4826:GLY:O	2.41	0.54
1:B:1267:HIS:HB3	1:B:1294:ASN:HD21	1.73	0.54
1:C:123:HIS:HD2	1:C:126:SER:H	1.56	0.54
1:C:1267:HIS:HB3	1:C:1294:ASN:HD21	1.73	0.54
1:C:1629:SER:HA	1:C:1640:ASP:HA	1.90	0.54
1:D:1601:ASN:ND2	1:D:1643:GLU:OE2	2.41	0.54
1:D:1629:SER:HA	1:D:1640:ASP:HA	1.90	0.54
1:A:243:GLU:HA	1:A:264:GLY:HA2	1.89	0.53
1:A:776:GLN:HB3	1:A:1470:GLY:HA3	1.89	0.53
1:B:1431:ARG:HB3	1:B:1554:GLN:HB2	1.90	0.53
1:B:2489:LEU:O	1:B:2492:GLY:N	2.41	0.53
1:B:4171:ARG:HH21	1:B:4171:ARG:HG3	1.72	0.53
1:D:1267:HIS:HB3	1:D:1294:ASN:HD21	1.73	0.53
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.90	0.53
1:A:2071:ALA:HA	1:A:2076:ILE:HD11	1.90	0.53
1:A:800:VAL:HG23	1:A:1619:VAL:HG13	1.90	0.53
1:B:3670:LEU:HD22	1:B:3674:ARG:HH21	1.73	0.53
1:B:4810:MET:HB3	1:C:4519:LEU:O	2.08	0.53
1:A:4780:TYR:HA	1:A:4783:THR:HG22	1.89	0.53
1:B:800:VAL:HG23	1:B:1619:VAL:HG13	1.90	0.53
1:C:1510:VAL:HG12	1:C:1511:VAL:HG23	1.90	0.53
1:D:123:HIS:HD2	1:D:126:SER:H	1.55	0.53
1:D:1690:GLU:OE2	1:D:1790:LYS:NZ	2.39	0.53
1:A:1690:GLU:OE2	1:A:1790:LYS:NZ	2.39	0.53
1:B:1252:SER:HB2	1:B:1598:ARG:HB2	1.90	0.53
1:B:4191:VAL:HA	1:B:4194:CYS:HB2	1.91	0.53
1:D:3670:LEU:HD22	1:D:3674:ARG:HH21	1.74	0.53
1:A:4800:GLY:HA2	1:A:4804:ASP:HB3	1.90	0.53
1:B:1629:SER:HA	1:B:1640:ASP:HA	1.90	0.53
1:B:4188:GLU:O	1:B:4192:ASN:ND2	2.42	0.53
1:A:1442:TRP:HD1	1:A:1488:VAL:HG13	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4826:GLY:O	1:B:4823:ARG:NH1	2.42	0.53
1:D:800:VAL:HG23	1:D:1619:VAL:HG13	1.91	0.53
1:A:1267:HIS:HB3	1:A:1294:ASN:HD21	1.74	0.53
1:B:1128:LEU:HD13	1:B:1206:SER:HB2	1.90	0.53
1:C:1128:LEU:HD13	1:C:1206:SER:HB2	1.91	0.53
1:D:2489:LEU:O	1:D:2492:GLY:N	2.41	0.53
1:D:4888:LYS:HA	1:D:4895:GLY:HA2	1.90	0.53
1:B:4752:LYS:HG3	1:B:4755:ARG:HE	1.74	0.53
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.89	0.53
1:C:243:GLU:HA	1:C:264:GLY:HA2	1.90	0.53
1:C:228:LEU:HD12	1:C:354:ILE:HB	1.89	0.53
1:B:4791:ARG:HH12	1:C:4559:HIS:HE1	1.53	0.53
1:D:1607:ASP:HB3	1:D:1608:VAL:HG23	1.90	0.53
1:D:243:GLU:HA	1:D:264:GLY:HA2	1.89	0.53
1:A:1128:LEU:HD13	1:A:1206:SER:HB2	1.90	0.53
1:A:1431:ARG:HB3	1:A:1554:GLN:HB2	1.90	0.53
1:C:3670:LEU:HD22	1:C:3674:ARG:HH21	1.72	0.53
1:D:1442:TRP:HB2	1:D:1544:PHE:HB2	1.91	0.53
1:A:1442:TRP:HB2	1:A:1544:PHE:HB2	1.91	0.53
1:D:1245:ARG:HE	1:D:1692:LYS:HG2	1.74	0.53
1:D:4780:TYR:HA	1:D:4783:THR:HG22	1.90	0.53
1:C:1431:ARG:HB3	1:C:1554:GLN:HB2	1.91	0.52
1:C:800:VAL:HG23	1:C:1619:VAL:HG13	1.91	0.52
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.91	0.52
1:B:652:VAL:HG11	1:B:715:GLY:HA2	1.90	0.52
1:C:3645:LEU:HB2	1:C:3665:LEU:HD12	1.91	0.52
1:C:4810:MET:HB3	1:D:4519:LEU:O	2.09	0.52
1:D:1431:ARG:HB3	1:D:1554:GLN:HB2	1.91	0.52
1:B:243:GLU:HA	1:B:264:GLY:HA2	1.90	0.52
1:B:776:GLN:HB3	1:B:1470:GLY:HA3	1.90	0.52
1:C:712:GLU:OE2	1:C:1636:ASN:ND2	2.43	0.52
1:C:4014:ILE:HA	1:C:4017:PHE:HB3	1.92	0.52
1:D:1128:LEU:HD13	1:D:1206:SER:HB2	1.91	0.52
1:D:1266:GLU:O	1:D:1294:ASN:ND2	2.43	0.52
1:D:4014:ILE:HA	1:D:4017:PHE:HB3	1.92	0.52
1:D:4188:GLU:O	1:D:4192:ASN:ND2	2.43	0.52
1:A:4519:LEU:O	1:D:4810:MET:HB3	2.09	0.52
1:C:4191:VAL:HA	1:C:4194:CYS:HB2	1.92	0.52
1:B:2794:ARG:HB2	1:B:2901:GLY:HA3	1.92	0.52
1:B:3645:LEU:HB2	1:B:3665:LEU:HD12	1.92	0.52
1:C:1442:TRP:HB2	1:C:1544:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1442:TRP:HB2	1:B:1544:PHE:HB2	1.92	0.52
1:B:2130:LEU:HD12	1:B:2133:VAL:HG21	1.92	0.52
1:B:2404:ALA:HB3	1:B:2475:ARG:HH21	1.74	0.52
1:B:227:TYR:CE1	1:B:355:LYS:HG2	2.45	0.52
1:C:2130:LEU:HD12	1:C:2133:VAL:HG21	1.92	0.52
1:D:3924:TYR:O	1:D:3932:ASN:ND2	2.43	0.52
1:A:4188:GLU:O	1:A:4192:ASN:ND2	2.42	0.52
1:A:4810:MET:HB3	1:B:4519:LEU:O	2.09	0.52
1:C:776:GLN:HB3	1:C:1470:GLY:HA3	1.90	0.52
1:D:281:ARG:NH1	1:D:346:VAL:O	2.42	0.52
1:C:2794:ARG:HB2	1:C:2901:GLY:HA3	1.92	0.52
1:C:4817:HIS:HA	1:C:4821:GLY:H	1.75	0.52
1:D:1252:SER:HB2	1:D:1598:ARG:HB2	1.91	0.52
1:D:3730:ALA:HA	1:D:3733:HIS:CE1	2.45	0.52
1:A:4559:HIS:HE1	1:D:4791:ARG:HH12	1.54	0.52
1:A:3665:LEU:HD22	1:A:3735:ARG:HH11	1.75	0.52
1:A:4608:ALA:HB1	1:A:4650:VAL:HG11	1.92	0.52
1:C:4770:LEU:HB3	1:D:4754:LEU:CD1	2.37	0.52
1:D:1272:ARG:NH2	1:D:1590:PHE:O	2.43	0.52
1:D:3645:LEU:HB2	1:D:3665:LEU:HD12	1.92	0.52
1:D:4817:HIS:HA	1:D:4821:GLY:H	1.74	0.52
1:D:652:VAL:HG11	1:D:715:GLY:HA2	1.92	0.52
1:A:2794:ARG:HB2	1:A:2901:GLY:HA3	1.92	0.52
1:B:1442:TRP:HD1	1:B:1488:VAL:HG13	1.75	0.52
1:C:227:TYR:CE1	1:C:355:LYS:HG2	2.44	0.52
1:C:3665:LEU:HD22	1:C:3735:ARG:HH11	1.75	0.52
1:C:4188:GLU:O	1:C:4192:ASN:ND2	2.42	0.52
1:D:598:ILE:HG23	1:D:636:LEU:HD12	1.92	0.52
1:A:3730:ALA:HA	1:A:3733:HIS:CE1	2.45	0.51
1:B:2071:ALA:HA	1:B:2076:ILE:HD11	1.91	0.51
1:D:1442:TRP:HD1	1:D:1488:VAL:HG13	1.75	0.51
1:D:1703:TYR:HD2	1:D:1820:PRO:HB2	1.75	0.51
1:D:2076:ILE:HG21	1:D:2081:LEU:HD22	1.92	0.51
1:D:4170:LYS:HE2	1:D:4916:LEU:HD23	1.91	0.51
1:A:227:TYR:CE1	1:A:355:LYS:HG2	2.45	0.51
1:A:4752:LYS:HG3	1:A:4755:ARG:HE	1.76	0.51
1:B:3730:ALA:HA	1:B:3733:HIS:CE1	2.46	0.51
1:B:3665:LEU:HD22	1:B:3735:ARG:HH11	1.75	0.51
1:C:2076:ILE:HG21	1:C:2081:LEU:HD22	1.92	0.51
1:C:2083:ARG:HG3	1:C:3688:LEU:HD22	1.92	0.51
1:D:3665:LEU:HD22	1:D:3735:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4608:ALA:HB1	1:D:4650:VAL:HG11	1.91	0.51
1:A:2130:LEU:HD12	1:A:2133:VAL:HG21	1.93	0.51
1:A:3645:LEU:HB2	1:A:3665:LEU:HD12	1.93	0.51
1:A:4014:ILE:HA	1:A:4017:PHE:HB3	1.91	0.51
1:A:4191:VAL:HA	1:A:4194:CYS:HB2	1.93	0.51
1:B:3742:LEU:HD23	1:B:3781:TYR:HB3	1.92	0.51
1:D:227:TYR:CE1	1:D:355:LYS:HG2	2.45	0.51
1:A:1266:GLU:O	1:A:1294:ASN:ND2	2.43	0.51
1:B:4824:ALA:HB3	1:B:4827:GLY:H	1.75	0.51
1:C:1124:PRO:HB2	1:C:1252:SER:HB3	1.93	0.51
1:C:1272:ARG:NH2	1:C:1590:PHE:O	2.44	0.51
1:D:866:PRO:HD2	1:D:1009:ARG:HD2	1.92	0.51
1:D:2794:ARG:HB2	1:D:2901:GLY:HA3	1.92	0.51
1:D:2083:ARG:HG3	1:D:3688:LEU:HD22	1.92	0.51
1:A:1252:SER:HB2	1:A:1598:ARG:HB2	1.91	0.51
1:A:1272:ARG:NH2	1:A:1590:PHE:O	2.44	0.51
1:C:866:PRO:HD2	1:C:1009:ARG:HD2	1.92	0.51
1:C:1266:GLU:O	1:C:1294:ASN:ND2	2.43	0.51
1:C:3730:ALA:HA	1:C:3733:HIS:CE1	2.45	0.51
1:C:3924:TYR:O	1:C:3932:ASN:ND2	2.43	0.51
1:A:281:ARG:NH1	1:A:346:VAL:O	2.42	0.51
1:A:4817:HIS:HA	1:A:4821:GLY:H	1.74	0.51
1:D:1124:PRO:HB2	1:D:1252:SER:HB3	1.93	0.51
1:A:866:PRO:HD2	1:A:1009:ARG:HD2	1.92	0.51
1:B:1272:ARG:NH2	1:B:1590:PHE:O	2.44	0.51
1:B:2076:ILE:HG21	1:B:2081:LEU:HD22	1.91	0.51
1:C:598:ILE:HG23	1:C:636:LEU:HD12	1.93	0.51
1:A:1124:PRO:HB2	1:A:1252:SER:HB3	1.93	0.51
1:B:1124:PRO:HB2	1:B:1252:SER:HB3	1.93	0.51
1:C:1245:ARG:HE	1:C:1692:LYS:HG2	1.75	0.51
1:C:1442:TRP:HD1	1:C:1488:VAL:HG13	1.75	0.51
1:D:712:GLU:OE2	1:D:1636:ASN:ND2	2.43	0.51
1:A:677:LEU:HD23	1:A:802:PHE:HA	1.93	0.51
1:B:866:PRO:HD2	1:B:1009:ARG:HD2	1.93	0.51
1:B:4817:HIS:HA	1:B:4821:GLY:H	1.75	0.51
1:B:598:ILE:HG23	1:B:636:LEU:HD12	1.93	0.51
1:D:2226:SER:HB2	1:D:2241:LEU:HB2	1.93	0.51
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.29	0.51
1:A:3924:TYR:O	1:A:3932:ASN:ND2	2.44	0.51
1:A:394:HIS:HD2	1:A:397:GLY:H	1.59	0.51
1:D:2130:LEU:HD12	1:D:2133:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1703:TYR:HD2	1:A:1820:PRO:HB2	1.76	0.50
1:A:2076:ILE:HG21	1:A:2081:LEU:HD22	1.92	0.50
1:A:2083:ARG:HG3	1:A:3688:LEU:HD22	1.93	0.50
