



Full wwPDB EM Validation Report ⓘ

Jan 27, 2025 – 07:39 PM EST

PDB ID : 9CGP
EMDB ID : EMD-45584
Title : RyR1 disease mutant Y523S with FKBP12.6, nanodisc and inhibitor dantrolene in the absence of calcium with refined P1 domain
Authors : Iyer, K.A.; Samso, M.
Deposited on : 2024-06-30
Resolution : 3.34 Å(reported)
Based on initial model : 7T64

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

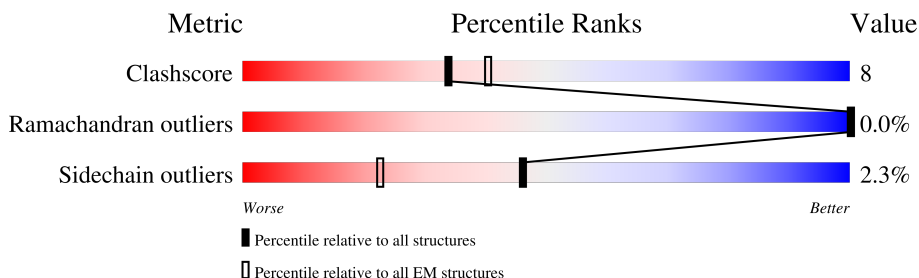
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.34 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	
2	E	107	
2	F	107	
2	G	107	
2	H	107	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 132860 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4258	Total	C	N	O	S	0	0
			32374	20609	5541	6025	199		
1	B	4258	Total	C	N	O	S	0	0
			32374	20609	5541	6025	199		
1	C	4258	Total	C	N	O	S	0	0
			32374	20609	5541	6025	199		
1	D	4258	Total	C	N	O	S	0	0
			32374	20609	5541	6025	199		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	TYR	engineered mutation	UNP P11716
B	523	SER	TYR	engineered mutation	UNP P11716
C	523	SER	TYR	engineered mutation	UNP P11716
D	523	SER	TYR	engineered mutation	UNP P11716

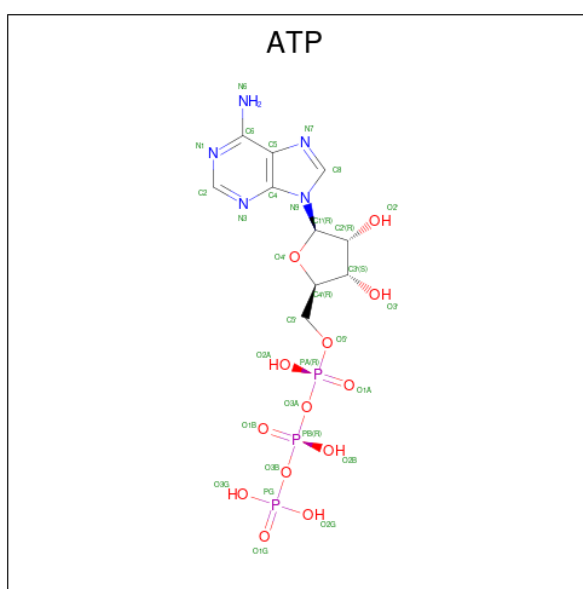
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			786	498	137	148	3		
2	F	107	Total	C	N	O	S	0	0
			786	498	137	148	3		
2	G	107	Total	C	N	O	S	0	0
			786	498	137	148	3		
2	H	107	Total	C	N	O	S	0	0
			786	498	137	148	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

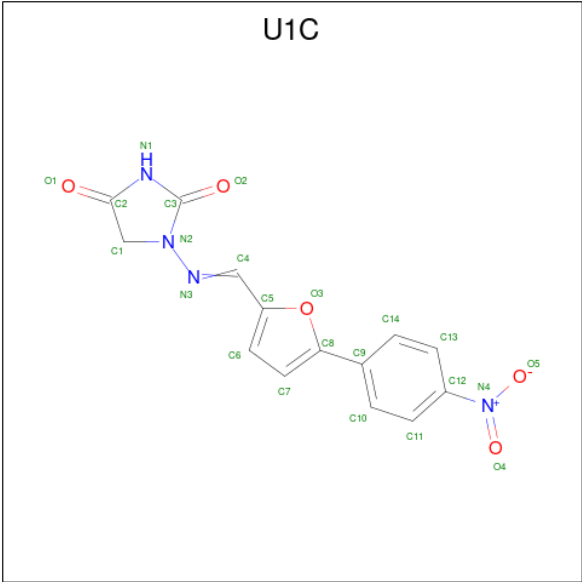
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is Dantrolene (three-letter code: U1C) (formula: $C_{14}H_{10}N_4O_5$) (labeled as "Ligand of Interest" by depositor).

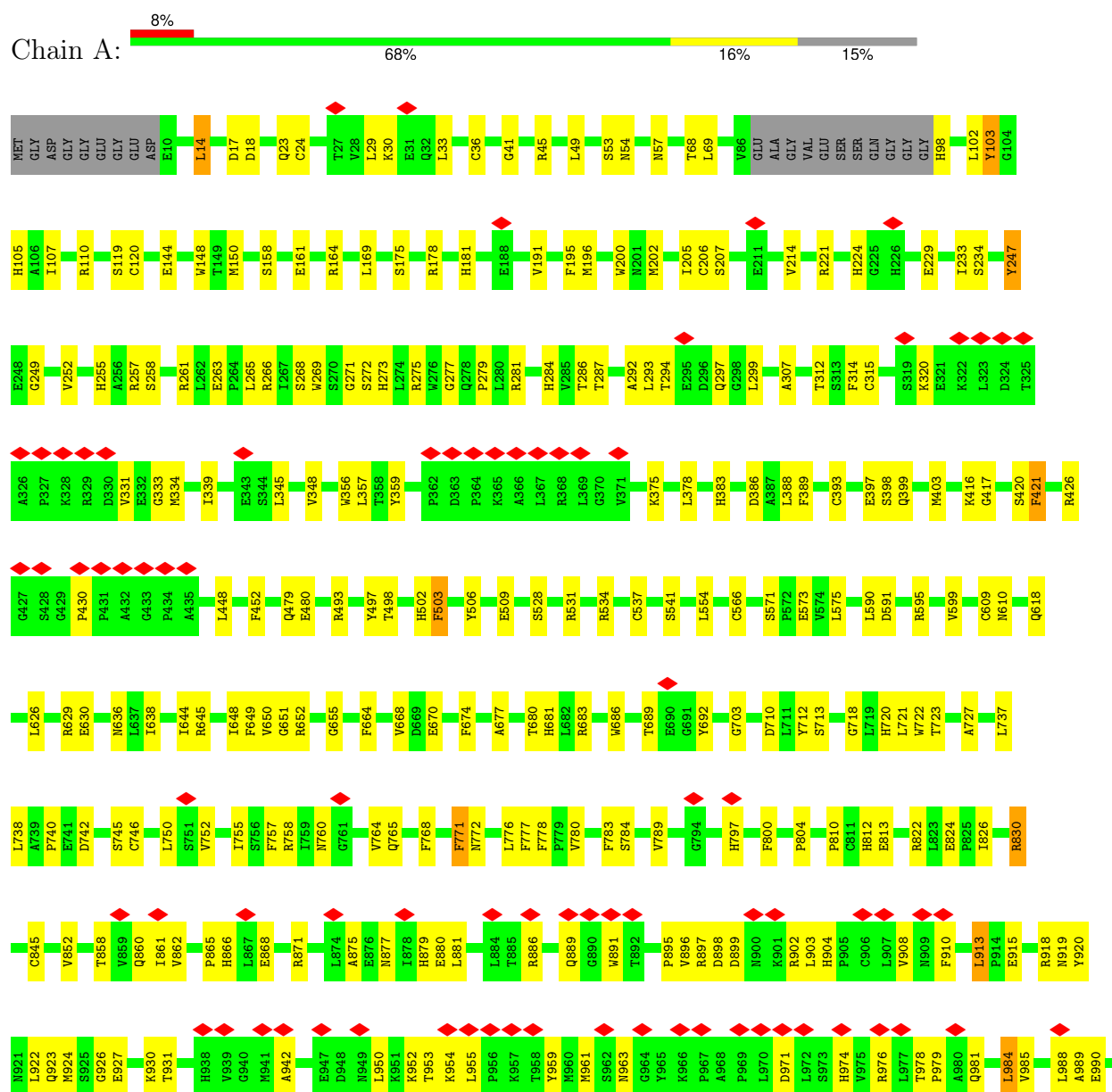


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			23	14	4	5	
5	B	1	Total	C	N	O	0
			23	14	4	5	
5	C	1	Total	C	N	O	0
			23	14	4	5	
5	D	1	Total	C	N	O	0
			23	14	4	5	

3 Residue-property plots

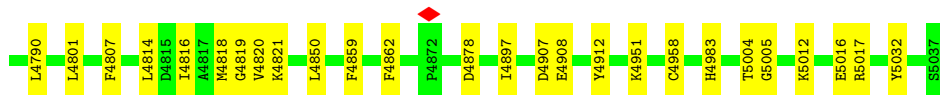
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Ryanodine receptor 1