1:B:2163:MET:HA	1:B:2166:LEU:HD12	1.93	0.50
1:B:394:HIS:HD2	1:B:397:GLY:H	1.59	0.50
1:B:4014:ILE:HA	1:B:4017:PHE:HB3	1.91	0.50
1:B:4170:LYS:HE2	1:B:4174:ILE:HD11	1.93	0.50
1:C:1690:GLU:OE2	1:C:1790:LYS:NZ	2.39	0.50
1:C:2226:SER:HB2	1:C:2241:LEU:HB2	1.94	0.50
1:C:4891:ILE:HD13	1:C:4914:HIS:HB3	1.92	0.50
1:A:2226:SER:HB2	1:A:2241:LEU:HB2	1.93	0.50
1:B:1703:TYR:HD2	1:B:1820:PRO:HB2	1.76	0.50
1:B:3924:TYR:O	1:B:3932:ASN:ND2	2.44	0.50
1:A:598:ILE:HG23	1:A:636:LEU:HD12	1.92	0.50
1:B:1266:GLU:O	1:B:1294:ASN:ND2	2.44	0.50
1:B:2083:ARG:HG3	1:B:3688:LEU:HD22	1.93	0.50
1:C:598:ILE:HD13	1:C:636:LEU:HB2	1.94	0.50
1:D:2163:MET:HA	1:D:2166:LEU:HD12	1.93	0.50
1:B:712:GLU:OE2	1:B:1636:ASN:ND2	2.44	0.50
1:A:3779:LEU:HD11	1:A:3783:LYS:HE2	1.94	0.50
1:A:4780:TYR:O	1:A:4784:VAL:HG23	2.12	0.50
1:C:1703:TYR:HD2	1:C:1820:PRO:HB2	1.76	0.50
1:C:2163:MET:HA	1:C:2166:LEU:HD12	1.94	0.50
1:C:281:ARG:NH1	1:C:346:VAL:O	2.41	0.50
1:D:4191:VAL:HA	1:D:4194:CYS:HB2	1.93	0.50
1:D:677:LEU:HD23	1:D:802:PHE:HA	1.93	0.50
1:A:652:VAL:HG11	1:A:715:GLY:HA2	1.92	0.50
1:B:4608:ALA:HB1	1:B:4650:VAL:HG11	1.93	0.50
1:D:394:HIS:HD2	1:D:397:GLY:H	1.60	0.50
1:D:3779:LEU:HD11	1:D:3783:LYS:HE2	1.94	0.50
1:D:4891:ILE:HD13	1:D:4914:HIS:HB3	1.93	0.50
1:A:2521:LEU:HD22	1:A:2565:ALA:HB2	1.94	0.50
1:B:1690:GLU:OE2	1:B:1790:LYS:NZ	2.39	0.50
1:B:3779:LEU:HD11	1:B:3783:LYS:HE2	1.94	0.50
1:C:2723:ASN:OD1	1:C:2773:ARG:NH2	2.45	0.50
1:D:1706:LEU:HD21	1:D:1787:LEU:HD21	1.94	0.50
1:A:2163:MET:HA	1:A:2166:LEU:HD12	1.92	0.50
1:A:4824:ALA:HB3	1:A:4827:GLY:H	1.77	0.50
1:C:3742:LEU:HD23	1:C:3781:TYR:HB3	1.93	0.50
1:A:3879:LEU:HD13	1:A:3921:LEU:HD12	1.94	0.49
1:C:3779:LEU:HD11	1:C:3783:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4060:THR:OG1	1:C:4063:GLU:OE1	2.26	0.49
1:C:4780:TYR:O	1:C:4784:VAL:HG23	2.12	0.49
1:C:677:LEU:HD23	1:C:802:PHE:HA	1.93	0.49
1:D:1184:ASP:HB3	1:D:1186:SER:H	1.77	0.49
1:D:2723:ASN:OD1	1:D:2773:ARG:NH2	2.45	0.49
1:B:1160:ASP:OD1	1:B:1178:ASN:ND2	2.43	0.49
1:B:677:LEU:HD23	1:B:802:PHE:HA	1.93	0.49
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.29	0.49
1:C:3990:ASN:ND2	1:C:3991:VAL:O	2.45	0.49
1:A:4627:ILE:O	1:A:4631:TRP:N	2.46	0.49
1:A:4640:SER:OG	1:A:4703:ASP:OD2	2.29	0.49
1:A:4891:ILE:HD13	1:A:4914:HIS:HB3	1.93	0.49
1:C:1706:LEU:HD21	1:C:1787:LEU:HD21	1.95	0.49
1:D:4114:THR:HA	1:D:4117:GLN:HB2	1.95	0.49
1:D:4780:TYR:O	1:D:4784:VAL:HG23	2.11	0.49
1:D:4824:ALA:HB3	1:D:4827:GLY:H	1.77	0.49
1:D:598:ILE:HD13	1:D:636:LEU:HB2	1.94	0.49
1:A:2222:LEU:HD21	1:A:2243:VAL:HB	1.94	0.49
1:A:235:ARG:HE	1:A:274:LEU:HD21	1.77	0.49
1:B:2226:SER:HB2	1:B:2241:LEU:HB2	1.94	0.49
1:B:2723:ASN:OD1	1:B:2773:ARG:NH2	2.45	0.49
1:B:4780:TYR:O	1:B:4784:VAL:HG23	2.13	0.49
1:C:4824:ALA:HB3	1:C:4827:GLY:H	1.77	0.49
1:D:2521:LEU:HD22	1:D:2565:ALA:HB2	1.94	0.49
1:A:4114:THR:HA	1:A:4117:GLN:HB2	1.95	0.49
1:A:4189:LEU:HA	1:A:4192:ASN:HD22	1.77	0.49
1:B:4060:THR:OG1	1:B:4063:GLU:OE1	2.26	0.49
1:D:3879:LEU:HD13	1:D:3921:LEU:HD12	1.95	0.49
1:A:1706:LEU:HD21	1:A:1787:LEU:HD21	1.93	0.49
1:A:712:GLU:OE2	1:A:1636:ASN:ND2	2.44	0.49
1:C:1184:ASP:HB3	1:C:1186:SER:H	1.77	0.49
1:D:2222:LEU:HD21	1:D:2243:VAL:HB	1.94	0.49
1:A:1716:THR:HA	1:A:1719:LEU:HD12	1.95	0.49
1:B:2222:LEU:HD21	1:B:2243:VAL:HB	1.94	0.49
1:B:218:SER:HB3	1:B:286:GLY:HA3	1.94	0.49
1:B:4627:ILE:O	1:B:4631:TRP:N	2.46	0.49
1:C:1938:GLN:HE22	1:C:3614:ARG:HA	1.77	0.49
1:B:298:ARG:HA	1:B:305:TYR:HA	1.94	0.49
1:C:1244:ASN:HD22	1:C:1801:GLU:HG2	1.78	0.49
1:C:4608:ALA:HB1	1:C:4650:VAL:HG11	1.93	0.49
1:C:843:GLU:HA	1:C:848:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1692:LYS:HA	1:D:1810:VAL:HG13	1.95	0.49
1:D:4189:LEU:HA	1:D:4192:ASN:HD22	1.78	0.49
1:A:1160:ASP:OD1	1:A:1178:ASN:ND2	2.43	0.49
1:A:1654:HIS:O	1:A:1657:THR:OG1	2.27	0.49
1:A:2723:ASN:OD1	1:A:2773:ARG:NH2	2.45	0.49
1:B:4189:LEU:HA	1:B:4192:ASN:HD22	1.78	0.49
1:B:843:GLU:HA	1:B:848:ARG:HG2	1.94	0.49
1:C:2213:LYS:HA	1:C:2254:LEU:HD21	1.94	0.49
1:C:4627:ILE:O	1:C:4631:TRP:N	2.45	0.49
1:A:218:SER:HB3	1:A:286:GLY:HA3	1.95	0.49
1:A:3990:ASN:ND2	1:A:3991:VAL:O	2.46	0.49
1:B:4891:ILE:HD13	1:B:4914:HIS:HB3	1.94	0.49
1:C:2222:LEU:HD21	1:C:2243:VAL:HB	1.95	0.49
1:C:4171:ARG:NH2	1:C:4171:ARG:CG	2.73	0.49
1:D:2857:LYS:HE3	1:D:2861:LEU:HD11	1.95	0.49
1:D:3742:LEU:HD23	1:D:3781:TYR:HB3	1.95	0.49
1:A:3729:GLN:NE2	1:A:3767:LEU:O	2.47	0.48
1:A:4796:LYS:NZ	1:A:4807:CYS:SG	2.82	0.48
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.43	0.48
1:B:1184:ASP:OD2	1:B:1188:SER:OG	2.29	0.48
1:B:3990:ASN:ND2	1:B:3991:VAL:O	2.46	0.48
1:B:598:ILE:HD13	1:B:636:LEU:HB2	1.95	0.48
1:B:678:MET:HG3	1:B:754:VAL:HG22	1.94	0.48
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.43	0.48
1:C:1692:LYS:HA	1:C:1810:VAL:HG13	1.95	0.48
1:C:218:SER:HB3	1:C:286:GLY:HA3	1.95	0.48
1:A:843:GLU:HA	1:A:848:ARG:HG2	1.94	0.48
1:B:290:ARG:HH22	1:B:343:ARG:HG3	1.78	0.48
1:B:4114:THR:HA	1:B:4117:GLN:HB2	1.95	0.48
1:D:1160:ASP:OD1	1:D:1178:ASN:ND2	2.42	0.48
1:D:128:MET:HB3	1:D:149:LEU:HB3	1.95	0.48
1:A:4770:LEU:HB3	1:B:4754:LEU:CD1	2.40	0.48
1:C:4826:GLY:O	1:D:4823:ARG:NH1	2.46	0.48
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.29	0.48
1:D:1931:ASP:O	1:D:3614:ARG:NH1	2.42	0.48
1:D:3990:ASN:ND2	1:D:3991:VAL:O	2.46	0.48
1:D:4060:THR:OG1	1:D:4063:GLU:OE1	2.26	0.48
1:D:4627:ILE:O	1:D:4631:TRP:N	2.45	0.48
1:D:4796:LYS:NZ	1:D:4807:CYS:SG	2.82	0.48
1:A:1184:ASP:HB3	1:A:1186:SER:H	1.78	0.48
1:C:1160:ASP:OD1	1:C:1178:ASN:ND2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:MET:HB3	1:C:149:LEU:HB3	1.95	0.48
1:C:678:MET:HG3	1:C:754:VAL:HG22	1.96	0.48
1:D:2213:LYS:HA	1:D:2254:LEU:HD21	1.95	0.48
1:A:2857:LYS:HE3	1:A:2861:LEU:HD11	1.95	0.48
1:B:4826:GLY:O	1:C:4823:ARG:NH1	2.46	0.48
1:C:394:HIS:HD2	1:C:397:GLY:H	1.60	0.48
1:D:218:SER:HB3	1:D:286:GLY:HA3	1.96	0.48
1:D:843:GLU:HA	1:D:848:ARG:HG2	1.94	0.48
1:B:1184:ASP:HB3	1:B:1186:SER:H	1.77	0.48
1:D:235:ARG:HE	1:D:274:LEU:HD21	1.78	0.48
1:D:3690:MET:HE1	1:D:3754:PRO:HB2	1.96	0.48
1:D:4794:TYR:HB3	1:D:4807:CYS:HB2	1.95	0.48
1:A:4931:GLU:OE2	1:A:4942:TRP:NE1	2.46	0.48
1:B:4770:LEU:HB3	1:C:4754:LEU:CD1	2.39	0.48
1:C:2521:LEU:HD22	1:C:2565:ALA:HB2	1.95	0.48
1:A:2843:GLU:OE1	1:A:2887:ARG:NH2	2.47	0.48
1:B:1706:LEU:HD21	1:B:1787:LEU:HD21	1.94	0.48
1:D:1716:THR:HA	1:D:1719:LEU:HD12	1.95	0.48
1:D:3729:GLN:NE2	1:D:3767:LEU:O	2.47	0.48
1:D:4610:LYS:O	1:D:4615:GLY:N	2.46	0.48
1:A:4794:TYR:HB3	1:A:4807:CYS:HB2	1.96	0.48
1:A:678:MET:HG3	1:A:754:VAL:HG22	1.95	0.48
1:B:1654:HIS:O	1:B:1657:THR:OG1	2.28	0.48
1:B:1716:THR:HA	1:B:1719:LEU:HD12	1.96	0.48
1:B:235:ARG:HE	1:B:274:LEU:HD21	1.79	0.48
1:B:3729:GLN:NE2	1:B:3767:LEU:O	2.47	0.48
1:C:2857:LYS:HE3	1:C:2861:LEU:HD11	1.95	0.48
1:D:2528:LEU:HD11	1:D:2568:ASP:HA	1.96	0.48
1:B:1611:ILE:N	1:B:1620:GLN:O	2.43	0.48
1:B:1664:VAL:HG12	1:B:1672:VAL:HG11	1.96	0.48
1:C:235:ARG:HE	1:C:274:LEU:HD21	1.79	0.48
1:C:4114:THR:HA	1:C:4117:GLN:HB2	1.96	0.48
1:C:4610:LYS:O	1:C:4615:GLY:N	2.46	0.48
1:A:128:MET:HB3	1:A:149:LEU:HB3	1.96	0.47
1:B:1726:ILE:HB	1:B:2109:ILE:HD11	1.96	0.47
1:B:2521:LEU:HD22	1:B:2565:ALA:HB2	1.95	0.47
1:C:2843:GLU:OE1	1:C:2887:ARG:NH2	2.47	0.47
1:C:3729:GLN:NE2	1:C:3767:LEU:O	2.47	0.47
1:C:650:ASN:ND2	1:C:795:SER:O	2.47	0.47
1:D:2843:GLU:OE1	1:D:2887:ARG:NH2	2.47	0.47
1:A:298:ARG:HA	1:A:305:TYR:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3748:SER:HB2	1:A:3751:GLU:HB2	1.96	0.47
1:A:804:LEU:HD22	1:A:822:CYS:HB3	1.96	0.47
1:B:165:ALA:HB3	1:B:211:LEU:HD21	1.96	0.47
1:D:678:MET:HG3	1:D:754:VAL:HG22	1.96	0.47
1:B:2857:LYS:HE3	1:B:2861:LEU:HD11	1.95	0.47
1:B:3875:THR:HG21	1:B:3924:TYR:HE2	1.79	0.47
1:C:1716:THR:HA	1:C:1719:LEU:HD12	1.95	0.47
1:C:1931:ASP:O	1:C:3614:ARG:NH1	2.42	0.47
1:C:3952:PHE:HZ	1:C:3975:LEU:HD22	1.78	0.47
1:C:4931:GLU:OE2	1:C:4942:TRP:NE1	2.47	0.47
1:B:4046:LYS:HG3	1:B:4068:LEU:HD22	1.96	0.47
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.79	0.47
1:D:3748:SER:HB2	1:D:3751:GLU:HB2	1.96	0.47
1:D:4931:GLU:OE2	1:D:4942:TRP:NE1	2.46	0.47
1:D:718:VAL:HA	1:D:736:CYS:HB2	1.96	0.47
1:A:3742:LEU:HD23	1:A:3781:TYR:HB3	1.95	0.47
1:A:718:VAL:HA	1:A:736:CYS:HB2	1.96	0.47
1:B:128:MET:HB3	1:B:149:LEU:HB3	1.96	0.47
1:B:4733:GLY:HA3	1:B:4740:PHE:CD1	2.50	0.47
1:C:165:ALA:HB3	1:C:211:LEU:HD21	1.96	0.47
1:C:3879:LEU:HD13	1:C:3921:LEU:HD12	1.96	0.47
1:C:4189:LEU:HA	1:C:4192:ASN:HD22	1.79	0.47
1:D:298:ARG:HA	1:D:305:TYR:HA	1.95	0.47
1:B:2843:GLU:OE1	1:B:2887:ARG:NH2	2.47	0.47
1:B:718:VAL:HA	1:B:736:CYS:HB2	1.97	0.47
1:C:1654:HIS:O	1:C:1657:THR:OG1	2.28	0.47
1:C:1707:ILE:HA	1:C:1711:LEU:HB2	1.96	0.47
1:C:2528:LEU:HD11	1:C:2568:ASP:HA	1.97	0.47
1:C:25:THR:HB	1:C:32:GLN:HB3	1.97	0.47
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.43	0.47
1:A:1132:GLU:HG2	1:A:1133:ARG:HG3	1.97	0.47
1:A:1611:ILE:N	1:A:1620:GLN:O	2.43	0.47
1:A:1664:VAL:HG12	1:A:1672:VAL:HG11	1.97	0.47
1:A:260:VAL:HG12	1:A:391:ALA:HB3	1.97	0.47
1:A:598:ILE:HD13	1:A:636:LEU:HB2	1.96	0.47
1:D:25:THR:HB	1:D:32:GLN:HB3	1.97	0.47
1:D:260:VAL:HG12	1:D:391:ALA:HB3	1.97	0.47
1:A:290:ARG:HH22	1:A:343:ARG:HG3	1.79	0.47
1:C:4796:LYS:NZ	1:C:4807:CYS:SG	2.82	0.47
1:B:1244:ASN:HD22	1:B:1801:GLU:HG2	1.79	0.47
1:B:2213:LYS:HA	1:B:2254:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ARG:HA	1:C:305:TYR:HA	1.95	0.47
1:C:4046:LYS:HG3	1:C:4068:LEU:HD22	1.96	0.47
1:C:718:VAL:HA	1:C:736:CYS:HB2	1.97	0.47
1:C:804:LEU:HD22	1:C:822:CYS:HB3	1.97	0.47
1:D:165:ALA:HB3	1:D:211:LEU:HD21	1.96	0.47
1:D:3797:LEU:O	1:D:3800:SER:OG	2.32	0.47
1:B:207:PHE:CE2	1:C:2326:ILE:HG21	2.50	0.47
1:B:4931:GLU:OE2	1:B:4942:TRP:NE1	2.46	0.47
1:C:1833:ILE:HG22	1:C:1834:PHE:H	1.79	0.47
1:C:1726:ILE:HB	1:C:2109:ILE:HD11	1.97	0.47
1:D:1132:GLU:HG2	1:D:1133:ARG:HG3	1.97	0.47
1:D:1432:ILE:HD13	1:D:1441:VAL:HG21	1.97	0.47
1:D:1611:ILE:N	1:D:1620:GLN:O	2.43	0.47
1:D:3952:PHE:HZ	1:D:3975:LEU:HD22	1.80	0.47
1:D:4733:GLY:HA3	1:D:4740:PHE:CD1	2.50	0.47
1:A:1707:ILE:HA	1:A:1711:LEU:HB2	1.96	0.47
1:A:1692:LYS:HA	1:A:1810:VAL:HG13	1.98	0.47
1:A:2213:LYS:HA	1:A:2254:LEU:HD21	1.96	0.47
1:A:2390:MET:HG3	1:A:2465:HIS:CE1	2.50	0.47
1:A:4046:LYS:HG3	1:A:4068:LEU:HD22	1.96	0.47
1:B:260:VAL:HG12	1:B:391:ALA:HB3	1.96	0.47
1:B:559:ILE:HA	1:B:562:LEU:HB2	1.98	0.47
1:C:260:VAL:HG12	1:C:391:ALA:HB3	1.97	0.47
1:D:1172:THR:HG21	1:D:1190:LEU:HD13	1.97	0.47
1:D:1833:ILE:HG22	1:D:1834:PHE:H	1.79	0.47
1:D:2264:GLU:OE2	1:D:2268:ARG:NH2	2.47	0.47
1:D:4046:LYS:HG3	1:D:4068:LEU:HD22	1.96	0.47
1:D:650:ASN:ND2	1:D:795:SER:O	2.47	0.47
1:A:1833:ILE:HG22	1:A:1834:PHE:H	1.79	0.46
1:A:2528:LEU:HD11	1:A:2568:ASP:HA	1.97	0.46
1:A:4610:LYS:O	1:A:4615:GLY:N	2.46	0.46
1:B:802:PHE:HB2	1:B:1617:TRP:HB2	1.97	0.46
1:B:1707:ILE:HA	1:B:1711:LEU:HB2	1.96	0.46
1:A:207:PHE:CE2	1:B:2326:ILE:HG21	2.51	0.46
1:B:3879:LEU:HD13	1:B:3921:LEU:HD12	1.96	0.46
1:B:804:LEU:HD22	1:B:822:CYS:HB3	1.96	0.46
1:D:170:SER:OG	1:D:171:GLU:N	2.49	0.46
1:D:1244:ASN:HD22	1:D:1801:GLU:HG2	1.79	0.46
1:D:4170:LYS:HE2	1:D:4916:LEU:CD2	2.45	0.46
1:A:1219:LYS:NZ	1:A:1244:ASN:O	2.49	0.46
1:A:314:LEU:HB2	1:A:393:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4733:GLY:HA3	1:A:4740:PHE:CD1	2.50	0.46
1:B:4794:TYR:HB3	1:B:4807:CYS:HB2	1.97	0.46
1:C:2390:MET:HG3	1:C:2465:HIS:CE1	2.50	0.46
1:C:3748:SER:HB2	1:C:3751:GLU:HB2	1.97	0.46
1:B:1833:ILE:HG22	1:B:1834:PHE:H	1.79	0.46
1:B:25:THR:HB	1:B:32:GLN:HB3	1.97	0.46
1:B:2773:ARG:HA	1:B:2776:ILE:HD12	1.97	0.46
1:C:1132:GLU:HG2	1:C:1133:ARG:HG3	1.97	0.46
1:C:4018:PHE:O	1:C:4022:LEU:N	2.40	0.46
1:C:4733:GLY:HA3	1:C:4740:PHE:CD1	2.50	0.46
1:A:2773:ARG:HA	1:A:2776:ILE:HD12	1.97	0.46
1:A:25:THR:HB	1:A:32:GLN:HB3	1.97	0.46
1:B:1172:THR:HG21	1:B:1190:LEU:HD13	1.96	0.46
1:B:2390:MET:HG3	1:B:2465:HIS:CE1	2.51	0.46
1:C:1172:THR:HG21	1:C:1190:LEU:HD13	1.96	0.46
1:C:180:ASP:HB3	1:C:211:LEU:HD22	1.98	0.46
1:D:14:LEU:HD12	1:D:175:VAL:HG12	1.97	0.46
1:D:1707:ILE:HA	1:D:1711:LEU:HB2	1.96	0.46
1:D:2390:MET:HG3	1:D:2465:HIS:CE1	2.50	0.46
1:A:165:ALA:HB3	1:A:211:LEU:HD21	1.97	0.46
1:A:3904:GLN:NE2	1:A:3965:GLN:OE1	2.47	0.46
1:A:4018:PHE:O	1:A:4022:LEU:N	2.40	0.46
1:B:1692:LYS:HA	1:B:1810:VAL:HG13	1.98	0.46
1:C:170:SER:OG	1:C:171:GLU:N	2.48	0.46
1:C:20:VAL:HG12	1:C:216:PRO:HA	1.97	0.46
1:C:2264:GLU:OE2	1:C:2268:ARG:NH2	2.48	0.46
1:D:2773:ARG:HA	1:D:2776:ILE:HD12	1.98	0.46
1:D:649:VAL:HG21	1:D:713:TRP:HB3	1.98	0.46
1:A:1172:THR:HG21	1:A:1190:LEU:HD13	1.97	0.46
1:B:1165:MET:HB2	1:B:1174:MET:HB2	1.98	0.46
1:B:1219:LYS:H	1:B:1240:ALA:HB3	1.80	0.46
1:B:2264:GLU:OE2	1:B:2268:ARG:NH2	2.47	0.46
1:B:2897:LEU:HB3	1:B:2904:VAL:HG21	1.98	0.46
1:B:4052:ALA:O	1:B:4056:HIS:ND1	2.48	0.46
1:B:4640:SER:OG	1:B:4703:ASP:OD2	2.30	0.46
1:B:4796:LYS:NZ	1:B:4807:CYS:SG	2.82	0.46
1:C:290:ARG:HH22	1:C:343:ARG:HG3	1.81	0.46
1:D:686:VAL:O	1:D:687:THR:OG1	2.33	0.46
1:D:804:LEU:HD22	1:D:822:CYS:HB3	1.97	0.46
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.81	0.46
1:B:1432:ILE:HD13	1:B:1441:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1449:ASP:N	1:B:1449:ASP:OD1	2.49	0.46
1:B:1689:ILE:HA	1:B:1703:TYR:HE1	1.81	0.46
1:C:4616:LEU:HA	1:C:4620:GLU:HB2	1.98	0.46
1:C:695:VAL:HG21	1:C:755:ILE:HD13	1.98	0.46
1:D:717:GLY:O	1:D:736:CYS:N	2.45	0.46
1:D:695:VAL:HG21	1:D:755:ILE:HD13	1.98	0.46
1:A:1165:MET:HB2	1:A:1174:MET:HB2	1.97	0.46
1:A:1258:PHE:HB3	1:A:1303:ARG:NH2	2.31	0.46
1:A:4171:ARG:HH11	1:A:4752:LYS:CD	2.23	0.46
1:A:650:ASN:ND2	1:A:795:SER:O	2.48	0.46
1:B:14:LEU:HD12	1:B:175:VAL:HG12	1.98	0.46
1:B:20:VAL:HG12	1:B:216:PRO:HA	1.97	0.46
1:B:2528:LEU:HD11	1:B:2568:ASP:HA	1.97	0.46
1:B:1938:GLN:HE22	1:B:3614:ARG:HA	1.81	0.46
1:C:3904:GLN:NE2	1:C:3965:GLN:OE1	2.48	0.46
1:D:20:VAL:HG12	1:D:216:PRO:HA	1.98	0.46
1:A:2897:LEU:HB3	1:A:2904:VAL:HG21	1.98	0.46
1:B:3794:LEU:HA	1:B:3797:LEU:HD12	1.97	0.46
1:B:650:ASN:ND2	1:B:795:SER:O	2.48	0.46
1:C:1091:GLU:HA	1:C:1250:TRP:CZ3	2.51	0.46
1:D:1219:LYS:NZ	1:D:1244:ASN:O	2.49	0.46
1:D:238:HIS:HB3	1:D:243:GLU:HB3	1.98	0.46
1:D:3919:ASN:O	1:D:3922:THR:OG1	2.32	0.46
1:D:4018:PHE:O	1:D:4022:LEU:N	2.40	0.46
1:A:1219:LYS:H	1:A:1240:ALA:HB3	1.81	0.46
1:A:3952:PHE:HZ	1:A:3975:LEU:HD22	1.81	0.46
1:B:1132:GLU:HG2	1:B:1133:ARG:HG3	1.97	0.46
1:B:4018:PHE:O	1:B:4022:LEU:N	2.40	0.46
1:C:1219:LYS:H	1:C:1240:ALA:HB3	1.81	0.46
1:C:1449:ASP:OD1	1:C:1449:ASP:N	2.49	0.46
1:C:1664:VAL:HG12	1:C:1672:VAL:HG11	1.97	0.46
1:C:4794:TYR:HB3	1:C:4807:CYS:HB2	1.97	0.46
1:D:1219:LYS:H	1:D:1240:ALA:HB3	1.81	0.46
1:D:2897:LEU:HB3	1:D:2904:VAL:HG21	1.98	0.46