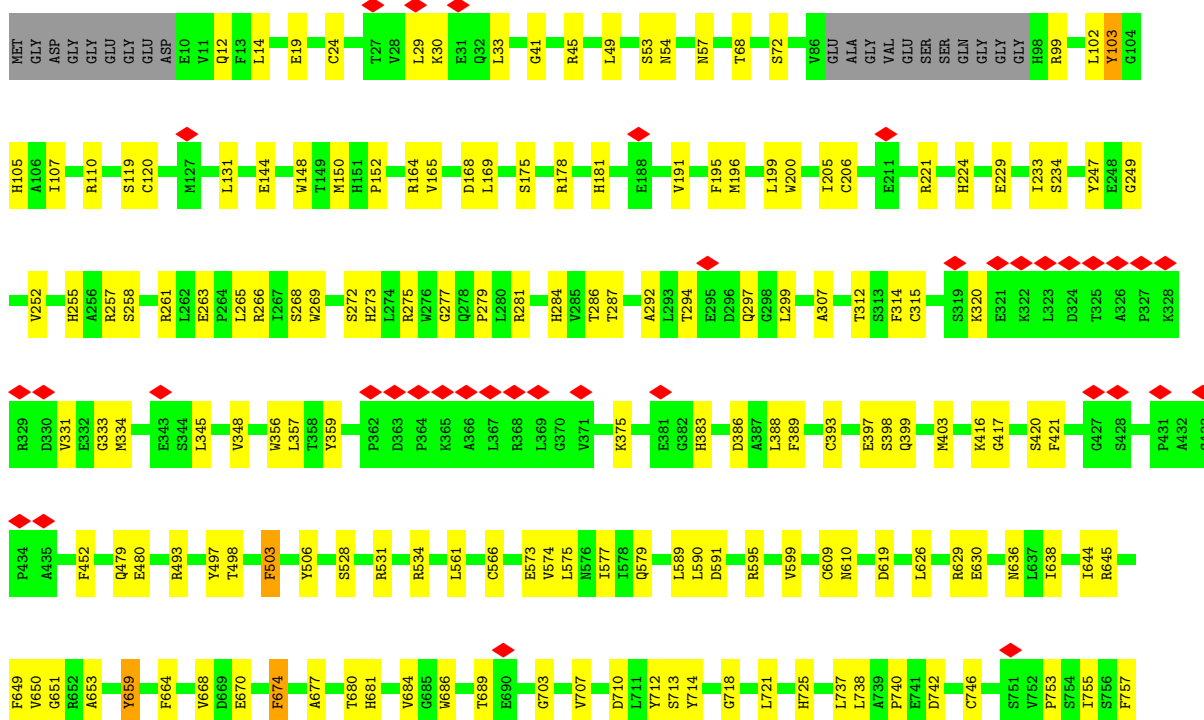


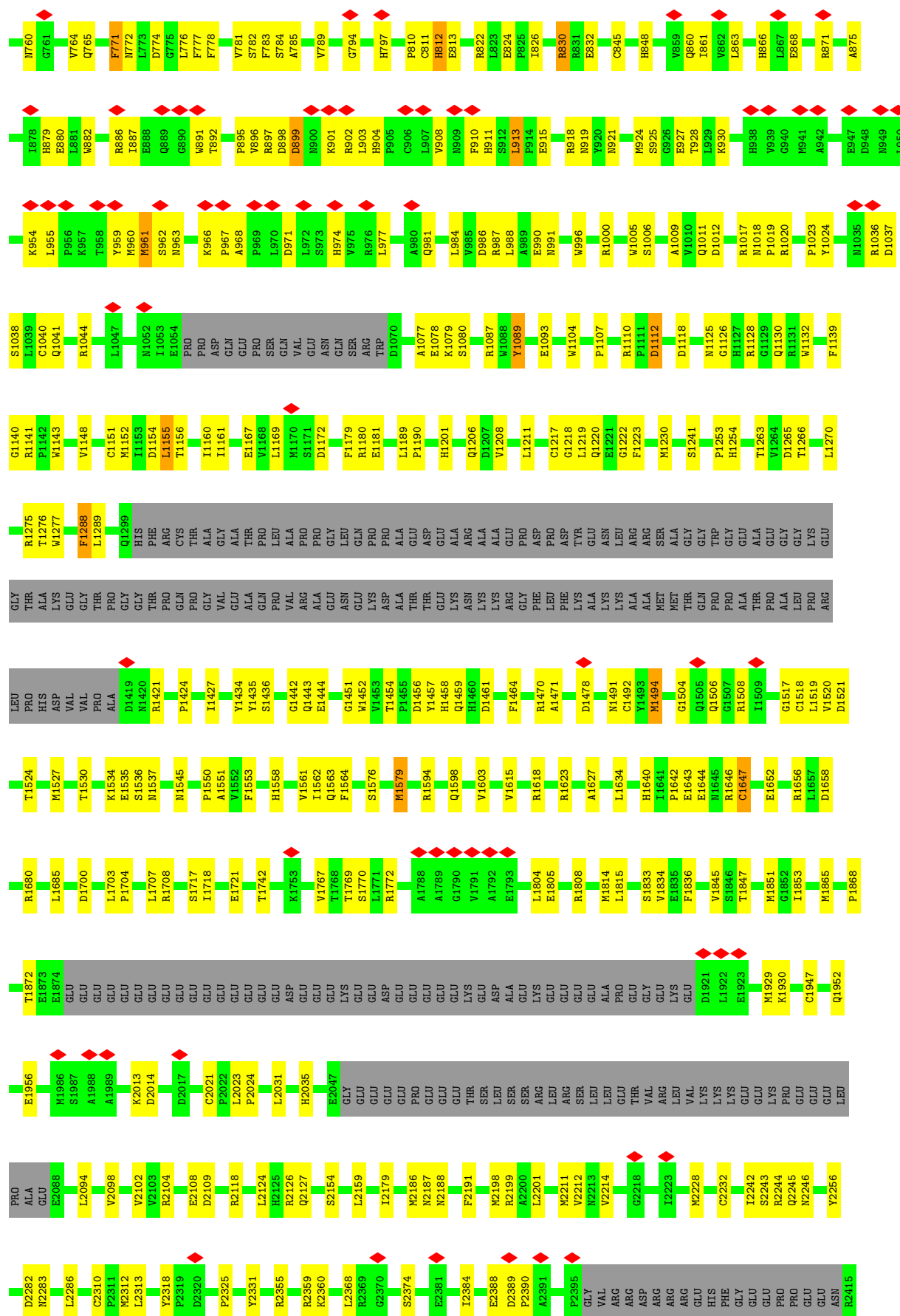
H993	E1093	E1921	TYR	LYS	N1482	V1615	M1814	GLU	SER	R2199	T2384	I2476	H2584
R1000	E1093	G1222	GLY	ALA	S1486	R1618	L1815	GLU	LEU	A2200	E2388	P2477	T2585
W1005	W1104	F1223	ASN	LYS	S1833	R1623	S1833	ALA	GLY	L2201	D2389	T2478	T2585
S1006	P1107	M1230	LEU	LYS	N1491	R1623	E1835	PRO	THR	M2211	D2390	L2478	R2591
A1009	R1110	S1241	ARG	ALA	M1494	A1627	F1836	GLY	VAL	V2212	A2391	L2478	S2594
V1010	P1111	P1253	ALA	THR	G1504	L1634	V1845	LYS	LEU	G2218	P2395	A2487	K2597
Q1011	D1112	H1254	GLY	GLN	Q1505	H1640	T1847	LVS	GLY	I2223	VAL	LEU	C2606
D1012	D1012	T1263	TRP	PRO	R1508	P1642	L1848	LVS	LVS	M2228	ARG	VAL	L2607
I1013	D1118	T1266	GLY	PRO	I1509	E1643	V1850	GLU	GLU	L2233	ARG	Q2487	I2614
V1022	N1125	T1266	ALA	THR	G1517	E1643	M1851	LYS	GLU	M2238	ASP	S2491	R2615
P1023	G1126	L1270	GLU	PRO	C1518	E1644	M1865	PRO	PRO	L2236	ARG	A2492	P2618
Y1024	W1132	L1270	GLY	LEU	L1519	E1646	P1868	ARG	GLU	L2266	ARG	F2494	S2617
L1027	F1139	R1275	LVS	PRO	D1521	C1647	T1872	GLU	GLU	I2242	GLU	D2497	N2618
D1028	G1140	T1276	GLY	ARG	T1524	E1652	E1873	LEU	LEU	S2243	HIS	A2500	L2622
K1032	W1143	W1277	THR	LEU	M1527	R1656	E1874	ALA	ALA	R2244	PHE	L2506	L2626
N1035	V1148	V1284	LVS	HIS	M1527	D1658	E1874	ALA	ALA	Q2245	GLY	L2507	L2627
R1036	C1151	F1288	GLY	VAL	T1530	M1678	E1874	GLU	GLU	N2246	GLU	E2088	F2628
L1039	M1152	L1289	THR	PRO	T1530	N1678	E1874	GLU	GLU	M2250	PRO	L2094	L2633
R1044	I1153	Q1299	GLY	ALA	E1535	D1700	E1874	GLU	GLU	Y2256	GLU	L2098	R2650
L1047	D1154	PHE	THR	THR	S1536	L1703	E1874	GLU	GLU	L2257	GLU	V2098	C2651
G1048	T1156	ARG	PRO	PRO	N1537	P1704	E1874	GLU	GLU	L2258	ASN	V2102	T2652
N1052	T1160	CYS	GLN	GLN	N1545	L1707	E1874	GLU	GLU	V2275	GLU	V2103	R2653
E1054	I1161	THR	GLY	VAL	L1548	R1708	E1874	GLU	GLU	D2282	GLU	R2104	Y2654
PRO	L1169	ALA	ALA	ALA	F1549	A1717	E1874	GLU	GLU	N2283	GLU	E2108	L2657
ASP	M1170	THR	GLN	GLN	P1550	S1717	E1874	GLU	GLU	L2286	PRO	R2118	T2659
GLN	S1171	ALA	GLY	ALA	A1551	E1721	E1874	GLU	GLU	C2310	GLU	L2124	N2663
PRO	D1172	LEU	VAL	VAL	V1554	T1742	E1874	GLU	GLU	M2312	GLU	H2125	M2530
GLU	F1179	PRO	ALA	ALA	L1555	K1753	E1874	GLU	GLU	L2313	GLU	Q2127	R2531
PRO	R1180	GLY	GLY	GLY	H1558	V1767	E1874	GLU	GLU	Y2318	GLU	Y2128	A2437
SER	E1181	LEU	ASN	ASN	V1561	T1768	E1874	GLU	GLU	P2319	GLU	V2149	K2440
GLN	L1189	ASP	GLN	GLN	I1562	T1769	E1874	GLU	GLU	D2320	GLU	E2150	H2441
VAL	P1190	THR	GLY	ALA	Q1563	R1772	E1874	GLU	GLU	P2325	GLU	M2153	L2442
GLN	H1201	THR	THR	THR	F1564	R1772	E1874	GLU	GLU	Y2331	GLU	S2154	Q2444
ARG	Q1206	GLY	THR	THR	T1572	A1788	E1874	GLU	GLU	R2355	GLU	L2159	R2452
TRP	D1207	ASP	THR	THR	S1576	A1789	E1874	GLU	GLU	R2359	GLU	M2170	R2454
A1077	V1208	ARG	GLY	GLY	M1579	V1791	E1874	GLU	GLU	L2368	GLU	L2179	R2458
E1078	S1209	ALA	ASN	ASN	P1583	A1792	E1874	GLU	GLU	R2369	GLU	N2188	D2464
K1079	L1211	ALA	LVS	LVS	R1593	E1793	E1874	GLU	GLU	G2370	GLU	F2191	L2472
S1080	C1217	ALA	ARG	ARG	R1598	E1805	E1874	GLU	GLU	S2374	GLU	M2198	L2474
R1087	L1219	PRO	PHE	PHE	Q1598	R1808	E1874	GLU	GLU	E2381	GLU	Q2475	Q2475
V1088	Q1220	ASP	LEU	LEU	V1603	R1808	E1874	GLU	GLU		GLU		
Y1089			PHE	PHE				ARG	ARG				





- Molecule 1: Ryanodine receptor 1









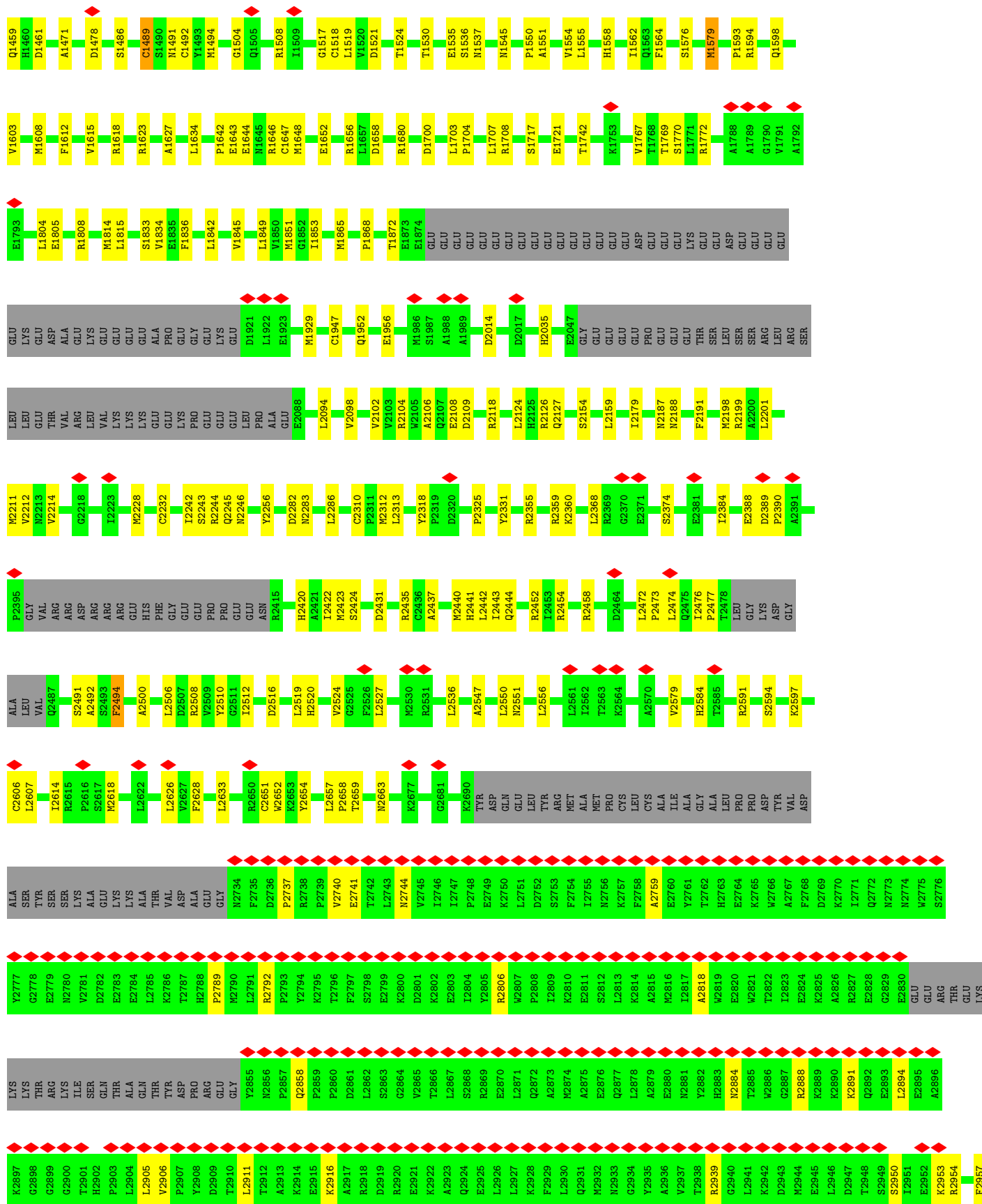
Metabolites									
V252	H105	MET	H106	GLY	E10	H107	V11	ASP	E11
H255	A106	GLY	A107	GLY	Q12	R110	F13	ASP	F14
A256	R110	GLU	R111	GLU	F15	S119	L14	ASP	D18
S258	S119	GLU	C120	GLU	Q23	C120	C24	ASP	Q23
R261	C120	GLU	M127	GLU	C24	T27	E31	ASP	C24
L262	M127	GLU	E144	GLU	T27	K30	Q32	ASP	L33
E263	E144	GLU	W148	GLU	K30	E31	L33	ASP	C36
P264	W148	GLU	T149	GLU	E31	Q32	L33	ASP	Q41
L265	T149	GLU	H151	GLU	Q32	L33	B45	ASP	L49
S268	H151	GLU	P152	GLU	L33	B45	L49	ASP	S53
W269	P152	GLU	R164	GLU	B45	L49	S53	ASP	N54
S272	R164	GLU	V165	GLU	L49	S53	N54	ASP	N57
H273	V165	GLU	D168	GLU	S53	N54	N57	ASP	T68
L274	D168	GLU	L169	GLU	N54	N57	T68	ASP	L69
R275	L169	GLU	S175	GLU	N57	T68	L69	ASP	V86
W276	S175	GLU	R178	GLU	T68	L69	V86	ASP	GLU
Q277	R178	GLU	H181	GLU	V86	GLU	ALA	ASP	ALA
K278	H181	GLU	E188	GLU	GLU	ALA	GLY	ASP	GLY
P279	E188	GLU	V191	GLU	ALA	GLY	VAL	ASP	VAL
L280	V191	GLU	M196	GLU	VAL	VAL	GLU	ASP	GLU
R281	M196	GLU	Q197	GLU	GLU	GLU	SER	ASP	SER
H284	Q197	GLU	T198	GLU	SER	SER	GLN	ASP	GLN
W285	T198	GLU	L199	GLU	GLN	GLN	GLY	ASP	GLY
T286	L199	GLU	W200	GLU	GLY	GLY	H98	ASP	GLY
T287	W200	GLU	T205	GLU	H98	L102	L103	ASP	L103
T294	T205	GLU	C206	GLU	L102	L103	G109	ASP	G109
E295	C206	GLU	S207	GLU	L103	G109		ASP	
D296	S207	GLU	E211	GLU				ASP	
Q297	E211	GLU	R221	GLU				ASP	
G298	R221	GLU	H224	GLU				ASP	
L299	H224	GLU	E229	GLU				ASP	
A307	E229	GLU	T233	GLU				ASP	
T312	T233	GLU	S234	GLU				ASP	
S313	S234	GLU	Y247	GLU				ASP	
F314	Y247	GLU	E248	GLU				ASP	
C315	E248	GLU	G249	GLU				ASP	
S319	G249	GLU						ASP	
K320		GLU						ASP	
E321		GLU						ASP	
K322		GLU						ASP	
L323		GLU						ASP	
D324		GLU						ASP	
T325		GLU						ASP	
A326		GLU						ASP	
F327		GLU						ASP	
K329		GLU						ASP	



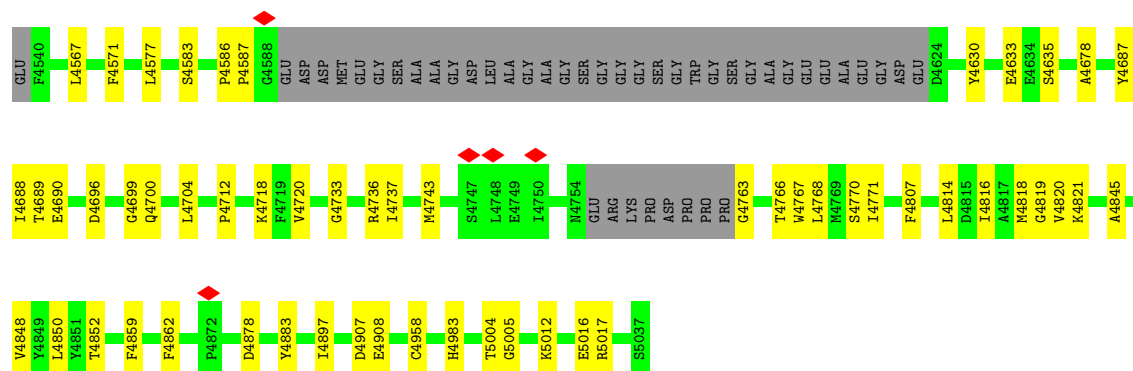




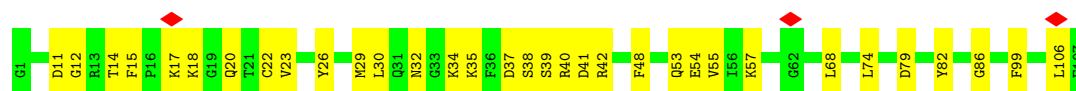




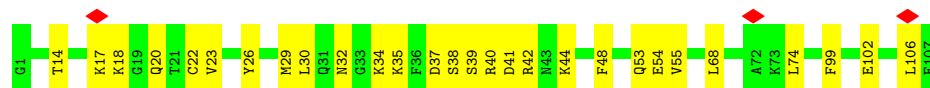




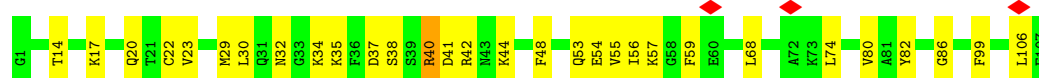
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



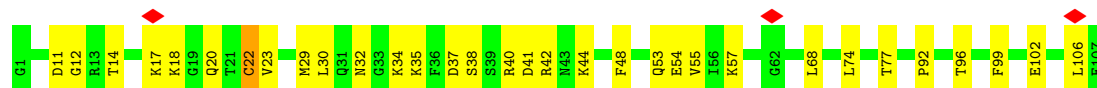
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249034	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.277	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.32	Depositor
Map size (\AA)	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U1C, ATP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/33082	0.48	3/45015 (0.0%)
1	B	0.24	0/33082	0.47	2/45015 (0.0%)
1	C	0.24	0/33082	0.48	4/45015 (0.0%)
1	D	0.25	0/33082	0.48	5/45015 (0.0%)
2	E	0.26	0/802	0.52	0/1086
2	F	0.27	0/802	0.54	0/1086
2	G	0.27	0/802	0.55	0/1086
2	H	0.26	0/802	0.52	0/1086
All	All	0.25	0/135536	0.48	14/184404 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3003	LEU	CA-CB-CG	7.13	131.69	115.30
1	C	3003	LEU	CA-CB-CG	7.11	131.64	115.30
1	D	3003	LEU	CA-CB-CG	7.03	131.48	115.30
1	A	3003	LEU	CA-CB-CG	7.00	131.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	922	LEU	CA-CB-CG	6.73	130.77	115.30
1	D	922	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	984	LEU	CA-CB-CG	5.78	128.60	115.30
1	B	3274	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	2644	LEU	CA-CB-CG	5.41	127.75	115.30
1	C	14	LEU	CA-CB-CG	5.40	127.73	115.30
1	D	3274	LEU	CA-CB-CG	5.33	127.55	115.30
1	D	988	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	14	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	832	GLU	CB-CA-C	5.06	120.52	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	626	LEU	Peptide
1	B	626	LEU	Peptide
1	C	626	LEU	Peptide
1	D	626	LEU	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	32374	0	30869	505	0
1	B	32374	0	30869	488	0
1	C	32374	0	30869	498	0
1	D	32374	0	30869	514	0
2	E	786	0	766	22	0
2	F	786	0	766	20	0
2	G	786	0	766	21	0
2	H	786	0	766	26	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
All	All	132860	0	126588	2070	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 8.