1:A:14:LEU:HD12	1:A:175:VAL:HG12	1.97	0.45
1:A:649:VAL:HG21	1:A:713:TRP:HB3	1.98	0.45
1:A:686:VAL:O	1:A:687:THR:OG1	2.33	0.45
1:B:1091:GLU:HA	1:B:1250:TRP:CZ3	2.51	0.45
1:B:3748:SER:HB2	1:B:3751:GLU:HB2	1.97	0.45
1:B:3952:PHE:HZ	1:B:3975:LEU:HD22	1.81	0.45
1:B:449:ILE:HG13	1:B:522:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4610:LYS:O	1:B:4615:GLY:N	2.46	0.45
1:C:3794:LEU:HA	1:C:3797:LEU:HD12	1.98	0.45
1:D:1258:PHE:HB3	1:D:1303:ARG:NH2	2.32	0.45
1:D:1938:GLN:HE22	1:D:3614:ARG:HA	1.81	0.45
1:D:954:ASP:HB3	1:D:1061:GLY:HA3	1.98	0.45
1:A:1432:ILE:HD13	1:A:1441:VAL:HG21	1.98	0.45
1:A:4616:LEU:HA	1:A:4620:GLU:HB2	1.99	0.45
1:B:1611:ILE:HB	1:B:1620:GLN:HB3	1.98	0.45
1:C:1570:LEU:HD13	1:C:1584:PRO:HG3	1.98	0.45
1:C:1611:ILE:N	1:C:1620:GLN:O	2.44	0.45
1:C:23:GLN:HA	1:C:36:CYS:HA	1.99	0.45
1:C:4130:PHE:O	1:C:4134:LEU:N	2.50	0.45
1:D:3875:THR:HG21	1:D:3924:TYR:HE2	1.81	0.45
1:A:1570:LEU:HD13	1:A:1584:PRO:HG3	1.98	0.45
1:A:4757:ILE:HG21	1:A:4757:ILE:HD13	1.71	0.45
1:B:180:ASP:HB3	1:B:211:LEU:HD22	1.98	0.45
1:B:480:ARG:NH2	1:B:3677:LEU:O	2.50	0.45
1:C:954:ASP:HB3	1:C:1061:GLY:HA3	1.99	0.45
1:C:1089:ARG:HH21	1:C:1600:PRO:HG3	1.81	0.45
1:C:1219:LYS:NZ	1:C:1244:ASN:O	2.49	0.45
1:C:1689:ILE:HA	1:C:1703:TYR:HE1	1.81	0.45
1:C:14:LEU:HD12	1:C:175:VAL:HG12	1.97	0.45
1:C:234:LEU:HD13	1:C:405:LEU:HD22	1.98	0.45
1:C:238:HIS:HB3	1:C:243:GLU:HB3	1.98	0.45
1:A:3794:LEU:HA	1:A:3797:LEU:HD12	1.98	0.45
1:A:954:ASP:HB3	1:A:1061:GLY:HA3	1.98	0.45
1:C:207:PHE:CE2	1:D:2326:ILE:HG21	2.51	0.45
1:C:2773:ARG:HA	1:C:2776:ILE:HD12	1.98	0.45
1:C:433:LEU:HD21	1:C:505:LEU:HG	1.99	0.45
1:D:2436:VAL:HG21	1:D:2469:MET:HE3	1.98	0.45
1:D:472:HIS:CE1	1:D:3674:ARG:HB2	2.52	0.45
1:A:1611:ILE:HB	1:A:1620:GLN:HB3	1.99	0.45
1:A:20:VAL:HG12	1:A:216:PRO:HA	1.97	0.45
1:A:472:HIS:CE1	1:A:3674:ARG:HB2	2.52	0.45
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.97	0.45
1:C:1432:ILE:HD13	1:C:1441:VAL:HG21	1.97	0.45
1:C:1899:LEU:O	1:C:1904:LYS:NZ	2.37	0.45
1:D:1664:VAL:HG12	1:D:1672:VAL:HG11	1.98	0.45
1:A:1244:ASN:HD22	1:A:1801:GLU:HG2	1.79	0.45
1:A:2264:GLU:OE2	1:A:2268:ARG:NH2	2.48	0.45
1:A:23:GLN:HA	1:A:36:CYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.32	0.45
1:B:1219:LYS:NZ	1:B:1244:ASN:O	2.49	0.45
1:B:1258:PHE:HB3	1:B:1303:ARG:NH2	2.32	0.45
1:B:1570:LEU:HD13	1:B:1584:PRO:HG3	1.98	0.45
1:B:170:SER:OG	1:B:171:GLU:N	2.48	0.45
1:B:1931:ASP:O	1:B:3614:ARG:NH1	2.41	0.45
1:B:472:HIS:CE1	1:B:3674:ARG:HB2	2.51	0.45
1:C:1165:MET:HB2	1:C:1174:MET:HB2	1.98	0.45
1:C:2436:VAL:HG21	1:C:2469:MET:HE3	1.97	0.45
1:C:248:PRO:HG2	1:C:257:ARG:HA	1.98	0.45
1:C:472:HIS:CE1	1:C:3674:ARG:HB2	2.51	0.45
1:C:3696:MET:O	1:C:3699:SER:OG	2.32	0.45
1:D:1091:GLU:HA	1:D:1250:TRP:CZ3	2.52	0.45
1:D:1689:ILE:HA	1:D:1703:TYR:HE1	1.81	0.45
1:D:23:GLN:HA	1:D:36:CYS:HA	1.99	0.45
1:D:3794:LEU:HA	1:D:3797:LEU:HD12	1.99	0.45
1:D:4196:ASP:O	1:D:4200:GLU:N	2.49	0.45
1:D:737:ILE:HG22	1:D:739:ARG:HG3	1.99	0.45
1:A:1938:GLN:HE22	1:A:3614:ARG:HA	1.82	0.45
1:B:23:GLN:HA	1:B:36:CYS:HA	1.98	0.45
1:B:262:TYR:N	1:B:389:ARG:O	2.49	0.45
1:C:2897:LEU:HB3	1:C:2904:VAL:HG21	1.98	0.45
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.47	0.45
1:D:1174:MET:SD	1:D:1236:TYR:OH	2.74	0.45
1:D:1469:LEU:HG	1:D:1480:ILE:HD11	1.98	0.45
1:D:1726:ILE:HB	1:D:2109:ILE:HD11	1.99	0.45
1:D:480:ARG:NH2	1:D:3677:LEU:O	2.49	0.45
1:D:3729:GLN:O	1:D:3733:HIS:ND1	2.47	0.45
1:B:248:PRO:HG2	1:B:257:ARG:HA	1.99	0.45
1:B:3919:ASN:O	1:B:3922:THR:OG1	2.32	0.45
1:C:559:ILE:HA	1:C:562:LEU:HB2	1.99	0.45
1:D:1449:ASP:OD1	1:D:1449:ASP:N	2.49	0.45
1:D:4616:LEU:HA	1:D:4620:GLU:HB2	1.99	0.45
1:D:4851:PHE:O	1:D:4855:VAL:HB	2.17	0.45
1:A:1091:GLU:HA	1:A:1250:TRP:CZ3	2.52	0.45
1:A:1689:ILE:HA	1:A:1703:TYR:HE1	1.81	0.45
1:A:1726:ILE:HB	1:A:2109:ILE:HD11	1.99	0.45
1:A:3737:ALA:O	1:A:3740:MET:HG2	2.17	0.45
1:A:4904:HIS:NE2	1:A:4907:GLU:OE1	2.50	0.45
1:B:4616:LEU:HA	1:B:4620:GLU:HB2	1.99	0.45
1:C:1699:ARG:NH1	1:C:1816:PHE:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3737:ALA:O	1:C:3740:MET:HG2	2.17	0.45
1:C:480:ARG:NH2	1:C:3677:LEU:O	2.49	0.45
1:A:1087:ILE:HG23	1:A:1128:LEU:HD12	1.98	0.45
1:A:1640:ASP:N	1:A:1640:ASP:OD1	2.49	0.45
1:A:217:ILE:HG23	1:A:285:SER:HB3	1.99	0.45
1:A:480:ARG:NH2	1:A:3677:LEU:O	2.49	0.45
1:A:4060:THR:OG1	1:A:4063:GLU:OE1	2.26	0.45
1:A:559:ILE:HA	1:A:562:LEU:HB2	1.99	0.45
1:B:3904:GLN:NE2	1:B:3965:GLN:OE1	2.48	0.45
1:B:4904:HIS:NE2	1:B:4907:GLU:OE1	2.50	0.45
1:B:532:SER:HA	1:B:535:GLU:HB2	1.99	0.45
1:C:1258:PHE:HB3	1:C:1303:ARG:NH2	2.32	0.45
1:C:1736:ILE:HG23	1:C:1753:LEU:HD12	1.99	0.45
1:C:314:LEU:HB2	1:C:393:MET:HG2	1.98	0.45
1:C:649:VAL:HG21	1:C:713:TRP:HB3	1.98	0.45
1:D:1165:MET:HB2	1:D:1174:MET:HB2	1.98	0.45
1:D:709:GLY:O	1:D:1253:LYS:NZ	2.50	0.45
1:D:1570:LEU:HD13	1:D:1584:PRO:HG3	1.98	0.45
1:D:290:ARG:HH22	1:D:343:ARG:HG3	1.81	0.45
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.98	0.45
1:A:2326:ILE:HG21	1:D:207:PHE:CE2	2.52	0.44
1:A:433:LEU:HD21	1:A:505:LEU:HG	1.98	0.44
1:A:449:ILE:HG13	1:A:522:ALA:HB1	1.98	0.44
1:B:16:THR:HB	1:B:110:HIS:HA	1.99	0.44
1:D:1699:ARG:NH1	1:D:1816:PHE:O	2.48	0.44
1:D:1926:ILE:HD11	1:D:3625:TYR:CE2	2.53	0.44
1:D:3737:ALA:O	1:D:3740:MET:HG2	2.17	0.44
1:A:248:PRO:HG2	1:A:257:ARG:HA	1.98	0.44
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.48	0.44
1:A:4832:ILE:HG21	1:A:4844:ARG:NH2	2.30	0.44
1:B:4892:CYS:SG	1:B:4909:HIS:NE2	2.80	0.44
1:C:802:PHE:HB2	1:C:1617:TRP:HB2	1.99	0.44
1:C:1613:GLU:HB2	1:C:1618:LEU:H	1.82	0.44
1:C:4196:ASP:O	1:C:4200:GLU:N	2.49	0.44
1:C:4904:HIS:NE2	1:C:4907:GLU:OE1	2.50	0.44
1:C:510:SER:O	1:C:520:ARG:NH2	2.51	0.44
1:D:234:LEU:HD13	1:D:405:LEU:HD22	1.98	0.44
1:D:248:PRO:HG2	1:D:257:ARG:HA	1.98	0.44
1:D:532:SER:HA	1:D:535:GLU:HB2	1.99	0.44
1:A:1174:MET:SD	1:A:1236:TYR:OH	2.75	0.44
1:A:238:HIS:HB3	1:A:243:GLU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4153:ILE:HD13	1:A:4158:ARG:HH11	1.82	0.44
1:A:4196:ASP:O	1:A:4200:GLU:N	2.49	0.44
1:B:954:ASP:HB3	1:B:1061:GLY:HA3	1.99	0.44
1:B:234:LEU:HD13	1:B:405:LEU:HD22	2.00	0.44
1:C:16:THR:HB	1:C:110:HIS:HA	2.00	0.44
1:C:1611:ILE:HB	1:C:1620:GLN:HB3	1.99	0.44
1:C:3919:ASN:O	1:C:3922:THR:OG1	2.32	0.44
1:C:737:ILE:HG22	1:C:739:ARG:HG3	2.00	0.44
1:D:4153:ILE:HD13	1:D:4158:ARG:HH11	1.83	0.44
1:D:4904:HIS:NE2	1:D:4907:GLU:OE1	2.50	0.44
1:D:449:ILE:HG13	1:D:522:ALA:HB1	1.99	0.44
1:A:1736:ILE:HG23	1:A:1753:LEU:HD12	1.99	0.44
1:A:1931:ASP:O	1:A:3614:ARG:NH1	2.42	0.44
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.48	0.44
1:A:262:TYR:N	1:A:389:ARG:O	2.49	0.44
1:A:555:LEU:HD13	1:A:585:ALA:HB1	1.99	0.44
1:B:1089:ARG:HH21	1:B:1600:PRO:HG3	1.83	0.44
1:B:305:TYR:HE1	1:B:319:LYS:HG2	1.83	0.44
1:B:4130:PHE:O	1:B:4134:LEU:N	2.50	0.44
1:B:4153:ILE:HD13	1:B:4158:ARG:HH11	1.82	0.44
1:B:590:LYS:HB2	1:B:593:HIS:HD2	1.82	0.44
1:C:262:TYR:N	1:C:389:ARG:O	2.49	0.44
1:C:591:GLU:HA	1:C:631:LEU:HD21	1.99	0.44
1:D:3904:GLN:NE2	1:D:3965:GLN:OE1	2.48	0.44
1:D:4130:PHE:O	1:D:4134:LEU:N	2.50	0.44
1:D:555:LEU:HD13	1:D:585:ALA:HB1	1.99	0.44
1:A:1469:LEU:HG	1:A:1480:ILE:HD11	1.98	0.44
1:A:3893:TYR:CE2	1:A:3899:ILE:HG23	2.53	0.44
1:A:4130:PHE:O	1:A:4134:LEU:N	2.50	0.44