All (2070) 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:830:ARG:HD3	1:D:1612:PHE:CE2	1.70	1.26
1:D:1454:THR:CG2	1:D:1456:ASP:OD1	2.09	0.99
1:D:830:ARG:CD	1:D:1612:PHE:CE2	2.45	0.99
1:D:1454:THR:HG23	1:D:1456:ASP:OD1	1.63	0.97
1:B:4763:GLY:N	1:B:4766:THR:HG1	1.62	0.95
1:D:833:GLY:HA3	1:D:838:HIS:HD2	1.32	0.92
1:D:830:ARG:NH1	1:D:1612:PHE:CD2	2.39	0.91
1:C:4763:GLY:N	1:C:4766:THR:HG1	1.75	0.85
1:C:707:VAL:HG23	1:C:713:SER:OG	1.78	0.83
1:D:4763:GLY:N	1:D:4766:THR:HG1	1.76	0.83
1:D:3003:LEU:HD12	1:D:3004:PRO:HD3	1.60	0.83
1:D:897:ARG:HG2	1:D:898:ASP:H	1.44	0.82
1:C:911:HIS:ND1	1:C:911:HIS:O	2.12	0.82
1:B:3003:LEU:HD12	1:B:3004:PRO:HD3	1.61	0.81
1:B:609:CYS:SG	1:B:610:ASN:N	2.53	0.81
1:B:1451:GLY:HA3	1:B:1494:MET:HB3	1.62	0.81
1:C:69:LEU:HD11	1:C:107:ILE:HD11	1.63	0.81
1:C:3003:LEU:HD12	1:C:3004:PRO:HD3	1.60	0.81
1:A:3003:LEU:HD12	1:A:3004:PRO:HD3	1.61	0.81
1:C:609:CYS:SG	1:C:610:ASN:N	2.53	0.81
1:B:707:VAL:HG23	1:B:713:SER:OG	1.81	0.80
1:D:609:CYS:SG	1:D:610:ASN:N	2.53	0.80
1:D:1454:THR:HG21	1:D:1456:ASP:OD1	1.81	0.79
1:D:830:ARG:NH1	1:D:1612:PHE:HD2	1.82	0.78
1:A:609:CYS:SG	1:A:610:ASN:N	2.53	0.78
1:C:1437:VAL:HG13	1:C:1562:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.67	0.76
1:D:3277:LEU:HA	1:D:3280:TYR:HB3	1.66	0.76
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.67	0.76
1:D:833:GLY:HA3	1:D:838:HIS:CD2	2.20	0.76
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.66	0.76
1:B:3277:LEU:HA	1:B:3280:TYR:HB3	1.68	0.75
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.67	0.75
1:C:3277:LEU:HA	1:C:3280:TYR:HB3	1.68	0.75
1:A:4763:GLY:N	1:A:4766:THR:HG1	1.83	0.74
1:D:686:TRP:HE1	1:D:746:CYS:HG	1.36	0.74
1:A:3277:LEU:HA	1:A:3280:TYR:HB3	1.69	0.73
1:B:205:ILE:HG22	1:B:206:CYS:H	1.54	0.72
1:C:3651:ASN:HA	1:C:3654:LEU:HD12	1.71	0.72
1:B:1018:ASN:HD21	1:B:1020:ARG:HG2	1.53	0.72
1:D:1130:GLN:NE2	1:D:1136:SER:OG	2.23	0.72
1:D:3651:ASN:HA	1:D:3654:LEU:HD12	1.72	0.72
1:B:897:ARG:HG2	1:B:898:ASP:H	1.55	0.71
1:C:897:ARG:HG2	1:C:898:ASP:H	1.56	0.71
1:A:897:ARG:HG2	1:A:898:ASP:H	1.56	0.71
1:A:3651:ASN:HA	1:A:3654:LEU:HD12	1.71	0.71
1:D:102:LEU:HB3	1:D:105:HIS:CD2	2.25	0.71
1:D:205:ILE:HG22	1:D:206:CYS:H	1.54	0.71
1:A:638:ILE:HG21	1:A:703:GLY:HA3	1.73	0.70
1:A:942:ALA:HB2	1:A:1052:ASN:HB3	1.73	0.70
1:A:2651:CYS:SG	1:A:2652:TRP:N	2.65	0.70
1:B:686:TRP:HE1	1:B:746:CYS:HG	1.38	0.70
1:D:794:GLY:O	1:D:812:HIS:ND1	2.25	0.69
1:D:2651:CYS:SG	1:D:2652:TRP:N	2.65	0.69
1:B:2651:CYS:SG	1:B:2652:TRP:N	2.65	0.69
1:B:3651:ASN:HA	1:B:3654:LEU:HD12	1.72	0.69
1:A:4850:LEU:HD11	1:B:4814:LEU:HB2	1.74	0.69
1:B:2626:LEU:HG	1:B:2628:PHE:H	1.58	0.69
1:D:830:ARG:CD	1:D:1612:PHE:HE2	2.04	0.69
1:A:4814:LEU:HB2	1:D:4850:LEU:HD11	1.75	0.69
1:B:681:HIS:HB3	1:B:784:SER:HB3	1.73	0.69
1:A:2524:VAL:HA	1:A:2527:LEU:HD23	1.74	0.69
1:C:2651:CYS:SG	1:C:2652:TRP:N	2.64	0.69
1:B:1128:ARG:HB2	1:B:1130:GLN:HE21	1.58	0.69
1:A:2626:LEU:HG	1:A:2628:PHE:H	1.58	0.68
1:B:4850:LEU:HD11	1:C:4814:LEU:HB2	1.74	0.68
1:C:2626:LEU:HG	1:C:2628:PHE:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:ILE:HG21	1:D:703:GLY:HA3	1.75	0.68
1:D:4820:VAL:HG23	1:D:4821:LYS:H	1.59	0.68
1:C:4850:LEU:HD11	1:D:4814:LEU:HB2	1.75	0.68
1:B:638:ILE:HG21	1:B:703:GLY:HA3	1.76	0.68
1:A:4820:VAL:HG23	1:A:4821:LYS:H	1.59	0.68
1:C:629:ARG:O	1:C:630:GLU:HG3	1.93	0.68
1:C:861:ILE:HB	1:C:930:LYS:HZ2	1.58	0.68
1:B:4820:VAL:HG23	1:B:4821:LYS:H	1.59	0.68
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.76	0.68
1:D:830:ARG:HD3	1:D:1612:PHE:CZ	2.26	0.67
1:D:961:MET:HE2	1:D:963:ASN:H	1.58	0.67
1:B:2441:HIS:HA	1:B:2444:GLN:HB3	1.76	0.67
1:C:14:LEU:HD11	1:C:69:LEU:HD13	1.75	0.67
1:D:2626:LEU:HG	1:D:2628:PHE:H	1.58	0.67
1:B:629:ARG:O	1:B:630:GLU:HG3	1.95	0.67
1:A:102:LEU:HB3	1:A:105:HIS:CD2	2.30	0.67
1:C:4820:VAL:HG23	1:C:4821:LYS:H	1.61	0.66
1:D:2579:VAL:HG22	1:D:2594:SER:HB2	1.78	0.66
1:A:590:LEU:HB2	1:A:599:VAL:HG11	1.78	0.66
1:C:638:ILE:HG21	1:C:703:GLY:HA3	1.77	0.66
1:D:23:GLN:NE2	1:D:36:CYS:SG	2.69	0.66
1:C:977:LEU:HB3	1:C:981:GLN:HB2	1.78	0.66
1:C:2579:VAL:HG22	1:C:2594:SER:HB2	1.77	0.66
1:D:102:LEU:HB3	1:D:105:HIS:HD2	1.61	0.66
1:D:3716:LEU:HD13	1:D:3793:MET:HG2	1.78	0.66
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.76	0.65
1:B:2214:VAL:HG21	1:B:2228:MET:HE1	1.77	0.65
1:C:12:GLN:HE22	1:C:14:LEU:HD22	1.61	0.65
1:C:3697:PRO:O	1:C:3701:LEU:N	2.24	0.65
1:A:3716:LEU:HD13	1:A:3793:MET:HG2	1.78	0.65
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.76	0.65
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.77	0.65
1:B:772:ASN:HD22	1:B:1471:ALA:H	1.42	0.65
2:F:37:ASP:OD1	2:F:42:ARG:NH2	2.30	0.65
1:C:23:GLN:NE2	1:C:36:CYS:SG	2.69	0.65
1:D:590:LEU:HB2	1:D:599:VAL:HG11	1.79	0.65
1:D:2442:LEU:HG	1:D:2443:ILE:HG12	1.79	0.65
1:A:868:GLU:O	1:A:871:ARG:HG3	1.95	0.65
1:C:590:LEU:HB2	1:C:599:VAL:HG11	1.78	0.65
1:A:2579:VAL:HG22	1:A:2594:SER:HB2	1.77	0.65
1:A:3697:PRO:O	1:A:3701:LEU:N	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2579:VAL:HG22	1:B:2594:SER:HB2	1.78	0.64
1:A:3080:VAL:HG13	1:A:3081:MET:HE3	1.79	0.64
1:A:879:HIS:NE2	1:A:908:VAL:O	2.29	0.64
1:D:861:ILE:O	1:D:930:LYS:NZ	2.31	0.64
1:D:664:PHE:HB3	1:D:746:CYS:HB3	1.78	0.64
1:D:1804:LEU:HD12	1:D:1853:ILE:HG21	1.79	0.64
1:C:3052:HIS:NE2	1:C:3128:ASN:O	2.30	0.63
1:A:629:ARG:O	1:A:630:GLU:HG3	1.98	0.63
1:C:1459:GLN:HE22	1:C:1461:ASP:HB2	1.63	0.63
1:D:681:HIS:HB3	1:D:784:SER:HB3	1.80	0.63
1:D:1459:GLN:HE22	1:D:1461:ASP:HB2	1.63	0.63
1:A:23:GLN:NE2	1:A:36:CYS:SG	2.72	0.63
1:B:3319:ILE:HD11	1:B:3338:LEU:HD11	1.79	0.63
1:D:977:LEU:HB3	1:D:981:GLN:HB2	1.80	0.63
1:C:2214:VAL:HG21	1:C:2228:MET:HE1	1.80	0.63
1:A:348:VAL:HG13	1:A:357:LEU:HD23	1.80	0.63
1:B:348:VAL:HG13	1:B:357:LEU:HD23	1.81	0.63
1:B:3080:VAL:HG13	1:B:3081:MET:HE3	1.80	0.63
2:G:23:VAL:HG21	2:G:106:LEU:HB2	1.80	0.63
2:E:37:ASP:OD1	2:E:42:ARG:NH2	2.32	0.63
1:A:2961:GLN:HA	1:A:2964:LEU:HB3	1.81	0.63
1:A:664:PHE:HB3	1:A:746:CYS:HB3	1.81	0.63
1:A:1457:TYR:HA	1:A:1491:ASN:HD22	1.63	0.63
1:C:879:HIS:NE2	1:C:908:VAL:O	2.31	0.63
1:A:722:TRP:CD1	1:A:727:ALA:HA	2.34	0.62
1:B:794:GLY:O	1:B:812:HIS:ND1	2.27	0.62
1:D:3697:PRO:O	1:D:3701:LEU:N	2.26	0.62
2:H:37:ASP:OD1	2:H:42:ARG:NH2	2.32	0.62
1:A:2441:HIS:HA	1:A:2444:GLN:HB3	1.81	0.62
1:B:1804:LEU:HD12	1:B:1853:ILE:HG21	1.80	0.62
1:C:2961:GLN:HA	1:C:2964:LEU:HB3	1.81	0.62
1:C:4166:LEU:HD23	1:C:4166:LEU:H	1.64	0.62
1:B:4088:ILE:HB	1:B:4092:ASP:HB2	1.81	0.62
2:F:23:VAL:HG21	2:F:106:LEU:HB2	1.80	0.62
2:H:23:VAL:HG21	2:H:106:LEU:HB2	1.79	0.62
1:A:1576:SER:HA	1:A:1579:MET:HB2	1.82	0.62
1:B:590:LEU:HB2	1:B:599:VAL:HG11	1.80	0.62
1:C:3592:ILE:HA	1:C:3595:ARG:HE	1.64	0.62
1:D:879:HIS:NE2	1:D:908:VAL:O	2.28	0.62
2:G:37:ASP:OD1	2:G:42:ARG:NH2	2.32	0.62
1:A:1289:LEU:HB2	1:A:1550:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4003:LEU:HG	1:B:4009:GLN:HG3	1.82	0.62
1:D:3592:ILE:HA	1:D:3595:ARG:HE	1.64	0.62
1:B:961:MET:HE2	1:B:963:ASN:H	1.64	0.62
1:D:2214:VAL:HG21	1:D:2228:MET:HE1	1.82	0.62
1:D:4088:ILE:HB	1:D:4092:ASP:HB2	1.82	0.62
1:A:2214:VAL:HG21	1:A:2228:MET:HE1	1.81	0.62
2:E:74:LEU:HB2	2:E:99:PHE:HB2	1.82	0.62
1:A:1742:THR:HG22	1:A:1769:THR:HG21	1.82	0.61
1:A:205:ILE:HG22	1:A:206:CYS:H	1.65	0.61
1:A:988:LEU:HG	1:A:1039:LEU:HD12	1.81	0.61
1:B:1289:LEU:HB2	1:B:1550:PRO:HD2	1.81	0.61
1:B:3697:PRO:O	1:B:3701:LEU:N	2.30	0.61
1:C:1457:TYR:HA	1:C:1491:ASN:HD22	1.65	0.61
1:A:681:HIS:HB3	1:A:784:SER:HB3	1.82	0.61
1:C:3016:TYR:HA	1:C:3029:GLY:HA2	1.82	0.61
1:A:737:LEU:HD23	1:A:738:LEU:H	1.65	0.61
1:D:348:VAL:HG13	1:D:357:LEU:HD23	1.81	0.61
1:D:677:ALA:HB1	2:H:40:ARG:HB3	1.82	0.61
1:D:1457:TYR:HA	1:D:1491:ASN:HD22	1.65	0.61
1:A:4088:ILE:HB	1:A:4092:ASP:HB2	1.83	0.61
1:D:1576:SER:HA	1:D:1579:MET:HB2	1.81	0.61
2:G:74:LEU:HB2	2:G:99:PHE:HB2	1.83	0.61
1:A:2472:LEU:HD12	1:A:2473:PRO:HD2	1.83	0.61
1:A:4003:LEU:HG	1:A:4009:GLN:HG3	1.83	0.61
1:C:4003:LEU:HG	1:C:4009:GLN:HG3	1.82	0.61
1:A:895:PRO:HG2	1:A:896:VAL:HG23	1.83	0.61
1:B:645:ARG:HB3	1:B:826:ILE:HD11	1.83	0.61
1:D:299:LEU:HD11	1:D:314:PHE:HZ	1.66	0.61
1:B:765:GLN:NE2	1:B:1478:ASP:OD1	2.34	0.61
1:D:1742:THR:HG22	1:D:1769:THR:HG21	1.83	0.61
1:B:1576:SER:HA	1:B:1579:MET:HB2	1.82	0.60
1:C:645:ARG:HB3	1:C:826:ILE:HD11	1.83	0.60
1:B:1742:THR:HG22	1:B:1769:THR:HG21	1.83	0.60
1:C:1742:THR:HG22	1:C:1769:THR:HG21	1.83	0.60
1:D:737:LEU:HD23	1:D:738:LEU:H	1.65	0.60
1:D:4712:PRO:O	1:D:4718:LYS:NZ	2.34	0.60
2:F:74:LEU:HB2	2:F:99:PHE:HB2	1.83	0.60
1:B:892:THR:OG1	1:B:902:ARG:O	2.18	0.60
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.34	0.60
1:B:2472:LEU:HD12	1:B:2473:PRO:HD2	1.84	0.60
1:C:1545:ASN:OD1	2:G:32:ASN:ND2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:765:GLN:NE2	1:D:1478:ASP:OD1	2.34	0.60