1:A:4817:HIS:O	1:A:4822:VAL:N	2.45	0.44
1:A:695:VAL:HG21	1:A:755:ILE:HD13	1.99	0.44
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.72	0.44
1:B:314:LEU:HB2	1:B:393:MET:HG2	1.98	0.44
1:B:510:SER:O	1:B:520:ARG:NH2	2.50	0.44
1:D:217:ILE:HG23	1:D:285:SER:HB3	1.99	0.44
1:D:4804:ASP:N	1:D:4804:ASP:OD1	2.50	0.44
1:A:1219:LYS:N	1:A:1240:ALA:HB3	2.33	0.44
1:A:299:HIS:CD2	1:A:301:THR:HG1	2.34	0.44
1:A:3642:ILE:HG23	1:A:3642:ILE:HD12	1.79	0.44
1:A:510:SER:O	1:A:520:ARG:NH2	2.51	0.44
1:B:3696:MET:O	1:B:3699:SER:OG	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3936:LEU:HD21	1:B:3941:LEU:HD13	1.99	0.44
1:B:433:LEU:HD21	1:B:505:LEU:HG	1.98	0.44
1:B:4752:LYS:HG2	1:B:4755:ARG:HH21	1.83	0.44
1:B:565:LEU:HG	1:B:604:HIS:CE1	2.53	0.44
1:C:1174:MET:SD	1:C:1236:TYR:OH	2.74	0.44
1:D:30:LYS:HB2	1:D:30:LYS:HE3	1.82	0.44
1:A:16:THR:HB	1:A:110:HIS:HA	1.99	0.44
1:A:1272:ARG:HH12	1:A:1588:VAL:HA	1.83	0.44
1:A:565:LEU:HD23	1:A:1588:VAL:HG23	1.99	0.44
1:A:2436:VAL:HG21	1:A:2469:MET:HE3	1.99	0.44
1:A:3921:LEU:HD23	1:A:3921:LEU:HA	1.78	0.44
1:B:1753:LEU:HD23	1:B:1753:LEU:HA	1.84	0.44
1:B:236:LEU:HD23	1:B:245:LEU:HD22	2.00	0.44
1:B:238:HIS:HB3	1:B:243:GLU:HB3	1.99	0.44
1:B:3737:ALA:O	1:B:3740:MET:HG2	2.17	0.44
1:B:695:VAL:HG21	1:B:755:ILE:HD13	1.99	0.44
1:C:305:TYR:HE1	1:C:319:LYS:HG2	1.83	0.44
1:D:433:LEU:HD21	1:D:505:LEU:HG	1.99	0.44
1:A:4804:ASP:N	1:A:4804:ASP:OD1	2.50	0.44
1:B:1219:LYS:N	1:B:1240:ALA:HB3	2.33	0.44
1:B:4862:ILE:O	1:B:4866:LEU:N	2.50	0.44
1:C:1899:LEU:HD23	1:C:1903:VAL:HG12	2.00	0.44
1:C:4052:ALA:O	1:C:4056:HIS:ND1	2.48	0.44
1:C:4851:PHE:O	1:C:4855:VAL:HB	2.18	0.44
1:D:1219:LYS:N	1:D:1240:ALA:HB3	2.33	0.44
1:D:180:ASP:HB3	1:D:211:LEU:HD22	1.98	0.44
1:D:3893:TYR:CE2	1:D:3899:ILE:HG23	2.53	0.44
1:D:510:SER:O	1:D:520:ARG:NH2	2.51	0.44
1:A:1926:ILE:HD11	1:A:3625:TYR:CE2	2.52	0.44
1:B:1613:GLU:HB2	1:B:1618:LEU:H	1.82	0.44
1:B:2301:ASP:OD1	1:B:2304:ARG:NH2	2.51	0.44
1:B:3642:ILE:HD12	1:B:3642:ILE:HG23	1.78	0.44
1:B:464:HIS:HA	1:B:465:PRO:HD3	1.86	0.44
1:B:591:GLU:HA	1:B:631:LEU:HD21	1.99	0.44
1:B:709:GLY:O	1:B:1253:LYS:NZ	2.51	0.44
1:C:1087:ILE:HG23	1:C:1128:LEU:HD12	1.98	0.44
1:C:2770:GLU:HA	1:C:2773:ARG:HB2	2.00	0.44
1:C:4153:ILE:HD13	1:C:4158:ARG:HH11	1.82	0.44
1:C:4862:ILE:O	1:C:4866:LEU:N	2.50	0.44
1:C:709:GLY:O	1:C:1253:LYS:NZ	2.50	0.44
1:D:1087:ILE:HG23	1:D:1128:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LEU:HB2	1:D:393:MET:HG2	1.99	0.44
1:A:1089:ARG:HH21	1:A:1600:PRO:HG3	1.83	0.43
1:A:1613:GLU:HB2	1:A:1618:LEU:H	1.82	0.43
1:B:1736:ILE:HG23	1:B:1753:LEU:HD12	1.99	0.43
1:B:649:VAL:HG21	1:B:713:TRP:HB3	1.98	0.43
1:C:565:LEU:HD23	1:C:1588:VAL:HG23	2.00	0.43
1:C:565:LEU:HG	1:C:604:HIS:CE1	2.53	0.43
1:D:1611:ILE:HB	1:D:1620:GLN:HB3	1.99	0.43
1:D:2738:LEU:HD22	1:D:2819:ALA:HB3	2.00	0.43
1:A:2770:GLU:HA	1:A:2773:ARG:HB2	2.00	0.43
1:A:305:TYR:HE1	1:A:319:LYS:HG2	1.83	0.43
1:B:1170:GLU:O	1:B:1172:THR:N	2.51	0.43
1:B:565:LEU:HD23	1:B:1588:VAL:HG23	1.99	0.43
1:B:1699:ARG:HH22	1:B:1821:LEU:HD11	1.83	0.43
1:B:4187:MET:N	1:B:4187:MET:SD	2.91	0.43
1:C:1219:LYS:N	1:C:1240:ALA:HB3	2.33	0.43
1:C:2738:LEU:HD22	1:C:2819:ALA:HB3	2.00	0.43
1:C:2887:ARG:O	1:C:2891:GLN:N	2.49	0.43
1:D:1089:ARG:HH21	1:D:1600:PRO:HG3	1.82	0.43
1:D:1736:ILE:HG23	1:D:1753:LEU:HD12	1.99	0.43
1:D:305:TYR:HE1	1:D:319:LYS:HG2	1.83	0.43
1:A:3936:LEU:HD21	1:A:3941:LEU:HD13	1.99	0.43
1:A:234:LEU:HD13	1:A:405:LEU:HD22	1.99	0.43
1:B:1899:LEU:HD23	1:B:1903:VAL:HG12	2.00	0.43
1:C:1469:LEU:HG	1:C:1480:ILE:HD11	1.99	0.43
1:D:1613:GLU:HB2	1:D:1618:LEU:H	1.83	0.43
1:A:532:SER:HA	1:A:535:GLU:HB2	1.99	0.43
1:A:565:LEU:HG	1:A:604:HIS:CE1	2.53	0.43
1:B:4925:TYR:CZ	1:B:4929:LYS:HD2	2.54	0.43
1:C:4187:MET:SD	1:C:4187:MET:N	2.91	0.43
1:D:1445:TRP:H	1:D:1487:MET:HB2	1.83	0.43
1:D:2435:GLY:O	1:D:2438:SER:OG	2.29	0.43
1:D:559:ILE:HA	1:D:562:LEU:HB2	2.00	0.43
1:A:122:ARG:HE	1:A:127:GLY:HA2	1.83	0.43
1:A:1647:GLN:O	1:A:1651:LEU:N	2.52	0.43
1:A:180:ASP:HB3	1:A:211:LEU:HD22	2.00	0.43
1:A:2301:ASP:OD1	1:A:2304:ARG:NH2	2.51	0.43
1:A:4851:PHE:O	1:A:4855:VAL:HB	2.18	0.43
1:B:572:LEU:O	1:B:576:HIS:N	2.51	0.43
1:C:4804:ASP:OD1	1:C:4804:ASP:N	2.51	0.43
1:C:4892:CYS:SG	1:C:4909:HIS:NE2	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:SER:HA	1:C:535:GLU:HB2	1.99	0.43
1:D:16:THR:HB	1:D:110:HIS:HA	2.00	0.43
1:D:4665:ASP:HA	1:D:4668:SER:HB2	2.00	0.43
1:A:464:HIS:HA	1:A:465:PRO:HD3	1.87	0.43
1:A:4862:ILE:O	1:A:4866:LEU:N	2.50	0.43
1:A:4925:TYR:CZ	1:A:4929:LYS:HD2	2.53	0.43
1:B:1136:ALA:HB3	1:B:1145:TRP:HB2	2.01	0.43
1:B:1104:GLU:HA	1:B:1163:GLY:HA2	2.00	0.43
1:B:1272:ARG:HH12	1:B:1588:VAL:HA	1.83	0.43
1:C:2301:ASP:OD1	1:C:2304:ARG:NH2	2.51	0.43
1:C:217:ILE:HG23	1:C:285:SER:HB3	2.00	0.43
1:C:679:VAL:HA	1:C:800:VAL:HG12	2.00	0.43
1:C:920:GLU:HG2	1:C:976:TYR:CE1	2.54	0.43
1:D:565:LEU:HD23	1:D:1588:VAL:HG23	2.00	0.43
1:D:1899:LEU:HD23	1:D:1903:VAL:HG12	2.00	0.43
1:D:4862:ILE:O	1:D:4866:LEU:N	2.50	0.43
1:D:679:VAL:HA	1:D:800:VAL:HG12	2.00	0.43
1:A:170:SER:OG	1:A:171:GLU:N	2.49	0.43
1:A:1699:ARG:HH22	1:A:1821:LEU:HD11	1.82	0.43
1:A:4892:CYS:SG	1:A:4909:HIS:NE2	2.80	0.43
1:B:119:ILE:HD13	1:B:162:ILE:HD11	2.01	0.43
1:C:1640:ASP:N	1:C:1640:ASP:OD1	2.49	0.43
1:C:1764:SER:N	1:C:1779:SER:O	2.51	0.43
1:C:1926:ILE:HD11	1:C:3625:TYR:CE2	2.54	0.43
1:C:590:LYS:HB2	1:C:593:HIS:HD2	1.83	0.43
1:D:1699:ARG:HH22	1:D:1821:LEU:HD11	1.83	0.43
1:A:3891:TRP:CB	1:D:76:ARG:HD2	2.37	0.43
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.99	0.43
1:A:1753:LEU:HD23	1:A:1753:LEU:HA	1.85	0.43
1:A:4508:LEU:HD11	1:A:4747:ILE:HD12	2.00	0.43
1:A:590:LYS:HB2	1:A:593:HIS:HD2	1.83	0.43
1:A:717:GLY:O	1:A:736:CYS:N	2.45	0.43
1:B:2436:VAL:HG21	1:B:2469:MET:HE3	2.00	0.43
1:B:2770:GLU:HA	1:B:2773:ARG:HB2	2.00	0.43
1:B:217:ILE:HG23	1:B:285:SER:HB3	2.00	0.43
1:B:3729:GLN:O	1:B:3733:HIS:ND1	2.48	0.43
1:B:4851:PHE:O	1:B:4855:VAL:HB	2.18	0.43
1:B:737:ILE:HG22	1:B:739:ARG:HG3	2.00	0.43
1:C:1104:GLU:HA	1:C:1163:GLY:HA2	2.00	0.43
1:C:4072:GLU:HB3	1:C:4074:ASP:HB2	2.01	0.43
1:C:4591:TYR:HE1	1:C:4595:LYS:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:GLU:OE2	1:C:477:ASN:ND2	2.50	0.43
1:C:449:ILE:HG13	1:C:522:ALA:HB1	1.99	0.43
1:D:4187:MET:N	1:D:4187:MET:SD	2.91	0.43
1:D:565:LEU:HG	1:D:604:HIS:CE1	2.53	0.43
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.43	0.43
1:B:1172:THR:HG22	1:B:1193:LYS:HG3	2.01	0.43
1:B:4804:ASP:N	1:B:4804:ASP:OD1	2.51	0.43
1:C:119:ILE:HD13	1:C:162:ILE:HD11	2.01	0.43
1:C:1647:GLN:O	1:C:1651:LEU:N	2.52	0.43
1:D:2301:ASP:OD1	1:D:2304:ARG:NH2	2.51	0.43
1:D:920:GLU:HG2	1:D:976:TYR:CE1	2.54	0.43
1:A:591:GLU:HA	1:A:631:LEU:HD21	2.00	0.43
1:B:1087:ILE:HG23	1:B:1128:LEU:HD12	1.99	0.43
1:B:1174:MET:SD	1:B:1236:TYR:OH	2.74	0.43
1:B:1727:VAL:HG11	1:B:1927:VAL:HG21	2.00	0.43
1:C:1170:GLU:O	1:C:1172:THR:N	2.52	0.43
1:C:1172:THR:HG22	1:C:1193:LYS:HG3	2.01	0.43
1:C:3893:TYR:CE2	1:C:3899:ILE:HG23	2.54	0.43
1:C:719:GLY:H	1:C:722:LEU:HD12	1.84	0.43
1:D:1272:ARG:HH12	1:D:1588:VAL:HA	1.83	0.43
1:D:3936:LEU:HD21	1:D:3941:LEU:HD13	2.00	0.43
1:D:4508:LEU:HD11	1:D:4747:ILE:HD12	2.01	0.43
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.49	0.42
1:A:4011:VAL:HG12	1:A:4015:LEU:HG	2.01	0.42