1:B:3016:TYR:HA	1:B:3029:GLY:HA2	1.84	0.60
1:C:1451:GLY:HA3	1:C:1494:MET:HB3	1.82	0.60
1:D:797:HIS:HB3	1:D:1623:ARG:HH21	1.66	0.60
1:A:2967:MET:HA	1:A:2970:SER:HB3	1.84	0.60
1:A:3592:ILE:HA	1:A:3595:ARG:HE	1.65	0.60
1:C:2591:ARG:O	1:C:2594:SER:OG	2.18	0.60
1:D:2659:THR:O	1:D:2663:ASN:ND2	2.35	0.60
1:D:3016:TYR:HA	1:D:3029:GLY:HA2	1.82	0.60
1:A:2474:LEU:HA	1:A:2494:PHE:HD2	1.67	0.60
1:B:879:HIS:NE2	1:B:908:VAL:O	2.31	0.60
1:C:986:ASP:N	1:C:986:ASP:OD1	2.33	0.60
1:C:4088:ILE:HB	1:C:4092:ASP:HB2	1.83	0.60
1:C:4158:PRO:O	1:C:4162:ASN:ND2	2.35	0.60
1:B:299:LEU:HD11	1:B:314:PHE:HZ	1.67	0.60
1:B:3052:HIS:NE2	1:B:3128:ASN:O	2.34	0.60
1:C:205:ILE:HG22	1:C:206:CYS:H	1.66	0.60
1:C:348:VAL:HG13	1:C:357:LEU:HD23	1.83	0.60
1:C:765:GLN:NE2	1:C:1478:ASP:OD1	2.35	0.60
1:D:421:PHE:HB3	1:D:426:ARG:HH21	1.67	0.60
2:H:74:LEU:HB2	2:H:99:PHE:HB2	1.84	0.60
1:B:659:TYR:HE1	1:B:1006:SER:HB3	1.66	0.60
1:C:1289:LEU:HB2	1:C:1550:PRO:HD2	1.83	0.60
1:D:2911:LEU:HB2	1:D:2916:LYS:HD3	1.84	0.60
1:B:1012:ASP:HB3	1:B:1017:ARG:HG3	1.84	0.60
1:D:3080:VAL:HG13	1:D:3081:MET:HE3	1.82	0.60
1:A:645:ARG:HB3	1:A:826:ILE:HD11	1.84	0.59
1:C:2472:LEU:HD12	1:C:2473:PRO:HD2	1.83	0.59
1:D:1289:LEU:HB2	1:D:1550:PRO:HD2	1.83	0.59
1:D:2472:LEU:HD12	1:D:2473:PRO:HD2	1.84	0.59
2:G:53:GLN:HG2	2:G:54:GLU:H	1.66	0.59
1:A:961:MET:HE2	1:A:963:ASN:H	1.67	0.59
1:A:3016:TYR:HA	1:A:3029:GLY:HA2	1.83	0.59
1:C:3040:THR:HG21	1:C:3080:VAL:HG21	1.85	0.59
1:D:649:PHE:HB3	1:D:776:LEU:HD22	1.84	0.59
1:A:765:GLN:NE2	1:A:1478:ASP:OD1	2.34	0.59
1:A:4712:PRO:O	1:A:4718:LYS:NZ	2.34	0.59
1:B:630:GLU:HA	1:B:1642:PRO:HB2	1.84	0.59
1:B:668:VAL:HG22	1:B:789:VAL:HG12	1.85	0.59
1:D:645:ARG:HD3	1:D:826:ILE:HG12	1.83	0.59
1:D:686:TRP:NE1	1:D:746:CYS:SG	2.72	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:TYR:CE1	1:B:1006:SER:HB3	2.37	0.59
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.83	0.59
1:B:2961:GLN:HA	1:B:2964:LEU:HB3	1.82	0.59
1:C:1104:TRP:NE1	1:C:1151:CYS:SG	2.75	0.59
1:A:4158:PRO:O	1:A:4162:ASN:ND2	2.35	0.59
1:B:150:MET:HB3	1:B:169:LEU:HD13	1.84	0.59
1:B:649:PHE:HB3	1:B:776:LEU:HD22	1.85	0.59
1:B:1457:TYR:HA	1:B:1491:ASN:HD22	1.66	0.59
1:B:2967:MET:HA	1:B:2970:SER:HB3	1.84	0.59
1:D:265:LEU:HD23	1:D:279:PRO:HB2	1.85	0.59
1:D:1104:TRP:NE1	1:D:1151:CYS:SG	2.76	0.59
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.85	0.59
1:C:107:ILE:N	1:C:148:TRP:O	2.34	0.59
1:D:707:VAL:HG23	1:D:713:SER:HB2	1.85	0.59
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.36	0.59
1:A:797:HIS:HB3	1:A:1623:ARG:HH21	1.66	0.59
1:A:813:GLU:OE1	1:A:813:GLU:N	2.36	0.59
1:A:2659:THR:O	1:A:2663:ASN:ND2	2.36	0.59
1:B:4712:PRO:O	1:B:4718:LYS:NZ	2.34	0.59
1:C:4712:PRO:O	1:C:4718:LYS:NZ	2.33	0.59
1:D:709:ASP:OD1	1:D:713:SER:OG	2.20	0.59
1:D:772:ASN:HD22	1:D:1471:ALA:H	1.49	0.59
1:A:2452:ARG:NH1	1:D:175:SER:O	2.36	0.59
1:A:2911:LEU:HB2	1:A:2916:LYS:HD3	1.84	0.59
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.35	0.59
1:D:168:ASP:HB3	1:D:199:LEU:HB3	1.84	0.59
1:D:331:VAL:HG22	1:D:333:GLY:H	1.68	0.59
2:E:11:ASP:OD1	2:E:12:GLY:N	2.36	0.59
1:A:421:PHE:HB3	1:A:426:ARG:HH21	1.68	0.58
1:A:3409:TYR:HE2	1:A:3510:ILE:HG23	1.68	0.58
1:B:4158:PRO:O	1:B:4162:ASN:ND2	2.36	0.58
1:C:265:LEU:HD23	1:C:279:PRO:HB2	1.85	0.58
1:C:331:VAL:HG22	1:C:333:GLY:H	1.68	0.58
1:A:331:VAL:HG22	1:A:333:GLY:H	1.67	0.58
1:B:797:HIS:HB3	1:B:1623:ARG:HH21	1.66	0.58
1:B:895:PRO:HG2	1:B:896:VAL:HG23	1.84	0.58
1:D:986:ASP:OD1	1:D:986:ASP:N	2.36	0.58
1:A:1545:ASN:OD1	2:E:32:ASN:ND2	2.34	0.58
1:B:3096:PHE:O	1:B:3100:SER:N	2.36	0.58
1:D:574:VAL:HA	1:D:577:ILE:HD12	1.85	0.58
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:GLU:N	1:C:813:GLU:OE1	2.36	0.58
1:D:1118:ASP:OD1	1:D:1118:ASP:N	2.36	0.58
2:E:23:VAL:HG21	2:E:106:LEU:HB2	1.85	0.58
1:A:1451:GLY:HA3	1:A:1494:MET:HB3	1.84	0.58
1:D:3052:HIS:NE2	1:D:3128:ASN:O	2.36	0.58
1:B:2659:THR:O	1:B:2663:ASN:ND2	2.36	0.58
1:C:1576:SER:HA	1:C:1579:MET:HB2	1.83	0.58
1:C:3409:TYR:HE2	1:C:3510:ILE:HG23	1.67	0.58
1:D:4733:GLY:HA3	1:D:4736:ARG:HG3	1.85	0.58
2:E:53:GLN:HG2	2:E:54:GLU:H	1.67	0.58
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.84	0.58
1:C:686:TRP:HE1	1:C:746:CYS:HG	1.48	0.58
1:D:1545:ASN:OD1	2:H:32:ASN:ND2	2.35	0.58
2:H:17:LYS:NZ	2:H:18:LYS:O	2.36	0.58
1:B:4733:GLY:HA3	1:B:4736:ARG:HG3	1.86	0.58
1:C:668:VAL:HG22	1:C:789:VAL:HG12	1.85	0.58
1:C:2911:LEU:HB2	1:C:2916:LYS:HD3	1.84	0.58
2:G:17:LYS:H	2:G:20:GLN:HE22	1.50	0.58
2:H:11:ASP:OD1	2:H:12:GLY:N	2.37	0.58
1:A:1000:ARG:HG3	1:A:1005:TRP:HB2	1.86	0.58
1:C:393:CYS:SG	1:C:398:SER:OG	2.62	0.58
1:D:19:GLU:HB2	1:D:205:ILE:HB	1.86	0.58
1:D:150:MET:HB3	1:D:169:LEU:HD13	1.86	0.58
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.85	0.58
1:A:534:ARG:NH2	1:A:573:GLU:OE2	2.37	0.57
1:A:4733:GLY:HA3	1:A:4736:ARG:HG3	1.86	0.57
1:C:534:ARG:NH2	1:C:573:GLU:OE2	2.37	0.57
1:C:649:PHE:HB3	1:C:776:LEU:HD22	1.85	0.57
1:C:4733:GLY:HA3	1:C:4736:ARG:HG3	1.85	0.57
1:D:534:ARG:NH2	1:D:573:GLU:OE2	2.36	0.57
1:A:668:VAL:HG22	1:A:789:VAL:HG12	1.86	0.57
1:B:175:SER:O	1:C:2452:ARG:NH1	2.37	0.57
1:C:636:ASN:HD21	2:G:35:LYS:HE3	1.69	0.57
1:C:2659:THR:O	1:C:2663:ASN:ND2	2.37	0.57
1:D:668:VAL:HG22	1:D:789:VAL:HG12	1.86	0.57
1:D:927:GLU:O	1:D:931:THR:HG23	2.04	0.57
2:E:14:THR:HG21	2:E:68:LEU:HD12	1.86	0.57
2:F:53:GLN:HG2	2:F:54:GLU:H	1.68	0.57
1:A:175:SER:O	1:B:2452:ARG:NH1	2.38	0.57
1:B:331:VAL:HG22	1:B:333:GLY:H	1.68	0.57
1:B:1104:TRP:NE1	1:B:1151:CYS:SG	2.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1452:TRP:HE1	1:C:1518:CYS:HB3	1.70	0.57
1:A:1104:TRP:NE1	1:A:1151:CYS:SG	2.77	0.57
1:A:3980:LEU:HD23	1:A:3985:LEU:HD22	1.85	0.57
1:B:737:LEU:HD23	1:B:738:LEU:H	1.69	0.57
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.36	0.57
1:C:2967:MET:HA	1:C:2970:SER:HB3	1.86	0.57
1:C:3415:TYR:O	1:C:3419:ASN:ND2	2.37	0.57
1:D:2968:ASP:O	1:D:2971:GLN:NE2	2.29	0.57
1:B:3409:TYR:HE2	1:B:3510:ILE:HG23	1.70	0.57
1:C:3096:PHE:O	1:C:3100:SER:N	2.36	0.57
1:D:2961:GLN:HA	1:D:2964:LEU:HB3	1.87	0.57
1:B:651:GLY:HA3	1:B:776:LEU:HA	1.85	0.57
1:A:221:ARG:NH1	1:A:258:SER:OG	2.38	0.57
1:B:574:VAL:HA	1:B:577:ILE:HD12	1.85	0.57
1:B:2911:LEU:HB2	1:B:2916:LYS:HD3	1.86	0.57
1:C:221:ARG:NH1	1:C:258:SER:OG	2.37	0.57
1:C:865:PRO:HA	1:C:868:GLU:HB3	1.86	0.57
1:C:1164:LEU:HD23	1:C:1169:LEU:HB3	1.86	0.57
1:D:1241:SER:HA	1:D:1603:VAL:HG12	1.86	0.57
1:D:2524:VAL:HA	1:D:2527:LEU:HD23	1.85	0.57
1:D:4158:PRO:O	1:D:4162:ASN:ND2	2.37	0.57
1:A:651:GLY:HA3	1:A:776:LEU:HA	1.86	0.57
1:A:3666:ASP:OD1	1:A:3666:ASP:N	2.38	0.57
1:C:4567:LEU:HB2	1:C:4816:ILE:HG21	1.87	0.57
1:D:895:PRO:HD2	1:D:903:LEU:HD13	1.85	0.57
1:A:299:LEU:HD11	1:A:314:PHE:HZ	1.68	0.57
1:B:1140:GLY:HA3	1:B:1169:LEU:HD12	1.87	0.57
1:D:3409:TYR:HE2	1:D:3510:ILE:HG23	1.70	0.57
1:A:393:CYS:SG	1:A:398:SER:OG	2.62	0.57
1:B:636:ASN:HD21	2:F:35:LYS:HE3	1.69	0.57
1:B:737:LEU:HD23	1:B:738:LEU:N	2.20	0.57
1:B:4696:ASP:O	1:B:4700:GLN:NE2	2.38	0.57
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.87	0.57
1:D:2967:MET:HA	1:D:2970:SER:HB3	1.87	0.57
1:D:3366:ARG:HA	1:D:3441:ILE:HD11	1.86	0.57
1:A:3052:HIS:NE2	1:A:3128:ASN:O	2.37	0.56
1:B:393:CYS:SG	1:B:398:SER:OG	2.63	0.56
1:B:753:PRO:HB2	1:B:771:PHE:CD2	2.40	0.56
1:D:860:GLN:OE1	1:D:860:GLN:N	2.38	0.56
1:A:636:ASN:HD21	2:E:35:LYS:HE3	1.70	0.56
1:A:2737:PRO:HG3	1:A:2888:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LEU:HD23	1:B:279:PRO:HB2	1.87	0.56
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.37	0.56
1:C:14:LEU:HD12	1:C:18:ASP:HB3	1.86	0.56
1:D:3415:TYR:O	1:D:3419:ASN:ND2	2.38	0.56
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.38	0.56
1:A:644:ILE:HD11	1:A:1615:VAL:HG21	1.87	0.56
1:A:1140:GLY:HA3	1:A:1169:LEU:HD12	1.86	0.56
1:B:677:ALA:HB1	2:F:40:ARG:HB3	1.87	0.56
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.85	0.56
1:C:3270:ILE:HA	1:C:3274:LEU:HD21	1.86	0.56
1:D:1089:TYR:HB2	1:D:1152:MET:HG2	1.87	0.56
1:D:1140:GLY:HA3	1:D:1169:LEU:HD12	1.87	0.56
2:H:53:GLN:HG2	2:H:54:GLU:H	1.69	0.56
1:A:3415:TYR:O	1:A:3419:ASN:ND2	2.38	0.56
1:C:3335:MET:HB3	1:C:3407:ALA:HB2	1.87	0.56
1:D:636:ASN:HD21	2:H:35:LYS:HE3	1.70	0.56
1:D:910:PHE:HA	1:D:913:LEU:HD11	1.87	0.56
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.39	0.56
1:B:1241:SER:HA	1:B:1603:VAL:HG12	1.86	0.56
1:B:3980:LEU:HD23	1:B:3985:LEU:HD22	1.87	0.56
1:D:689:THR:HB	1:D:778:PHE:CZ	2.40	0.56
1:D:1424:PRO:HA	1:D:1427:ILE:HG22	1.87	0.56
1:D:2118:ARG:NH2	1:D:3719:ASP:OD1	2.37	0.56
1:B:977:LEU:HB3	1:B:981:GLN:HB2	1.88	0.56
1:B:4678:ALA:HB1	1:B:4720:VAL:HG21	1.87	0.56
1:C:860:GLN:N	1:C:860:GLN:OE1	2.38	0.56
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.87	0.56
1:A:4678:ALA:HB1	1:A:4720:VAL:HG21	1.87	0.56
1:B:860:GLN:OE1	1:B:860:GLN:N	2.39	0.56
1:C:664:PHE:HB3	1:C:746:CYS:HB3	1.88	0.56
1:D:221:ARG:NH1	1:D:258:SER:OG	2.38	0.56
1:A:150:MET:HB3	1:A:169:LEU:HD13	1.87	0.56
1:A:452:PHE:O	1:A:528:SER:OG	2.24	0.56
1:A:4567:LEU:HB2	1:A:4816:ILE:HG21	1.88	0.56
1:B:910:PHE:HA	1:B:913:LEU:HD11	1.86	0.56
1:C:651:GLY:HA3	1:C:776:LEU:HA	1.88	0.56
1:C:2884:ASN:OD1	1:C:2888:ARG:NH1	2.39	0.56
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.38	0.56
1:C:4769:MET:N	1:C:4769:MET:SD	2.79	0.56
1:D:1452:TRP:HE1	1:D:1518:CYS:HB3	1.71	0.56
1:D:2512:ILE:HG22	1:D:2516:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3980:LEU:HD23	1:D:3985:LEU:HD22	1.87	0.56
1:A:2591:ARG:O	1:A:2594:SER:OG	2.19	0.56
1:C:882:TRP:HZ3	1:C:921:ASN:HD21	1.53	0.56
1:C:895:PRO:HD2	1:C:903:LEU:HD13	1.86	0.56
1:C:3366:ARG:HA	1:C:3441:ILE:HD11	1.87	0.56
1:D:393:CYS:SG	1:D:398:SER:OG	2.63	0.56
1:D:2737:PRO:HG3	1:D:2888:ARG:HD2	1.88	0.56
1:D:4567:LEU:HB2	1:D:4816:ILE:HG21	1.88	0.56
1:A:1112:ASP:OD1	1:A:1112:ASP:N	2.36	0.56
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.36	0.56
1:A:2118:ARG:NH2	1:A:3719:ASP:OD1	2.37	0.56
1:A:2740:VAL:HG21	1:A:2818:ALA:HB1	1.88	0.56
1:B:221:ARG:NH1	1:B:258:SER:OG	2.38	0.56
1:B:2891:LYS:HA	1:B:2894:LEU:HD12	1.88	0.56
1:B:4232:GLU:OE2	1:B:5017:ARG:NH2	2.39	0.56
1:C:830:ARG:NH2	1:C:832:GLU:OE2	2.36	0.56
1:C:3980:LEU:HD23	1:C:3985:LEU:HD22	1.87	0.56
1:A:2884:ASN:OD1	1:A:2888:ARG:NH1	2.39	0.55
1:B:4567:LEU:HB2	1:B:4816:ILE:HG21	1.88	0.55
1:C:2740:VAL:HG21	1:C:2818:ALA:HB1	1.88	0.55
1:D:864:PRO:HD2	1:D:867:LEU:HD12	1.87	0.55
1:D:1003:GLN:O	1:D:1016:ARG:NH2	2.39	0.55
1:D:3319:ILE:HD11	1:D:3338:LEU:HD11	1.87	0.55
1:D:5012:LYS:NZ	1:D:5016:GLU:OE2	2.39	0.55
1:A:107:ILE:N	1:A:148:TRP:O	2.38	0.55
1:B:2512:ILE:HG22	1:B:2516:ASP:HB3	1.87	0.55
1:C:5012:LYS:NZ	1:C:5016:GLU:OE2	2.40	0.55
1:D:12:GLN:HG3	1:D:165:VAL:HA	1.88	0.55
1:D:4696:ASP:O	1:D:4700:GLN:NE2	2.40	0.55
1:A:229:GLU:HA	1:A:249:GLY:HA3	1.89	0.55
1:A:1241:SER:HA	1:A:1603:VAL:HG12	1.87	0.55
1:B:102:LEU:HB3	1:B:105:HIS:CD2	2.41	0.55
1:B:2740:VAL:HG21	1:B:2818:ALA:HB1	1.88	0.55
1:B:4087:LEU:HD22	1:B:4122:MET:HA	1.88	0.55
1:C:175:SER:O	1:D:2452:ARG:NH1	2.38	0.55
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.38	0.55
1:B:861:ILE:HB	1:B:930:LYS:HZ2	1.71	0.55
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.36	0.55
1:C:2737:PRO:HG3	1:C:2888:ARG:HD2	1.88	0.55
1:D:3666:ASP:OD1	1:D:3666:ASP:N	2.38	0.55
1:A:772:ASN:HD22	1:A:1471:ALA:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2737:PRO:HG3	1:B:2888:ARG:HD2	1.87	0.55
1:C:150:MET:HB3	1:C:169:LEU:HD13	1.88	0.55
1:C:299:LEU:HD11	1:C:314:PHE:HZ	1.71	0.55
1:C:452:PHE:O	1:C:528:SER:OG	2.24	0.55
1:C:755:ILE:HG13	1:C:771:PHE:CZ	2.42	0.55
1:A:677:ALA:HB1	2:E:40:ARG:HB3	1.88	0.55
1:A:4696:ASP:O	1:A:4700:GLN:NE2	2.40	0.55
1:B:1089:TYR:HB2	1:B:1152:MET:HG2	1.88	0.55
1:C:797:HIS:HB3	1:C:1623:ARG:HH21	1.70	0.55
1:C:2118:ARG:NH2	1:C:3719:ASP:OD1	2.38	0.55
1:C:4032:GLU:OE2	1:C:5004:THR:OG1	2.25	0.55
1:A:14:LEU:HD11	1:A:69:LEU:HD13	1.88	0.55
1:A:3270:ILE:HA	1:A:3274:LEU:HD21	1.88	0.55
1:B:2884:ASN:OD1	1:B:2888:ARG:NH1	2.39	0.55
1:B:5012:LYS:NZ	1:B:5016:GLU:OE2	2.39	0.55
1:C:689:THR:HB	1:C:778:PHE:CZ	2.42	0.55
1:C:2420:HIS:N	1:C:2492:ALA:O	2.40	0.55
1:D:107:ILE:N	1:D:148:TRP:O	2.38	0.55
1:D:4224:GLU:OE2	1:D:4224:GLU:N	2.40	0.55
1:A:399:GLN:O	1:A:403:MET:HG3	2.06	0.55
1:A:3366:ARG:HA	1:A:3441:ILE:HD11	1.88	0.55
1:A:5012:LYS:NZ	1:A:5016:GLU:OE2	2.39	0.55
1:B:2244:ARG:NH1	1:B:2283:ASN:OD1	2.40	0.55
1:B:3415:TYR:O	1:B:3419:ASN:ND2	2.40	0.55
1:C:4678:ALA:HB1	1:C:4720:VAL:HG21	1.89	0.55
1:D:2244:ARG:NH1	1:D:2283:ASN:OD1	2.40	0.55
1:D:2884:ASN:OD1	1:D:2888:ARG:NH1	2.39	0.55
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.39	0.55
1:A:3417:ASP:OD1	1:A:3417:ASP:N	2.40	0.55
1:B:103:TYR:HE2	1:B:152:PRO:HA	1.71	0.55
1:D:1530:THR:HG22	1:D:1535:GLU:HA	1.89	0.55
1:D:3335:MET:HB3	1:D:3407:ALA:HB2	1.89	0.55
1:D:3678:SER:OG	1:D:3773:ARG:NH2	2.39	0.55
1:A:2512:ILE:HG22	1:A:2516:ASP:HB3	1.87	0.55
1:B:2654:TYR:HA	1:B:2657:LEU:HD23	1.89	0.55
1:B:4166:LEU:HD23	1:B:4166:LEU:H	1.70	0.55
1:C:1504:GLY:O	1:C:1508:ARG:NH1	2.40	0.55
1:C:2098:VAL:HG11	1:C:2127:GLN:HG3	1.88	0.55
1:C:4224:GLU:N	1:C:4224:GLU:OE1	2.40	0.55
1:D:3245:VAL:HG12	1:D:3247:ASP:H	1.72	0.55
1:A:649:PHE:HB3	1:A:776:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3319:ILE:HD11	1:A:3338:LEU:HD11	1.89	0.54
1:A:4818:MET:SD	1:A:4819:GLY:N	2.81	0.54
1:B:229:GLU:HA	1:B:249:GLY:HA3	1.89	0.54
1:B:284:HIS:ND1	1:B:287:THR:OG1	2.33	0.54
1:B:1018:ASN:ND2	1:B:1020:ARG:HG2	2.22	0.54
1:C:1028:ASP:OD1	1:C:1028:ASP:N	2.40	0.54
1:C:1140:GLY:HA3	1:C:1169:LEU:HD12	1.89	0.54
1:C:1530:THR:HG22	1:C:1535:GLU:HA	1.89	0.54
1:D:2654:TYR:HA	1:D:2657:LEU:HD23	1.89	0.54
1:A:4032:GLU:OE2	1:A:5004:THR:OG1	2.24	0.54
1:B:534:ARG:NH2	1:B:573:GLU:OE2	2.35	0.54
1:B:2098:VAL:HG11	1:B:2127:GLN:HG3	1.89	0.54
1:B:4224:GLU:N	1:B:4224:GLU:OE2	2.40	0.54
1:D:580:GLU:HG3	1:D:620:LEU:HD21	1.89	0.54
1:D:867:LEU:HD22	1:D:929:LEU:HD11	1.88	0.54
1:A:910:PHE:HA	1:A:913:LEU:HD11	1.90	0.54
1:B:753:PRO:HB2	1:B:771:PHE:HD2	1.72	0.54
1:C:49:LEU:HD11	1:C:191:VAL:HG23	1.90	0.54
1:D:871:ARG:NH1	1:D:922:LEU:O	2.40	0.54
1:A:2891:LYS:HA	1:A:2894:LEU:HD12	1.90	0.54
1:A:3678:SER:OG	1:A:3773:ARG:NH2	2.41	0.54
1:B:4818:MET:SD	1:B:4819:GLY:N	2.81	0.54
1:C:3678:SER:OG	1:C:3773:ARG:NH2	2.41	0.54
1:C:4232:GLU:OE2	1:C:5017:ARG:NH2	2.40	0.54
1:A:144:GLU:O	1:A:175:SER:OG	2.25	0.54
1:D:2740:VAL:HG21	1:D:2818:ALA:HB1	1.89	0.54
1:D:4688:ILE:HD12	1:D:4737:ILE:HD12	1.90	0.54
1:A:54:ASN:HD22	1:A:57:ASN:HD21	1.54	0.54
1:A:1704:PRO:HG2	1:A:1707:LEU:HB2	1.90	0.54
1:A:3096:PHE:O	1:A:3100:SER:N	2.35	0.54
1:A:4688:ILE:HD12	1:A:4737:ILE:HD12	1.90	0.54
1:B:1152:MET:HB2	1:B:1161:ILE:O	2.08	0.54
1:B:1459:GLN:NE2	1:B:1470:ARG:HE	2.05	0.54
1:A:1658:ASP:N	1:A:1658:ASP:OD1	2.40	0.54
1:B:619:ASP:OD2	1:B:1680:ARG:NH2	2.37	0.54
1:D:4818:MET:SD	1:D:4819:GLY:N	2.81	0.54
1:B:1160:ILE:HB	1:B:1179:PHE:HD2	1.73	0.54
1:B:4768:LEU:HD12	1:B:4769:MET:SD	2.48	0.54
1:C:1089:TYR:HB2	1:C:1152:MET:HG2	1.89	0.54
1:C:3323:ILE:HD11	1:C:3338:LEU:HD22	1.90	0.54
1:D:2891:LYS:HA	1:D:2894:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.38	0.54
1:A:1089:TYR:HB2	1:A:1152:MET:HG2	1.89	0.54
1:A:3673:MET:O	1:A:3677:LEU:HB2	2.08	0.54
1:A:4224:GLU:N	1:A:4224:GLU:OE2	2.40	0.54
1:C:4087:LEU:HD22	1:C:4122:MET:HA	1.88	0.54
1:D:651:GLY:HA3	1:D:776:LEU:HA	1.88	0.54
1:A:1530:THR:HG22	1:A:1535:GLU:HA	1.90	0.54
1:A:2244:ARG:NH1	1:A:2283:ASN:OD1	2.40	0.54
1:B:659:TYR:OH	1:B:1017:ARG:HD3	2.07	0.54
1:B:1040:CYS:O	1:B:1044:ARG:HG2	2.07	0.54
1:B:2118:ARG:NH2	1:B:3719:ASP:OD1	2.37	0.54
1:C:2244:ARG:NH1	1:C:2283:ASN:OD1	2.40	0.54
1:C:2953:LYS:HA	1:C:2957:PHE:HB3	1.90	0.54
1:D:1704:PRO:HG2	1:D:1707:LEU:HB2	1.90	0.54
1:D:4032:GLU:OE2	1:D:5004:THR:OG1	2.25	0.54
1:A:1504:GLY:O	1:A:1508:ARG:NH1	2.41	0.53
1:A:2654:TYR:HA	1:A:2657:LEU:HD23	1.90	0.53
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.40	0.53
1:D:54:ASN:HD22	1:D:57:ASN:HD21	1.55	0.53
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.89	0.53
1:D:1443:GLN:NE2	1:D:1444:GLU:O	2.41	0.53
1:D:2420:HIS:N	1:D:2492:ALA:O	2.41	0.53
1:A:205:ILE:HG22	1:A:206:CYS:N	2.24	0.53
1:A:4162:ASN:HA	1:A:4165:GLU:HG2	1.89	0.53
1:B:644:ILE:HD11	1:B:1615:VAL:HG21	1.90	0.53
1:C:3319:ILE:HD11	1:C:3338:LEU:HD11	1.90	0.53
1:A:871:ARG:HH12	1:A:926:GLY:HA3	1.72	0.53
1:A:4769:MET:N	1:A:4769:MET:SD	2.81	0.53
1:B:813:GLU:HG3	1:B:1009:ALA:H	1.74	0.53
1:B:2420:HIS:CE1	1:B:2424:SER:HB3	2.43	0.53
1:B:2953:LYS:HA	1:B:2957:PHE:HB3	1.90	0.53
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.42	0.53
1:C:1241:SER:HA	1:C:1603:VAL:HG12	1.91	0.53
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.90	0.53
1:A:745:SER:HB3	1:A:758:ARG:HB2	1.91	0.53
1:B:1180:ARG:O	1:B:1181:GLU:HG2	2.09	0.53
1:B:4032:GLU:OE2	1:B:5004:THR:OG1	2.25	0.53
1:C:554:LEU:HD23	1:C:1593:PRO:HD3	1.90	0.53
1:C:681:HIS:HB3	1:C:784:SER:HB3	1.89	0.53
1:C:972:LEU:HD22	1:C:1044:ARG:HB3	1.90	0.53
1:C:2441:HIS:HA	1:C:2444:GLN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:GLU:HA	1:D:249:GLY:HA3	1.89	0.53
1:D:3133:THR:HA	1:D:3137:LEU:HD12	1.89	0.53
1:D:4003:LEU:HG	1:D:4009:GLN:HG3	1.90	0.53
1:B:1530:THR:HG22	1:B:1535:GLU:HA	1.91	0.53
1:C:54:ASN:HD22	1:C:57:ASN:HD21	1.56	0.53
1:C:4688:ILE:HD12	1:C:4737:ILE:HD12	1.91	0.53
1:D:24:CYS:HB2	1:D:200:TRP:HA	1.91	0.53
1:D:4055:VAL:HA	1:D:4058:ILE:HD12	1.90	0.53
2:H:17:LYS:H	2:H:20:GLN:HE22	1.56	0.53
1:B:3417:ASP:N	1:B:3417:ASP:OD1	2.42	0.53
1:C:1424:PRO:HA	1:C:1427:ILE:HG22	1.90	0.53
1:C:3417:ASP:N	1:C:3417:ASP:OD1	2.39	0.53
2:H:17:LYS:HG3	2:H:18:LYS:H	1.73	0.53
1:B:1772:ARG:NH2	1:B:1952:GLN:OE1	2.42	0.53