1:A:832:LEU:HG	1:A:1617:TRP:HE1	1.83	0.42
1:B:3893:TYR:CE2	1:B:3899:ILE:HG23	2.54	0.42
1:C:3988:GLU:HB2	1:C:4937:GLN:NE2	2.34	0.42
1:A:2738:LEU:HD22	1:A:2819:ALA:HB3	2.00	0.42
1:A:4187:MET:SD	1:A:4187:MET:N	2.92	0.42
1:B:1469:LEU:HG	1:B:1480:ILE:HD11	2.01	0.42
1:B:247:VAL:O	1:B:272:ARG:NH1	2.46	0.42
1:B:717:GLY:O	1:B:736:CYS:N	2.45	0.42
1:C:1272:ARG:HH12	1:C:1588:VAL:HA	1.83	0.42
1:C:1445:TRP:H	1:C:1487:MET:HB2	1.83	0.42
1:C:4665:ASP:HA	1:C:4668:SER:HB2	2.00	0.42
1:D:676:GLU:HB2	1:D:803:LEU:HB2	2.01	0.42
1:A:1136:ALA:HB3	1:A:1145:TRP:HB2	2.01	0.42
1:A:1300:MET:O	1:A:1545:ALA:N	2.44	0.42
1:A:119:ILE:HD13	1:A:162:ILE:HD11	2.02	0.42
1:B:122:ARG:HE	1:B:127:GLY:HA2	1.84	0.42
1:B:1094:TYR:OH	1:B:1808:ASP:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2738:LEU:HD22	1:B:2819:ALA:HB3	2.01	0.42
1:B:3642:ILE:HG22	1:B:3731:ARG:HD3	2.01	0.42
1:B:4508:LEU:HD11	1:B:4747:ILE:HD12	2.01	0.42
1:B:555:LEU:HD13	1:B:585:ALA:HB1	2.02	0.42
1:B:719:GLY:H	1:B:722:LEU:HD12	1.84	0.42
1:B:920:GLU:HG2	1:B:976:TYR:CE1	2.54	0.42
1:C:1457:PHE:HD1	1:C:1488:VAL:HG21	1.84	0.42
1:C:1699:ARG:HH22	1:C:1821:LEU:HD11	1.83	0.42
1:D:3907:PHE:HD2	1:D:3968:LEU:HD11	1.85	0.42
1:D:832:LEU:HG	1:D:1617:TRP:HE1	1.84	0.42
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.73	0.42
1:A:1727:VAL:HG11	1:A:1927:VAL:HG21	2.01	0.42
1:A:3955:MET:O	1:A:3959:LEU:N	2.48	0.42
1:B:308:LEU:N	1:B:326:SER:O	2.49	0.42
1:B:1926:ILE:HD11	1:B:3625:TYR:CE2	2.54	0.42
1:C:3642:ILE:HG22	1:C:3731:ARG:HD3	2.02	0.42
1:D:119:ILE:HD13	1:D:162:ILE:HD11	2.01	0.42
1:D:1647:GLN:O	1:D:1651:LEU:N	2.52	0.42
1:A:709:GLY:O	1:A:1253:LYS:NZ	2.51	0.42
1:B:3718:LYS:O	1:B:3722:LYS:N	2.50	0.42
1:B:679:VAL:HA	1:B:800:VAL:HG12	2.01	0.42
1:C:1136:ALA:HB3	1:C:1145:TRP:HB2	2.01	0.42
1:D:122:ARG:HE	1:D:127:GLY:HA2	1.84	0.42
1:D:4580:HIS:HB3	1:D:4740:PHE:HZ	1.84	0.42
1:D:4861:ALA:HA	1:D:4864:GLN:HB3	2.02	0.42
1:D:4925:TYR:CZ	1:D:4929:LYS:HD2	2.54	0.42
1:A:1445:TRP:H	1:A:1487:MET:HB2	1.84	0.42
1:A:1899:LEU:HD23	1:A:1903:VAL:HG12	2.01	0.42
1:A:236:LEU:HD23	1:A:245:LEU:HD22	2.01	0.42
1:A:530:LEU:HD23	1:A:533:LEU:HD12	2.02	0.42
1:A:679:VAL:HA	1:A:800:VAL:HG12	2.01	0.42
1:B:196:TYR:O	1:B:201:LEU:N	2.52	0.42
1:B:2884:ALA:HA	1:B:2887:ARG:HB3	2.02	0.42
1:B:4665:ASP:HA	1:B:4668:SER:HB2	2.00	0.42
1:C:1753:LEU:HD23	1:C:1753:LEU:HA	1.84	0.42
1:C:555:LEU:HD13	1:C:585:ALA:HB1	2.00	0.42
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.99	0.42
1:D:1764:SER:N	1:D:1779:SER:O	2.52	0.42
1:D:262:TYR:N	1:D:389:ARG:O	2.49	0.42
1:A:4864:GLN:HG3	1:D:4857:VAL:HG13	2.01	0.42
1:A:30:LYS:HE3	1:A:30:LYS:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:HG22	1:A:739:ARG:HG3	2.01	0.42
1:B:1699:ARG:NH1	1:B:1816:PHE:O	2.48	0.42
1:B:2587:GLN:O	1:B:2591:ARG:N	2.53	0.42
1:B:4207:ILE:O	1:B:4498:ARG:NH1	2.53	0.42
1:B:4580:HIS:HB3	1:B:4740:PHE:HZ	1.85	0.42
1:C:236:LEU:HD23	1:C:245:LEU:HD22	2.01	0.42
1:C:3921:LEU:HD23	1:C:3921:LEU:HA	1.79	0.42
1:C:4580:HIS:HB3	1:C:4740:PHE:HZ	1.85	0.42
1:D:1505:LEU:HB2	1:D:1523:ASN:HA	2.02	0.42
1:D:196:TYR:O	1:D:201:LEU:N	2.53	0.42
1:C:143:LEU:CD2	1:D:2426:SER:HB3	2.48	0.42
1:D:238:HIS:N	1:D:243:GLU:O	2.53	0.42
1:D:4591:TYR:HE1	1:D:4595:LYS:HD2	1.85	0.42
1:D:591:GLU:HA	1:D:631:LEU:HD21	2.00	0.42
1:A:4580:HIS:HB3	1:A:4740:PHE:HZ	1.84	0.42
1:A:4665:ASP:HA	1:A:4668:SER:HB2	2.01	0.42
1:B:4591:TYR:HE1	1:B:4595:LYS:HD2	1.84	0.42
1:C:4207:ILE:O	1:C:4498:ARG:NH1	2.53	0.42
1:D:1137:PHE:HD1	1:D:1144:ARG:HB3	1.85	0.42
1:A:1172:THR:HG22	1:A:1193:LYS:HG3	2.01	0.42
1:A:1094:TYR:OH	1:A:1808:ASP:OD1	2.38	0.42
1:A:191:TYR:N	1:A:206:ALA:O	2.48	0.42
1:A:2587:GLN:O	1:A:2591:ARG:N	2.53	0.42
1:A:4591:TYR:CE1	1:A:4595:LYS:HB2	2.55	0.42
1:A:4161:TRP:CZ2	1:A:4917:ALA:HB2	2.55	0.42
1:B:2143:MET:SD	1:B:2175:VAL:HG11	2.60	0.42
1:B:2796:GLY:HA2	1:B:2900:ASN:HA	2.02	0.42
1:B:4072:GLU:HB3	1:B:4074:ASP:HB2	2.02	0.42
1:B:76:ARG:HD2	1:C:3891:TRP:CB	2.38	0.42
1:B:832:LEU:HG	1:B:1617:TRP:HE1	1.84	0.42
1:C:2143:MET:SD	1:C:2175:VAL:HG11	2.60	0.42
1:C:717:GLY:O	1:C:736:CYS:N	2.45	0.42
1:D:2770:GLU:HA	1:D:2773:ARG:HB2	2.00	0.42
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.48	0.42
1:D:4072:GLU:HB3	1:D:4074:ASP:HB2	2.02	0.42
1:D:4640:SER:HB3	1:D:4643:ASN:HD21	1.85	0.42
1:D:727:PHE:N	1:D:749:LEU:HD13	2.35	0.42
1:A:626:ARG:HG2	1:A:1669:ASN:HD21	1.84	0.42
1:A:1799:VAL:HG22	1:A:1894:LEU:HD13	2.02	0.42
1:A:920:GLU:HG2	1:A:976:TYR:CE1	2.54	0.42
1:B:1799:VAL:HG22	1:B:1894:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:HIS:CE1	1:B:400:ASP:HB3	2.52	0.42
1:B:4196:ASP:O	1:B:4200:GLU:N	2.49	0.42
1:B:4591:TYR:CE1	1:B:4595:LYS:HB2	2.55	0.42
1:C:196:TYR:O	1:C:201:LEU:N	2.52	0.42
1:C:3936:LEU:HD21	1:C:3941:LEU:HD13	2.00	0.42
1:D:465:PRO:HA	1:D:466:PRO:HD3	1.87	0.42
1:D:590:LYS:HB2	1:D:593:HIS:HD2	1.83	0.42
1:A:1090:ALA:HA	1:A:1249:MET:HG2	2.01	0.41
1:B:1764:SER:N	1:B:1779:SER:O	2.52	0.41
1:B:30:LYS:HB2	1:B:30:LYS:HE3	1.82	0.41
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.72	0.41
1:C:3955:MET:O	1:C:3959:LEU:N	2.48	0.41
1:C:644:LEU:HB2	1:C:1654:HIS:CD2	2.48	0.41
1:C:852:GLY:HA2	1:C:853:PRO:HA	1.82	0.41
1:D:3718:LYS:O	1:D:3722:LYS:N	2.50	0.41
1:D:3988:GLU:HB2	1:D:4937:GLN:NE2	2.35	0.41
1:A:1137:PHE:HD1	1:A:1144:ARG:HB3	1.85	0.41
1:A:1764:SER:N	1:A:1779:SER:O	2.52	0.41
1:A:1752:GLY:HA3	1:A:1836:ASN:ND2	2.35	0.41
1:A:238:HIS:CE1	1:A:400:ASP:HB3	2.51	0.41
1:A:4640:SER:HB3	1:A:4643:ASN:HD21	1.85	0.41
1:A:3988:GLU:HB2	1:A:4937:GLN:NE2	2.35	0.41
1:C:1090:ALA:HB3	1:C:1203:PRO:HD2	2.03	0.41
1:C:191:TYR:N	1:C:206:ALA:O	2.48	0.41
1:C:2435:GLY:O	1:C:2438:SER:OG	2.29	0.41
1:C:3907:PHE:HD2	1:C:3968:LEU:HD11	1.84	0.41
1:D:4161:TRP:CZ2	1:D:4917:ALA:HB2	2.55	0.41
1:D:488:LEU:HA	1:D:488:LEU:HD23	1.93	0.41
1:A:1505:LEU:HB2	1:A:1523:ASN:HA	2.03	0.41
1:A:238:HIS:N	1:A:243:GLU:O	2.53	0.41
1:A:4591:TYR:HE1	1:A:4595:LYS:HD2	1.85	0.41
1:A:719:GLY:H	1:A:722:LEU:HD12	1.84	0.41
1:A:727:PHE:N	1:A:749:LEU:HD13	2.36	0.41
1:B:1445:TRP:H	1:B:1487:MET:HB2	1.85	0.41
1:B:2435:GLY:O	1:B:2438:SER:OG	2.29	0.41
1:C:4861:ALA:HA	1:C:4864:GLN:HB3	2.02	0.41
1:C:572:LEU:O	1:C:576:HIS:N	2.52	0.41
1:D:1136:ALA:HB3	1:D:1145:TRP:HB2	2.01	0.41
1:D:191:TYR:N	1:D:206:ALA:O	2.48	0.41
1:A:2123:SER:OG	1:A:2149:ASP:OD2	2.39	0.41
1:A:2435:GLY:O	1:A:2438:SER:OG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3907:PHE:HD2	1:A:3968:LEU:HD11	1.86	0.41
1:A:4011:VAL:HA	1:A:4014:ILE:HG12	2.03	0.41
1:A:4207:ILE:O	1:A:4498:ARG:NH1	2.53	0.41
1:A:773:GLN:HA	1:A:774:PRO:HD3	1.93	0.41
1:B:4011:VAL:HG12	1:B:4015:LEU:HG	2.02	0.41
1:B:855:VAL:HG22	1:B:1209:VAL:HG12	2.02	0.41
1:C:122:ARG:HE	1:C:127:GLY:HA2	1.84	0.41
1:C:1752:GLY:HA3	1:C:1836:ASN:ND2	2.36	0.41
1:C:4170:LYS:HE3	1:C:4916:LEU:CD2	2.49	0.41
1:C:4757:ILE:HG21	1:C:4757:ILE:HD13	1.69	0.41
1:D:1727:VAL:HG11	1:D:1927:VAL:HG21	2.01	0.41
1:D:236:LEU:HD23	1:D:245:LEU:HD22	2.01	0.41
1:D:4583:ILE:HD13	1:D:4583:ILE:HG21	1.81	0.41
1:D:719:GLY:H	1:D:722:LEU:HD12	1.84	0.41
1:A:196:TYR:O	1:A:201:LEU:N	2.53	0.41
1:A:4500:PHE:O	1:A:4504:ARG:N	2.52	0.41
1:B:1647:GLN:O	1:B:1651:LEU:N	2.52	0.41
1:B:1752:GLY:HA3	1:B:1836:ASN:ND2	2.35	0.41
1:B:717:GLY:H	1:B:722:LEU:HD13	1.85	0.41
1:B:727:PHE:N	1:B:749:LEU:HD13	2.36	0.41
1:C:727:PHE:N	1:C:749:LEU:HD13	2.36	0.41
1:D:626:ARG:HG2	1:D:1669:ASN:HD21	1.85	0.41
1:D:4011:VAL:HG12	1:D:4015:LEU:HG	2.01	0.41
1:D:473:GLU:OE2	1:D:477:ASN:ND2	2.50	0.41
1:D:847:THR:HG22	1:D:848:ARG:H	1.86	0.41
1:A:247:VAL:O	1:A:272:ARG:NH1	2.46	0.41
1:A:4609:ARG:HD3	1:A:4609:ARG:HH11	1.71	0.41
1:B:3907:PHE:HD2	1:B:3968:LEU:HD11	1.86	0.41
1:B:4499:ASN:ND2	1:B:4502:ASN:HB3	2.36	0.41
1:C:1137:PHE:HD1	1:C:1144:ARG:HB3	1.85	0.41
1:C:2587:GLN:O	1:C:2591:ARG:N	2.53	0.41
1:C:4020:MET:HB3	1:C:4067:LEU:HD11	2.02	0.41
1:C:832:LEU:HG	1:C:1617:TRP:HE1	1.85	0.41
1:A:2426:SER:HB3	1:D:143:LEU:CD2	2.47	0.41
1:A:3891:TRP:CG	1:D:76:ARG:CG	3.03	0.41
1:A:74:SER:HA	1:A:117:HIS:HA	2.03	0.41
1:B:626:ARG:HG2	1:B:1669:ASN:HD21	1.85	0.41
1:B:4020:MET:HB3	1:B:4067:LEU:HD11	2.01	0.41
1:B:852:GLY:HA2	1:B:853:PRO:HA	1.82	0.41
1:C:1228:THR:HA	1:C:1232:LEU:HD12	2.03	0.41
1:C:1090:ALA:HA	1:C:1249:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1094:TYR:OH	1:C:1808:ASP:OD1	2.38	0.41
1:C:745:ASN:ND2	1:C:773:GLN:OE1	2.54	0.41
1:C:676:GLU:HB2	1:C:803:LEU:HB2	2.01	0.41
1:C:847:THR:HG22	1:C:848:ARG:H	1.86	0.41
1:D:3642:ILE:HG22	1:D:3731:ARG:HD3	2.03	0.41
1:D:589:ILE:HG21	1:D:617:LEU:HD22	2.02	0.41
1:A:308:LEU:N	1:A:326:SER:O	2.50	0.41
1:A:465:PRO:HA	1:A:466:PRO:HD3	1.89	0.41
1:B:1137:PHE:HD1	1:B:1144:ARG:HB3	1.85	0.41
1:B:1090:ALA:HA	1:B:1249:MET:HG2	2.02	0.41
1:B:312:LYS:HD2	1:B:315:LEU:HD11	2.02	0.41
1:B:4161:TRP:CZ2	1:B:4917:ALA:HB2	2.56	0.41
1:B:706:TYR:HA	1:B:707:PRO:HD3	1.91	0.41
1:C:1727:VAL:HG11	1:C:1927:VAL:HG21	2.02	0.41
1:C:2273:CYS:HB3	1:C:2293:PRO:HD2	2.02	0.41
1:C:2884:ALA:HA	1:C:2887:ARG:HB3	2.02	0.41
1:C:4925:TYR:CZ	1:C:4929:LYS:HD2	2.55	0.41
1:C:589:ILE:HG21	1:C:617:LEU:HD22	2.02	0.41
1:D:1090:ALA:HB3	1:D:1203:PRO:HD2	2.03	0.41
1:D:1090:ALA:HA	1:D:1249:MET:HG2	2.02	0.41
1:D:2587:GLN:O	1:D:2591:ARG:N	2.53	0.41
1:D:4500:PHE:O	1:D:4504:ARG:N	2.52	0.41
1:D:4892:CYS:SG	1:D:4909:HIS:NE2	2.79	0.41
1:D:530:LEU:HD23	1:D:533:LEU:HD12	2.02	0.41
1:A:1170:GLU:O	1:A:1172:THR:N	2.52	0.41
1:A:363:ILE:HD12	1:A:403:LEU:HD12	2.03	0.41
1:A:4072:GLU:HB3	1:A:4074:ASP:HB2	2.03	0.41
1:A:745:ASN:ND2	1:A:773:GLN:OE1	2.54	0.41
1:B:137:ARG:HE	1:B:202:HIS:HB3	1.86	0.41
1:C:1799:VAL:HG22	1:C:1894:LEU:HD13	2.02	0.41
1:B:76:ARG:CG	1:C:3891:TRP:CG	3.04	0.41
1:C:4011:VAL:HG12	1:C:4015:LEU:HG	2.02	0.41
1:D:855:VAL:HG22	1:D:1209:VAL:HG12	2.03	0.41
1:D:312:LYS:HD2	1:D:315:LEU:HD11	2.02	0.41
1:D:3841:PHE:HB3	1:D:3920:THR:HG21	2.02	0.41
1:A:1137:PHE:CE2	1:A:1139:GLY:HA2	2.56	0.41
1:A:1184:ASP:HB2	1:A:1188:SER:H	1.86	0.41
1:A:3642:ILE:HG22	1:A:3731:ARG:HD3	2.03	0.41
1:B:238:HIS:N	1:B:243:GLU:O	2.53	0.41
1:B:2857:LYS:HE2	1:B:2869:HIS:CD2	2.56	0.41
1:B:363:ILE:HD12	1:B:403:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:CG	1:B:3891:TRP:CG	3.04	0.41
1:B:530:LEU:HD23	1:B:533:LEU:HD12	2.02	0.41
1:B:676:GLU:HB2	1:B:803:LEU:HB2	2.02	0.41
1:C:1505:LEU:HB2	1:C:1523:ASN:HA	2.03	0.41
1:C:363:ILE:HD12	1:C:403:LEU:HD12	2.03	0.41
1:C:4508:LEU:HD11	1:C:4747:ILE:HD12	2.03	0.41
1:C:4832:ILE:HG21	1:C:4844:ARG:NH2	2.30	0.41
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.73	0.41
1:D:1654:HIS:O	1:D:1657:THR:OG1	2.28	0.41
1:D:228:LEU:HD23	1:D:356:TYR:CE1	2.56	0.41
1:D:4020:MET:HB3	1:D:4067:LEU:HD11	2.03	0.41
1:D:646:THR:OG1	1:D:1684:GLN:NE2	2.51	0.41
1:D:745:ASN:ND2	1:D:773:GLN:OE1	2.54	0.41
1:A:1699:ARG:NH1	1:A:1816:PHE:O	2.48	0.41
1:A:4499:ASN:ND2	1:A:4502:ASN:HB3	2.36	0.41
1:A:717:GLY:H	1:A:722:LEU:HD13	1.85	0.41
1:B:1113:MET:HG3	1:B:1156:TRP:HZ2	1.86	0.41
1:B:1457:PHE:CD1	1:B:1488:VAL:HG21	2.56	0.41
1:B:3988:GLU:HB2	1:B:4937:GLN:NE2	2.35	0.41
1:B:4170:LYS:HE2	1:B:4916:LEU:CD2	2.51	0.41
1:B:4493:LEU:HA	1:B:4496:PHE:HD2	1.86	0.41
1:B:4861:ALA:HA	1:B:4864:GLN:HB3	2.03	0.41
1:B:745:ASN:ND2	1:B:773:GLN:OE1	2.54	0.41
1:C:1457:PHE:CD1	1:C:1488:VAL:HG21	2.55	0.41
1:C:2796:GLY:HA2	1:C:2900:ASN:HA	2.03	0.41
1:D:1172:THR:HG22	1:D:1193:LYS:HG3	2.02	0.41
1:D:1457:PHE:CD1	1:D:1488:VAL:HG21	2.56	0.41
1:D:2143:MET:SD	1:D:2175:VAL:HG11	2.61	0.41
1:D:23:GLN:HE21	1:D:34:LYS:HB3	1.86	0.41
1:C:76:ARG:CG	1:D:3891:TRP:CG	3.04	0.41
1:D:4011:VAL:HA	1:D:4014:ILE:HG12	2.03	0.41
1:D:4171:ARG:HH11	1:D:4752:LYS:CE	2.17	0.41
1:D:4591:TYR:CE1	1:D:4595:LYS:HB2	2.56	0.41
1:A:312:LYS:HD2	1:A:315:LEU:HD11	2.02	0.40
1:A:3760:LEU:HD13	1:A:3840:LEU:HA	2.02	0.40
1:A:4020:MET:HB3	1:A:4067:LEU:HD11	2.03	0.40
1:A:4036:TYR:HE2	1:A:4048:ASP:HB3	1.87	0.40
1:A:589:ILE:HG21	1:A:617:LEU:HD22	2.03	0.40
1:B:2424:LEU:HD23	1:B:2476:VAL:HG22	2.02	0.40
1:B:3768:ASN:H	1:B:3846:LEU:HD23	1.86	0.40
1:B:4640:SER:HB3	1:B:4643:ASN:HD21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:GLN:HA	1:B:774:PRO:HD3	1.94	0.40
1:D:1170:GLU:O	1:D:1172:THR:N	2.52	0.40
1:D:1300:MET:O	1:D:1545:ALA:N	2.45	0.40
1:D:1094:TYR:OH	1:D:1808:ASP:OD1	2.38	0.40
1:D:2520:TYR:HA	1:D:2523:THR:HB	2.03	0.40
1:A:228:LEU:HD23	1:A:356:TYR:CE1	2.56	0.40
1:A:426:PHE:O	1:A:430:ILE:N	2.54	0.40
1:A:847:THR:HG22	1:A:848:ARG:H	1.86	0.40
1:B:1505:LEU:HB2	1:B:1523:ASN:HA	2.03	0.40
1:B:4797:SER:HB3	1:B:4805:MET:H	1.85	0.40
1:C:1455:THR:HB	1:C:1546:GLN:NE2	2.36	0.40
1:C:3920:THR:O	1:C:3924:TYR:N	2.52	0.40
1:C:4640:SER:HB3	1:C:4643:ASN:HD21	1.85	0.40
1:C:4797:SER:HB3	1:C:4805:MET:H	1.86	0.40
1:D:1752:GLY:HA3	1:D:1836:ASN:ND2	2.36	0.40
1:D:3983:LEU:HD23	1:D:3983:LEU:H	1.86	0.40
1:D:4207:ILE:O	1:D:4498:ARG:NH1	2.54	0.40
1:A:2884:ALA:HA	1:A:2887:ARG:HB3	2.03	0.40
1:B:1090:ALA:HB3	1:B:1203:PRO:HD2	2.03	0.40
1:B:1220:ASP:O	1:B:1223:THR:N	2.36	0.40
1:C:2520:TYR:HA	1:C:2523:THR:HB	2.03	0.40
1:C:2857:LYS:HE2	1:C:2869:HIS:CD2	2.57	0.40
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	2.03	0.40
1:C:3983:LEU:H	1:C:3983:LEU:HD23	1.86	0.40
1:C:4499:ASN:ND2	1:C:4502:ASN:HB3	2.36	0.40
1:D:832:LEU:HB3	1:D:1614:ARG:NH1	2.37	0.40
1:D:1799:VAL:HG22	1:D:1894:LEU:HD13	2.03	0.40
1:D:644:LEU:HD12	1:D:1654:HIS:HB2	2.04	0.40
1:A:1228:THR:HA	1:A:1232:LEU:HD12	2.03	0.40
1:A:1761:MET:SD	1:A:1761:MET:N	2.92	0.40
1:A:299:HIS:N	1:A:304:LYS:O	2.50	0.40
1:A:4493:LEU:HA	1:A:4496:PHE:HD2	1.86	0.40
1:B:228:LEU:HD23	1:B:356:TYR:CE1	2.57	0.40
1:B:3797:LEU:O	1:B:3800:SER:OG	2.32	0.40
1:B:74:SER:HA	1:B:117:HIS:HA	2.03	0.40
1:C:30:LYS:HE3	1:C:30:LYS:HB2	1.82	0.40
1:C:686:VAL:O	1:C:687:THR:OG1	2.34	0.40
1:D:1457:PHE:HD1	1:D:1488:VAL:HG21	1.86	0.40
1:D:1506:GLU:HA	1:D:1522:ALA:HA	2.03	0.40
1:D:2857:LYS:HE2	1:D:2869:HIS:CD2	2.57	0.40
1:D:3955:MET:O	1:D:3959:LEU:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4182:GLY:O	1:D:4186:LYS:N	2.55	0.40
1:D:572:LEU:O	1:D:576:HIS:N	2.51	0.40
1:D:844:ARG:HD2	1:D:849:ASP:OD2	2.22	0.40
1:A:3690:MET:HB3	1:A:3690:MET:HE3	1.90	0.40
1:A:3980:VAL:HA	1:A:3983:LEU:HD23	2.04	0.40
1:A:489:PHE:HD2	1:A:540:LEU:HD21	1.87	0.40
1:B:1184:ASP:HB2	1:B:1188:SER:H	1.86	0.40
1:B:4054:GLU:HG3	1:B:4061:GLN:HG2	2.03	0.40
1:B:4182:GLY:O	1:B:4186:LYS:N	2.54	0.40
1:B:589:ILE:HG21	1:B:617:LEU:HD22	2.03	0.40
1:C:1138:ASP:HB2	1:C:1145:TRP:HE1	1.87	0.40
1:C:312:LYS:HD2	1:C:315:LEU:HD11	2.03	0.40
1:C:356:TYR:CE1	1:C:407:ARG:HB3	2.57	0.40
1:C:4591:TYR:CE1	1:C:4595:LYS:HB2	2.56	0.40
1:C:488:LEU:HA	1:C:488:LEU:HD23	1.94	0.40
1:D:1113:MET:HG3	1:D:1156:TRP:HZ2	1.86	0.40
1:D:1306:MET:HB3	1:D:1575:HIS:CE1	2.57	0.40