1:B:3366:ARG:HA	1:B:3441:ILE:HD11	1.90	0.53
1:B:4688:ILE:HD12	1:B:4737:ILE:HD12	1.91	0.53
1:C:3037:GLU:O	1:C:3040:THR:OG1	2.26	0.53
1:C:3673:MET:O	1:C:3677:LEU:HB2	2.08	0.53
1:D:3438:VAL:HG11	1:D:3517:MET:CE	2.39	0.53
1:B:984:LEU:O	1:B:988:LEU:HG	2.09	0.53
1:C:745:SER:HB3	1:C:758:ARG:HB2	1.90	0.53
1:C:1180:ARG:O	1:C:1181:GLU:HG2	2.09	0.53
1:C:2654:TYR:HA	1:C:2657:LEU:HD23	1.91	0.53
1:A:1424:PRO:HA	1:A:1427:ILE:HG22	1.90	0.53
1:A:5004:THR:OG1	1:A:5005:GLY:N	2.42	0.53
1:B:1461:ASP:HB3	1:B:1464:PHE:HB2	1.91	0.53
1:B:3245:VAL:HG12	1:B:3247:ASP:H	1.71	0.53
1:B:3794:VAL:HG21	1:B:3835:LEU:HD11	1.91	0.53
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.41	0.53
1:A:4087:LEU:HD22	1:A:4122:MET:HA	1.91	0.53
1:B:1079:LYS:HA	1:B:1189:LEU:HD11	1.91	0.53
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.42	0.53
1:B:4820:VAL:HG23	1:B:4821:LYS:N	2.24	0.53
1:C:1704:PRO:HG2	1:C:1707:LEU:HB2	1.91	0.53
1:D:2420:HIS:CE1	1:D:2424:SER:HB3	2.44	0.53
1:A:692:TYR:CD1	1:A:713:SER:OG	2.59	0.52
1:A:871:ARG:HH21	1:A:922:LEU:HD23	1.74	0.52
1:C:205:ILE:HG22	1:C:206:CYS:N	2.24	0.52
1:C:1160:ILE:HB	1:C:1179:PHE:HD2	1.74	0.52
1:C:1436:SER:HA	1:C:1517:GLY:HA2	1.90	0.52
1:D:1180:ARG:O	1:D:1181:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ARG:NH2	1:A:922:LEU:O	2.43	0.52
1:C:3545:THR:HG23	1:C:3548:GLU:H	1.73	0.52
1:C:4818:MET:SD	1:C:4819:GLY:N	2.82	0.52
1:C:5004:THR:OG1	1:C:5005:GLY:N	2.43	0.52
1:D:1079:LYS:HA	1:D:1189:LEU:HD11	1.91	0.52
1:D:1160:ILE:HB	1:D:1179:PHE:HD2	1.74	0.52
1:D:3673:MET:O	1:D:3677:LEU:HB2	2.09	0.52
1:A:265:LEU:HD11	1:A:281:ARG:HD3	1.91	0.52
1:B:1704:PRO:HG2	1:B:1707:LEU:HB2	1.91	0.52
1:D:119:SER:OG	1:D:120:CYS:N	2.43	0.52
1:D:981:GLN:O	1:D:985:VAL:HG23	2.10	0.52
1:A:3545:THR:HG23	1:A:3548:GLU:H	1.74	0.52
1:B:452:PHE:O	1:B:528:SER:OG	2.22	0.52
1:B:1504:GLY:O	1:B:1508:ARG:NH1	2.40	0.52
1:C:229:GLU:HA	1:C:249:GLY:HA3	1.90	0.52
1:C:913:LEU:HB2	1:C:918:ARG:HG2	1.92	0.52
1:C:2891:LYS:HA	1:C:2894:LEU:HD12	1.90	0.52
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.41	0.52
1:A:981:GLN:O	1:A:985:VAL:HG23	2.10	0.52
1:C:24:CYS:HB2	1:C:200:TRP:HA	1.91	0.52
1:D:3545:THR:HG23	1:D:3548:GLU:H	1.73	0.52
1:A:49:LEU:HD11	1:A:191:VAL:HG23	1.91	0.52
1:B:882:TRP:HZ3	1:B:921:ASN:HD21	1.58	0.52
1:B:1443:GLN:NE2	1:B:1444:GLU:O	2.41	0.52
1:C:119:SER:OG	1:C:120:CYS:N	2.43	0.52
1:D:41:GLY:O	1:D:45:ARG:NH1	2.43	0.52
1:D:4087:LEU:HD22	1:D:4122:MET:HA	1.91	0.52
1:A:1079:LYS:HA	1:A:1189:LEU:HD11	1.92	0.52
1:A:3453:ARG:O	1:A:3457:ASN:ND2	2.43	0.52
1:B:498:THR:H	1:B:503:PHE:HE2	1.57	0.52
1:B:4055:VAL:HA	1:B:4058:ILE:HD12	1.92	0.52
1:C:910:PHE:HA	1:C:913:LEU:HD11	1.92	0.52
1:D:3579:LEU:HG	1:D:3581:GLY:H	1.75	0.52
1:B:772:ASN:ND2	1:B:1471:ALA:H	2.08	0.52
1:C:1079:LYS:HA	1:C:1189:LEU:HD11	1.92	0.52
1:C:1435:TYR:HB3	1:C:1575:LEU:HG	1.92	0.52
1:C:4633:GLU:HG2	1:C:4635:SER:H	1.75	0.52
1:D:554:LEU:HD23	1:D:1593:PRO:HD3	1.91	0.52
1:D:1152:MET:HB2	1:D:1161:ILE:O	2.09	0.52
1:D:3453:ARG:O	1:D:3457:ASN:ND2	2.43	0.52
1:A:1443:GLN:NE2	1:A:1444:GLU:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2243:SER:OG	1:A:2245:GLN:OE1	2.28	0.52
1:A:2856:ASN:OD1	1:A:2856:ASN:N	2.43	0.52
1:B:49:LEU:HD11	1:B:191:VAL:HG23	1.92	0.52
1:B:2420:HIS:N	1:B:2492:ALA:O	2.42	0.52
1:D:674:PHE:N	1:D:680:THR:OG1	2.43	0.52
1:D:982:THR:HA	1:D:985:VAL:HG23	1.92	0.52
1:D:1772:ARG:NH2	1:D:1952:GLN:OE1	2.43	0.52
1:D:4696:ASP:OD1	1:D:4696:ASP:N	2.37	0.52
1:A:1110:ARG:NH2	1:A:1112:ASP:OD2	2.43	0.52
1:A:1180:ARG:O	1:A:1181:GLU:HG2	2.10	0.52
1:A:3037:GLU:O	1:A:3040:THR:OG1	2.26	0.52
1:B:830:ARG:NH2	1:B:832:GLU:OE2	2.38	0.52
1:B:1208:VAL:HA	1:B:1211:LEU:HD12	1.91	0.52
1:B:3545:THR:HG23	1:B:3548:GLU:H	1.74	0.52
1:C:1152:MET:HB2	1:C:1161:ILE:O	2.09	0.52
1:C:1277:TRP:CD1	1:C:1277:TRP:O	2.63	0.52
1:D:644:ILE:HD11	1:D:1615:VAL:HG21	1.92	0.52
1:D:1110:ARG:NH2	1:D:1112:ASP:OD2	2.43	0.52
1:D:1172:ASP:OD1	1:D:1172:ASP:N	2.43	0.52
1:D:5004:THR:OG1	1:D:5005:GLY:N	2.42	0.52
1:A:416:LYS:HD3	1:A:416:LYS:C	2.30	0.51
1:A:4633:GLU:HG2	1:A:4635:SER:H	1.75	0.51
1:C:984:LEU:O	1:C:988:LEU:HG	2.09	0.51
1:C:4055:VAL:HA	1:C:4058:ILE:HD12	1.92	0.51
1:D:3417:ASP:OD1	1:D:3417:ASP:N	2.40	0.51
1:A:976:ARG:HA	1:A:1044:ARG:HH12	1.74	0.51
1:A:2420:HIS:CE1	1:A:2424:SER:HB3	2.45	0.51
1:B:961:MET:CE	1:B:963:ASN:H	2.23	0.51
1:D:284:HIS:ND1	1:D:287:THR:OG1	2.34	0.51
1:D:1208:VAL:HA	1:D:1211:LEU:HD12	1.93	0.51
1:D:1504:GLY:O	1:D:1508:ARG:NH1	2.40	0.51
1:A:3110:LEU:HD12	1:A:3175:LEU:HD11	1.92	0.51
1:C:871:ARG:NH2	1:C:922:LEU:HB2	2.24	0.51
1:C:1562:ILE:HD12	1:C:1563:GLN:H	1.74	0.51
1:C:2420:HIS:CE1	1:C:2424:SER:HB3	2.46	0.51
1:D:3096:PHE:O	1:D:3100:SER:N	2.36	0.51
1:A:119:SER:OG	1:A:120:CYS:N	2.42	0.51
1:A:674:PHE:N	1:A:680:THR:OG1	2.42	0.51
1:A:1152:MET:HB2	1:A:1161:ILE:O	2.10	0.51
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.21	0.51
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.93	0.51
1:B:2154:SER:HB3	1:B:2188:ASN:HD21	1.75	0.51
1:B:3453:ARG:O	1:B:3457:ASN:ND2	2.43	0.51
1:C:1270:LEU:O	1:C:1564:PHE:N	2.36	0.51
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.78	0.51
1:D:1112:ASP:OD1	1:D:1112:ASP:N	2.36	0.51
1:D:4633:GLU:HG2	1:D:4635:SER:H	1.75	0.51
1:A:3065:VAL:O	1:A:3069:HIS:ND1	2.43	0.51
1:B:19:GLU:HB2	1:B:205:ILE:HB	1.91	0.51
1:B:1172:ASP:OD1	1:B:1172:ASP:N	2.44	0.51
1:B:4187:SER:OG	1:B:4191:GLU:OE2	2.27	0.51
1:B:4766:THR:HA	1:B:4769:MET:HE1	1.92	0.51
1:C:989:ALA:HA	1:C:1039:LEU:HG	1.92	0.51
1:D:745:SER:HB3	1:D:758:ARG:HB2	1.91	0.51
1:A:860:GLN:OE1	1:A:860:GLN:N	2.44	0.51
1:A:886:ARG:NH2	1:A:889:GLN:OE1	2.44	0.51
1:A:1078:GLU:OE1	1:A:1080:SER:OG	2.29	0.51
1:B:119:SER:OG	1:B:120:CYS:N	2.43	0.51
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.20	0.51
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.40	0.51
1:C:299:LEU:HD22	1:C:357:LEU:HD11	1.92	0.51
1:C:645:ARG:HD3	1:C:826:ILE:HG13	1.91	0.51
1:C:674:PHE:N	1:C:680:THR:OG1	2.36	0.51
1:C:686:TRP:NE1	1:C:746:CYS:SG	2.76	0.51
1:C:772:ASN:HD22	1:C:1471:ALA:H	1.59	0.51
1:C:2512:ILE:HG22	1:C:2516:ASP:HB3	1.91	0.51
1:C:3263:TYR:O	1:C:3267:PRO:HD2	2.11	0.51
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.43	0.51
1:D:452:PHE:O	1:D:528:SER:OG	2.24	0.51
1:D:1078:GLU:OE1	1:D:1080:SER:OG	2.29	0.51
1:D:4162:ASN:HA	1:D:4165:GLU:HG2	1.92	0.51
2:E:17:LYS:HG3	2:E:18:LYS:H	1.74	0.51
2:E:17:LYS:H	2:E:20:GLN:HE22	1.57	0.51
1:B:24:CYS:HB2	1:B:200:TRP:HA	1.92	0.51
1:B:181:HIS:CG	1:B:196:MET:HB2	2.46	0.51
1:B:1078:GLU:OE1	1:B:1080:SER:OG	2.29	0.51
1:B:2243:SER:OG	1:B:2245:GLN:OE1	2.29	0.51
1:B:5004:THR:OG1	1:B:5005:GLY:N	2.42	0.51
1:C:3453:ARG:O	1:C:3457:ASN:ND2	2.42	0.51
1:D:961:MET:CE	1:D:963:ASN:H	2.24	0.51
1:D:2243:SER:OG	1:D:2245:GLN:OE1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:ARG:HD3	1:A:826:ILE:HG13	1.93	0.51
1:A:895:PRO:HD2	1:A:903:LEU:HD23	1.93	0.51
1:A:2420:HIS:N	1:A:2492:ALA:O	2.43	0.51
1:B:1545:ASN:ND2	2:F:32:ASN:HD22	2.09	0.51
1:B:4633:GLU:HG2	1:B:4635:SER:H	1.76	0.51
1:C:320:LYS:HB3	1:C:356:TRP:NE1	2.26	0.51
1:C:1658:ASP:N	1:C:1658:ASP:OD1	2.41	0.51
1:A:554:LEU:HD23	1:A:1593:PRO:HD3	1.92	0.51
1:A:3969:ILE:HD13	1:A:4030:LEU:HD13	1.92	0.51
1:B:960:MET:SD	1:B:966:LYS:NZ	2.83	0.51
1:B:1110:ARG:NH2	1:B:1112:ASP:OD2	2.43	0.51
1:B:3666:ASP:OD1	1:B:3666:ASP:N	2.37	0.51
1:C:1139:PHE:CE1	1:C:1169:LEU:HD11	2.45	0.51
1:C:3337:ARG:HG2	1:C:3341:PHE:HE2	1.75	0.51
1:C:3965:LEU:HD22	1:C:3980:LEU:HD21	1.93	0.51
1:D:181:HIS:CG	1:D:196:MET:HB2	2.46	0.51
1:A:498:THR:H	1:A:503:PHE:HE2	1.57	0.51
1:A:2191:PHE:HA	1:A:2198:MET:HE3	1.92	0.51
1:A:4055:VAL:HA	1:A:4058:ILE:HD12	1.92	0.51
1:B:689:THR:HB	1:B:778:PHE:CZ	2.45	0.51
1:C:3395:ARG:HG2	1:C:3453:ARG:HH22	1.75	0.51
1:C:3579:LEU:HG	1:C:3581:GLY:H	1.76	0.51
2:G:48:PHE:CE1	2:G:55:VAL:HG21	2.46	0.51
1:A:3579:LEU:HG	1:A:3581:GLY:H	1.76	0.50
1:A:3965:LEU:HD22	1:A:3980:LEU:HD21	1.92	0.50
1:B:41:GLY:O	1:B:45:ARG:NH1	2.44	0.50
1:B:813:GLU:OE1	1:B:813:GLU:N	2.43	0.50
1:C:1284:VAL:HG22	1:C:1555:LEU:HD13	1.94	0.50
1:C:4187:SER:OG	1:C:4191:GLU:OE2	2.28	0.50
1:D:3037:GLU:O	1:D:3040:THR:OG1	2.25	0.50
1:A:668:VAL:HB	1:A:742:ASP:OD1	2.12	0.50
1:A:1717:SER:HA	1:A:1721:GLU:HB2	1.92	0.50
1:B:107:ILE:N	1:B:148:TRP:O	2.40	0.50
1:B:986:ASP:OD1	1:B:986:ASP:N	2.42	0.50
1:B:3674:ILE:HG13	1:B:3732:SER:HB2	1.92	0.50
1:C:990:GLU:HG2	1:C:1024:TYR:CE2	2.46	0.50
1:C:1717:SER:HA	1:C:1721:GLU:HB2	1.93	0.50
1:A:681:HIS:O	1:A:783:PHE:HA	2.10	0.50
1:A:989:ALA:HA	1:A:1039:LEU:HG	1.93	0.50
1:B:1452:TRP:HE1	1:B:1518:CYS:HB3	1.76	0.50
1:D:4187:SER:OG	1:D:4191:GLU:OE2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:HB3	1:A:356:TRP:NE1	2.27	0.50
1:A:1160:ILE:HB	1:A:1179:PHE:HD2	1.75	0.50
1:A:2104:ARG:NH1	1:A:2108:GLU:OE2	2.43	0.50