1:D:299:HIS:NE2	1:D:301:THR:OG1	2.47	0.40
1:D:363:ILE:HD12	1:D:403:LEU:HD12	2.04	0.40
1:D:426:PHE:O	1:D:430:ILE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3289/4968 (66%)	2988 (91%)	279 (8%)	22 (1%)	26	71
1	B	3289/4968 (66%)	2994 (91%)	273 (8%)	22 (1%)	26	71
1	C	3289/4968 (66%)	2988 (91%)	280 (8%)	21 (1%)	30	74
1	D	3289/4968 (66%)	2986 (91%)	282 (9%)	21 (1%)	30	74
All	All	13156/19872 (66%)	11956 (91%)	1114 (8%)	86 (1%)	31	71

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1737	THR
1	A	1756	SER
1	A	4071	ALA
1	B	1737	THR
1	B	1756	SER
1	B	4071	ALA
1	C	1737	THR
1	C	1756	SER
1	C	4071	ALA
1	D	1737	THR
1	D	1756	SER
1	D	4071	ALA
1	A	1580	PRO
1	A	3805	ASP
1	A	4916	LEU
1	B	1580	PRO
1	B	3805	ASP
1	B	4916	LEU
1	C	1580	PRO
1	C	3805	ASP
1	C	4916	LEU
1	D	1580	PRO
1	D	3805	ASP
1	D	4916	LEU
1	A	819	TYR
1	A	4164	PRO
1	B	819	TYR
1	B	4164	PRO
1	C	819	TYR
1	C	4164	PRO
1	D	819	TYR
1	D	4164	PRO
1	A	1738	LEU
1	A	3804	LEU
1	A	4030	SER
1	B	1738	LEU
1	B	2075	VAL
1	B	3804	LEU
1	B	4030	SER
1	C	1738	LEU
1	C	2075	VAL
1	C	3804	LEU

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Mol	Chain	Res	Type
1	C	4030	SER
1	D	1738	LEU
1	D	3804	LEU
1	D	4030	SER
1	A	792	VAL
1	A	839	GLU
1	A	1581	GLN
1	B	792	VAL
1	B	839	GLU
1	B	1581	GLN
1	C	792	VAL
1	C	839	GLU
1	D	792	VAL
1	D	839	GLU
1	D	2075	VAL
1	A	980	PRO
1	A	2075	VAL
1	A	4642	PRO
1	A	4958	CYS
1	B	980	PRO
1	B	4642	PRO
1	B	4958	CYS
1	C	980	PRO
1	C	1581	GLN
1	C	3769	GLY
1	C	4642	PRO
1	D	980	PRO
1	D	1581	GLN
1	D	4642	PRO
1	A	729	GLY
1	A	3769	GLY
1	B	729	GLY
1	B	3769	GLY
1	C	729	GLY
1	D	729	GLY
1	D	3769	GLY
1	A	1476	VAL
1	B	828	PRO
1	B	1476	VAL
1	C	1476	VAL
1	D	1476	VAL
1	A	828	PRO

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Mol	Chain	Res	Type
1	C	828	PRO
1	D	828	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2660/4355 (61%)	2616 (98%)	44 (2%)	68	88
1	B	2657/4355 (61%)	2617 (98%)	40 (2%)	72	89
1	C	2658/4355 (61%)	2615 (98%)	43 (2%)	70	88
1	D	2660/4355 (61%)	2616 (98%)	44 (2%)	68	88
All	All	10635/17420 (61%)	10464 (98%)	171 (2%)	72	88

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	84	ASN
1	A	192	LEU
1	A	298	ARG
1	A	439	LYS
1	A	475	LYS
1	A	531	ASN
1	A	606	ARG
1	A	628	ASN
1	A	658	ASN
1	A	678	MET
1	A	687	THR
1	A	841	LYS
1	A	854	THR
1	A	925	PRO
1	A	950	VAL
1	A	990	PRO
1	A	1089	ARG
1	A	1619	VAL

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Mol	Chain	Res	Type
1	A	1637	ARG
1	A	1739	PHE
1	A	1760	ARG
1	A	2080	GLU
1	A	2126	GLN
1	A	2206	ARG
1	A	2211	ASN
1	A	2293	PRO
1	A	2419	ARG
1	A	3670	LEU
1	A	3813	ASN
1	A	3906	ASN
1	A	3990	ASN
1	A	4032	THR
1	A	4122	LEU
1	A	4179	ASN
1	A	4184	LYS
1	A	4187	MET
1	A	4499	ASN
1	A	4515	ASN
1	A	4609	ARG
1	A	4727	MET
1	A	4752	LYS
1	A	4781	LEU
1	A	4844	ARG
1	B	44	ASN
1	B	84	ASN
1	B	298	ARG
1	B	439	LYS
1	B	475	LYS
1	B	531	ASN
1	B	606	ARG
1	B	628	ASN
1	B	658	ASN
1	B	678	MET
1	B	687	THR
1	B	841	LYS
1	B	854	THR
1	B	925	PRO
1	B	990	PRO
1	B	1089	ARG
1	B	1619	VAL

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Mol	Chain	Res	Type
1	B	1637	ARG
1	B	1739	PHE
1	B	1760	ARG
1	B	2126	GLN
1	B	2206	ARG
1	B	2211	ASN
1	B	2293	PRO
1	B	2419	ARG
1	B	3670	LEU
1	B	3813	ASN
1	B	3906	ASN
1	B	3990	ASN
1	B	4032	THR
1	B	4122	LEU
1	B	4179	ASN
1	B	4184	LYS
1	B	4187	MET
1	B	4499	ASN
1	B	4515	ASN
1	B	4609	ARG
1	B	4727	MET
1	B	4781	LEU
1	B	4844	ARG
1	C	44	ASN
1	C	84	ASN
1	C	192	LEU
1	C	298	ARG
1	C	439	LYS
1	C	531	ASN
1	C	606	ARG
1	C	628	ASN
1	C	658	ASN
1	C	678	MET
1	C	687	THR
1	C	841	LYS
1	C	854	THR
1	C	925	PRO
1	C	990	PRO
1	C	1089	ARG
1	C	1619	VAL
1	C	1637	ARG
1	C	1739	PHE

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Mol	Chain	Res	Type
1	C	1760	ARG
1	C	2126	GLN
1	C	2206	ARG
1	C	2211	ASN
1	C	2293	PRO
1	C	2419	ARG
1	C	3670	LEU
1	C	3813	ASN
1	C	3906	ASN
1	C	3990	ASN
1	C	4032	THR
1	C	4122	LEU
1	C	4168	GLU
1	C	4171	ARG
1	C	4179	ASN
1	C	4184	LYS
1	C	4187	MET
1	C	4499	ASN
1	C	4515	ASN
1	C	4609	ARG
1	C	4727	MET
1	C	4781	LEU
1	C	4844	ARG
1	C	4910	THR
1	D	44	ASN
1	D	84	ASN
1	D	192	LEU
1	D	298	ARG
1	D	439	LYS
1	D	475	LYS
1	D	531	ASN
1	D	606	ARG
1	D	628	ASN
1	D	658	ASN
1	D	678	MET
1	D	687	THR
1	D	841	LYS
1	D	854	THR
1	D	925	PRO
1	D	950	VAL
1	D	990	PRO
1	D	1089	ARG

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Mol	Chain	Res	Type
1	D	1619	VAL
1	D	1637	ARG
1	D	1739	PHE
1	D	1760	ARG
1	D	2080	GLU
1	D	2126	GLN
1	D	2206	ARG
1	D	2211	ASN
1	D	2293	PRO
1	D	2419	ARG
1	D	3670	LEU
1	D	3813	ASN
1	D	3906	ASN
1	D	3990	ASN
1	D	4032	THR
1	D	4122	LEU
1	D	4171	ARG
1	D	4179	ASN
1	D	4184	LYS
1	D	4187	MET
1	D	4499	ASN
1	D	4515	ASN
1	D	4609	ARG
1	D	4727	MET
1	D	4781	LEU
1	D	4844	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	44	ASN
1	A	84	ASN
1	A	123	HIS
1	A	238	HIS
1	A	293	GLN
1	A	364	GLN
1	A	394	HIS
1	A	486	GLN
1	A	490	GLN
1	A	531	ASN
1	A	544	ASN

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Mol	Chain	Res	Type
1	A	593	HIS
1	A	604	HIS
1	A	628	ASN
1	A	681	HIS
1	A	1244	ASN
1	A	1294	ASN
1	A	1602	GLN
1	A	1620	GLN
1	A	1654	HIS
1	A	1691	ASN
1	A	1938	GLN
1	A	2090	HIS
1	A	2211	ASN
1	A	2212	GLN
1	A	3666	HIS
1	A	3862	GLN
1	A	3906	ASN
1	A	3954	HIS
1	A	3990	ASN
1	A	4160	GLN
1	A	4179	ASN
1	A	4192	ASN
1	A	4499	ASN
1	A	4559	HIS
1	A	4630	GLN
1	A	4737	ASN
1	A	4767	GLN
1	A	4817	HIS
1	A	4880	GLN
1	A	4914	HIS
1	B	23	GLN
1	B	44	ASN
1	B	84	ASN
1	B	123	HIS
1	B	238	HIS
1	B	293	GLN
1	B	364	GLN
1	B	394	HIS
1	B	486	GLN
1	B	490	GLN
1	B	531	ASN
1	B	544	ASN

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Mol	Chain	Res	Type
1	B	593	HIS
1	B	604	HIS
1	B	628	ASN
1	B	681	HIS
1	B	1244	ASN
1	B	1294	ASN
1	B	1602	GLN
1	B	1620	GLN
1	B	1654	HIS
1	B	1691	ASN
1	B	1938	GLN
1	B	2090	HIS
1	B	2211	ASN
1	B	2212	GLN
1	B	3666	HIS
1	B	3862	GLN
1	B	3906	ASN
1	B	3954	HIS
1	B	3990	ASN
1	B	4179	ASN
1	B	4192	ASN
1	B	4499	ASN
1	B	4559	HIS
1	B	4630	GLN
1	B	4737	ASN
1	B	4767	GLN
1	B	4817	HIS
1	B	4880	GLN
1	B	4914	HIS
1	C	23	GLN
1	C	44	ASN
1	C	84	ASN
1	C	123	HIS
1	C	238	HIS
1	C	293	GLN
1	C	364	GLN
1	C	394	HIS
1	C	486	GLN
1	C	490	GLN
1	C	531	ASN
1	C	544	ASN
1	C	593	HIS

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Mol	Chain	Res	Type
1	C	604	HIS
1	C	628	ASN
1	C	681	HIS
1	C	1244	ASN
1	C	1294	ASN
1	C	1602	GLN
1	C	1620	GLN
1	C	1654	HIS
1	C	1691	ASN
1	C	1938	GLN
1	C	2090	HIS
1	C	2152	ASN
1	C	2211	ASN
1	C	2212	GLN
1	C	3666	HIS
1	C	3862	GLN
1	C	3906	ASN
1	C	3919	ASN
1	C	3954	HIS
1	C	3990	ASN
1	C	4179	ASN
1	C	4192	ASN
1	C	4499	ASN
1	C	4559	HIS
1	C	4630	GLN
1	C	4737	ASN
1	C	4767	GLN
1	C	4817	HIS
1	C	4880	GLN
1	C	4914	HIS
1	D	23	GLN
1	D	44	ASN
1	D	84	ASN
1	D	123	HIS
1	D	238	HIS
1	D	293	GLN
1	D	364	GLN
1	D	394	HIS
1	D	490	GLN
1	D	531	ASN
1	D	544	ASN
1	D	593	HIS

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Mol	Chain	Res	Type
1	D	604	HIS
1	D	628	ASN
1	D	681	HIS
1	D	1244	ASN
1	D	1294	ASN
1	D	1602	GLN
1	D	1620	GLN
1	D	1654	HIS
1	D	1691	ASN
1	D	1938	GLN
1	D	2090	HIS
1	D	2211	ASN
1	D	2212	GLN
1	D	2831	ASN
1	D	3666	HIS
1	D	3862	GLN
1	D	3906	ASN
1	D	3919	ASN
1	D	3954	HIS
1	D	3990	ASN
1	D	4179	ASN
1	D	4192	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4559	HIS
1	D	4630	GLN
1	D	4737	ASN
1	D	4767	GLN
1	D	4817	HIS
1	D	4880	GLN
1	D	4914	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.