1:A:2474:LEU:HA	1:A:2494:PHE:CD2	2.46	0.50
1:B:645:ARG:HD3	1:B:826:ILE:HG13	1.93	0.50
1:C:1263:THR:N	1:C:1266:THR:O	2.38	0.50
1:C:4958:CYS:SG	1:C:4983:HIS:HD2	2.34	0.50
1:D:1263:THR:N	1:D:1266:THR:O	2.38	0.50
1:A:3645:PRO:HG2	1:A:3648:ARG:HH11	1.77	0.50
1:B:1289:LEU:HD12	1:B:1550:PRO:HG2	1.94	0.50
1:B:3927:GLN:HE21	1:B:3991:GLY:HA3	1.76	0.50
1:C:1288:PHE:HE1	1:C:1598:GLN:HB2	1.77	0.50
1:C:3927:GLN:HE21	1:C:3991:GLY:HA3	1.77	0.50
1:C:4008:SER:OG	1:C:4009:GLN:OE1	2.26	0.50
1:D:718:GLY:HA3	1:D:737:LEU:HA	1.93	0.50
1:D:1717:SER:HA	1:D:1721:GLU:HB2	1.93	0.50
1:D:3065:VAL:O	1:D:3069:HIS:ND1	2.45	0.50
1:A:41:GLY:O	1:A:45:ARG:NH1	2.44	0.50
1:A:284:HIS:ND1	1:A:287:THR:OG1	2.34	0.50
1:A:4003:LEU:HD21	1:A:4012:LEU:HB3	1.93	0.50
1:C:1078:GLU:OE1	1:C:1080:SER:OG	2.29	0.50
1:C:1110:ARG:NH2	1:C:1112:ASP:OD2	2.43	0.50
1:C:4820:VAL:HG23	1:C:4821:LYS:N	2.24	0.50
1:D:4820:VAL:HG23	1:D:4821:LYS:N	2.24	0.50
2:E:48:PHE:CE1	2:E:55:VAL:HG21	2.47	0.50
1:A:1289:LEU:HD12	1:A:1550:PRO:HG2	1.94	0.50
1:A:2440:MET:SD	1:A:2442:LEU:N	2.84	0.50
1:A:3263:TYR:O	1:A:3267:PRO:HD2	2.12	0.50
1:B:307:ALA:HB1	1:B:312:THR:HG21	1.94	0.50
1:B:1263:THR:HG22	1:B:1266:THR:HB	1.94	0.50
1:B:1717:SER:HA	1:B:1721:GLU:HB2	1.93	0.50
1:C:884:LEU:HG	1:C:959:TYR:HE2	1.77	0.50
1:C:2243:SER:OG	1:C:2245:GLN:OE1	2.29	0.50
1:D:299:LEU:HD22	1:D:357:LEU:HD11	1.94	0.50
1:D:498:THR:H	1:D:503:PHE:HE2	1.59	0.50
1:D:4908:GLU:O	1:D:4908:GLU:HG2	2.12	0.50
2:H:30:LEU:HD21	2:H:92:PRO:HD2	1.93	0.50
1:A:3927:GLN:HE21	1:A:3991:GLY:HA3	1.77	0.50
1:B:144:GLU:O	1:B:175:SER:OG	2.26	0.50
1:B:4003:LEU:HD21	1:B:4012:LEU:HB3	1.93	0.50
1:C:1172:ASP:OD1	1:C:1172:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2963:LEU:HA	1:C:2966:TRP:HB2	1.93	0.50
1:D:320:LYS:HB3	1:D:356:TRP:NE1	2.27	0.50
1:D:2154:SER:HB3	1:D:2188:ASN:HD21	1.76	0.50
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.45	0.50
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.30	0.50
1:A:1155:LEU:H	1:A:1155:LEU:HD12	1.77	0.50
1:B:72:SER:O	1:B:105:HIS:ND1	2.45	0.50
1:B:2104:ARG:NH1	1:B:2108:GLU:OE2	2.44	0.50
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.38	0.50
1:C:1208:VAL:HA	1:C:1211:LEU:HD12	1.94	0.50
1:C:1644:GLU:OE1	1:C:1646:ARG:NE	2.43	0.50
1:C:3969:ILE:HD13	1:C:4030:LEU:HD13	1.92	0.50
1:D:3965:LEU:HD22	1:D:3980:LEU:HD21	1.94	0.50
2:F:14:THR:OG1	2:F:68:LEU:N	2.45	0.50
1:A:502:HIS:CE1	1:A:1263:THR:HA	2.47	0.49
1:A:4820:VAL:HG23	1:A:4821:LYS:N	2.25	0.49
1:B:895:PRO:HD2	1:B:903:LEU:HD23	1.94	0.49
1:C:3645:PRO:HG2	1:C:3648:ARG:HH11	1.77	0.49
1:D:2104:ARG:NH1	1:D:2108:GLU:OE2	2.43	0.49
1:B:1288:PHE:HE1	1:B:1598:GLN:HB2	1.77	0.49
1:B:1424:PRO:HA	1:B:1427:ILE:HG22	1.94	0.49
1:B:3677:LEU:HD22	1:B:3697:PRO:HG3	1.95	0.49
1:C:1289:LEU:HD12	1:C:1550:PRO:HG2	1.94	0.49
1:C:2187:ASN:OD1	1:C:2187:ASN:N	2.44	0.49
1:C:3390:GLY:HA2	1:C:3393:LEU:HD12	1.95	0.49
1:D:2591:ARG:O	1:D:2594:SER:OG	2.30	0.49
1:A:1703:LEU:HD23	1:A:1704:PRO:HD2	1.93	0.49
1:B:4696:ASP:OD1	1:B:4696:ASP:N	2.39	0.49
1:C:181:HIS:CG	1:C:196:MET:HB2	2.47	0.49
1:C:2104:ARG:NH1	1:C:2108:GLU:OE2	2.45	0.49
1:D:822:ARG:NH2	1:D:824:GLU:OE1	2.46	0.49
1:D:3927:GLN:HE21	1:D:3991:GLY:HA3	1.77	0.49
1:A:4908:GLU:O	1:A:4908:GLU:HG2	2.12	0.49
1:B:1277:TRP:O	1:B:1277:TRP:CD1	2.65	0.49
1:C:1155:LEU:H	1:C:1155:LEU:HD12	1.77	0.49
1:D:3695:PRO:HD2	1:D:3699:HIS:HB2	1.94	0.49
1:A:4878:ASP:OD1	1:A:4878:ASP:N	2.44	0.49
1:B:649:PHE:HE2	1:B:845:CYS:HB2	1.76	0.49
1:B:1703:LEU:HD23	1:B:1704:PRO:HD2	1.94	0.49
1:B:2474:LEU:HA	1:B:2494:PHE:HD2	1.76	0.49
1:C:252:VAL:HB	1:C:257:ARG:HH12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2556:LEU:HD21	1:C:2597:LYS:HA	1.95	0.49
1:D:224:HIS:HE2	1:D:386:ASP:HA	1.78	0.49
1:A:1087:ARG:NE	1:A:1222:GLY:O	2.46	0.49
1:A:1208:VAL:HA	1:A:1211:LEU:HD12	1.94	0.49
1:A:3136:LEU:HA	1:A:3139:VAL:HG22	1.94	0.49
1:A:3535:LEU:HD23	1:A:3535:LEU:H	1.77	0.49
1:A:3677:LEU:HG	1:A:3697:PRO:HG2	1.94	0.49
1:B:4878:ASP:OD1	1:B:4878:ASP:N	2.44	0.49
1:C:668:VAL:HB	1:C:742:ASP:OD1	2.13	0.49
1:D:4958:CYS:SG	1:D:4983:HIS:HD2	2.35	0.49
1:A:877:ASN:O	1:A:880:GLU:HG3	2.12	0.49
1:A:1270:LEU:O	1:A:1564:PHE:N	2.41	0.49
1:A:2431:ASP:OD1	1:A:2435:ARG:NE	2.46	0.49
1:B:320:LYS:HB3	1:B:356:TRP:NE1	2.27	0.49
1:B:684:VAL:HG12	1:B:781:VAL:HG12	1.95	0.49
1:B:990:GLU:HG2	1:B:1024:TYR:CZ	2.47	0.49
1:B:1112:ASP:OD1	1:B:1112:ASP:N	2.36	0.49
1:B:3535:LEU:HD23	1:B:3535:LEU:H	1.77	0.49
1:A:2098:VAL:HG11	1:A:2127:GLN:HG3	1.95	0.49
1:B:3698:LEU:HD12	1:B:3773:ARG:HG3	1.95	0.49
1:B:3965:LEU:HD22	1:B:3980:LEU:HD21	1.94	0.49
1:B:4000:MET:HE1	1:B:4058:ILE:HG12	1.95	0.49
1:C:41:GLY:O	1:C:45:ARG:NH1	2.46	0.49
1:A:307:ALA:HB1	1:A:312:THR:HG21	1.94	0.49
1:A:3395:ARG:HG2	1:A:3453:ARG:HH22	1.78	0.49
1:B:810:PRO:HD2	1:B:813:GLU:OE1	2.13	0.49
1:C:144:GLU:O	1:C:175:SER:OG	2.26	0.49
1:C:2657:LEU:N	1:C:2658:PRO:HD2	2.28	0.49
1:D:3395:ARG:HG2	1:D:3453:ARG:HH22	1.78	0.49
1:A:822:ARG:NH2	1:A:824:GLU:OE1	2.45	0.49
1:B:2325:PRO:HB3	1:B:2422:ILE:HA	1.94	0.49
1:B:3695:PRO:HD2	1:B:3699:HIS:HB2	1.95	0.49
1:C:644:ILE:HD11	1:C:1615:VAL:HG21	1.95	0.49
1:C:2474:LEU:HA	1:C:2494:PHE:HD2	1.78	0.49
1:D:668:VAL:HB	1:D:742:ASP:OD1	2.13	0.49
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.31	0.49
1:D:1459:GLN:NE2	1:D:1461:ASP:HB2	2.27	0.49
1:D:2950:SER:HB3	1:D:2954:ARG:HH21	1.78	0.49
1:D:4115:SER:OG	1:D:4116:GLU:N	2.46	0.49
1:A:649:PHE:HE2	1:A:845:CYS:HB2	1.78	0.48
1:B:252:VAL:HB	1:B:257:ARG:HH12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:ARG:NH2	1:B:824:GLU:OE1	2.46	0.48
1:B:971:ASP:O	1:B:974:HIS:NE2	2.46	0.48
1:B:2431:ASP:O	1:B:2435:ARG:HG2	2.13	0.48
1:B:2657:LEU:N	1:B:2658:PRO:HD2	2.28	0.48
1:C:1047:LEU:HD12	1:C:1053:ILE:HD12	1.95	0.48
1:C:3427:PRO:HG2	1:C:3579:LEU:HD12	1.95	0.48
1:D:1703:LEU:HD23	1:D:1704:PRO:HD2	1.93	0.48
1:D:2282:ASP:OD1	1:D:2282:ASP:N	2.46	0.48
1:D:2440:MET:HG3	1:D:2441:HIS:H	1.78	0.48
1:D:3390:GLY:HA2	1:D:3393:LEU:HD12	1.95	0.48
2:F:14:THR:HG21	2:F:68:LEU:HB2	1.95	0.48
1:A:689:THR:HB	1:A:778:PHE:CZ	2.48	0.48
1:A:993:HIS:ND1	1:A:1023:PRO:O	2.45	0.48
1:B:284:HIS:HD1	1:B:287:THR:HG1	1.56	0.48
1:B:1930:LYS:HE3	1:B:1930:LYS:HB3	1.69	0.48
1:B:3409:TYR:CE2	1:B:3510:ILE:HG23	2.48	0.48
1:C:1459:GLN:NE2	1:C:1461:ASP:HB2	2.27	0.48
1:D:144:GLU:O	1:D:175:SER:OG	2.24	0.48
1:D:307:ALA:HB1	1:D:312:THR:HG21	1.94	0.48
1:D:2191:PHE:HA	1:D:2198:MET:HE3	1.95	0.48
1:D:2953:LYS:HA	1:D:2957:PHE:HB3	1.94	0.48
1:A:813:GLU:HG3	1:A:1009:ALA:H	1.77	0.48
1:A:2282:ASP:OD1	1:A:2282:ASP:N	2.46	0.48
1:B:668:VAL:HB	1:B:742:ASP:OD1	2.14	0.48
1:B:977:LEU:HG	1:B:1044:ARG:HH11	1.77	0.48
1:B:3133:THR:HA	1:B:3137:LEU:HD12	1.94	0.48
1:C:294:THR:HG23	1:C:297:GLN:H	1.78	0.48
1:C:1112:ASP:OD1	1:C:1112:ASP:N	2.37	0.48
1:C:2154:SER:HB3	1:C:2188:ASN:HD21	1.78	0.48
1:D:689:THR:OG1	1:D:689:THR:O	2.30	0.48
1:D:1087:ARG:NE	1:D:1222:GLY:O	2.45	0.48
1:D:3263:TYR:O	1:D:3267:PRO:HD2	2.13	0.48
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.31	0.48
1:B:2191:PHE:HA	1:B:2198:MET:HE3	1.95	0.48
1:B:3645:PRO:HG2	1:B:3648:ARG:HH11	1.77	0.48
1:D:753:PRO:HB2	1:D:771:PHE:CD2	2.49	0.48
1:D:1277:TRP:O	1:D:1277:TRP:CD1	2.66	0.48
1:A:978:THR:HG22	1:A:979:PRO:HD2	1.95	0.48
1:A:2657:LEU:N	1:A:2658:PRO:HD2	2.28	0.48
1:B:653:ALA:HB2	1:B:848:HIS:HD2	1.79	0.48
1:B:4115:SER:OG	1:B:4116:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:875:ALA:HB1	1:C:910:PHE:CZ	2.48	0.48
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.31	0.48
1:C:2814:LYS:HD3	1:C:2814:LYS:HA	1.66	0.48
1:C:3245:VAL:HG12	1:C:3247:ASP:H	1.77	0.48
1:D:252:VAL:HB	1:D:257:ARG:HH12	1.78	0.48
1:D:920:TYR:HD1	1:D:923:GLN:HE21	1.62	0.48
1:D:3068:LEU:HA	1:D:3071:LEU:HB2	1.95	0.48
1:D:3794:VAL:HG21	1:D:3835:LEU:HD11	1.96	0.48
2:E:53:GLN:HG2	2:E:54:GLU:N	2.29	0.48
2:H:38:SER:OG	2:H:41:ASP:OD2	2.30	0.48
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.96	0.48
1:B:3068:LEU:HA	1:B:3071:LEU:HB2	1.96	0.48
1:C:677:ALA:HB1	2:G:40:ARG:HB3	1.96	0.48
1:C:2384:ILE:O	1:C:2388:GLU:HG2	2.14	0.48
1:C:4908:GLU:HG2	1:C:4908:GLU:O	2.14	0.48
1:D:2384:ILE:O	1:D:2388:GLU:HG2	2.13	0.48
2:E:30:LEU:N	2:E:34:LYS:O	2.46	0.48
1:A:718:GLY:HA3	1:A:737:LEU:HA	1.95	0.48
1:A:750:LEU:C	1:A:752:VAL:H	2.16	0.48
1:A:1772:ARG:NH2	1:A:1952:GLN:OE1	2.46	0.48
1:A:2506:LEU:HD12	1:A:2510:TYR:HB2	1.96	0.48
1:A:3794:VAL:HG21	1:A:3835:LEU:HD11	1.96	0.48
1:A:4166:LEU:HD23	1:A:4166:LEU:H	1.78	0.48
1:B:1087:ARG:NE	1:B:1222:GLY:O	2.46	0.48
1:C:102:LEU:HB3	1:C:105:HIS:CD2	2.49	0.48
1:D:49:LEU:HD11	1:D:191:VAL:HG23	1.95	0.48
1:D:416:LYS:HD3	1:D:416:LYS:C	2.34	0.48
1:D:1284:VAL:HG22	1:D:1555:LEU:HD13	1.95	0.48
1:D:1868:PRO:O	1:D:1872:THR:OG1	2.24	0.48
1:D:3535:LEU:HD23	1:D:3535:LEU:H	1.79	0.48
2:F:17:LYS:H	2:F:20:GLN:HE22	1.60	0.48
1:A:1435:TYR:HE1	1:A:1452:TRP:CZ2	2.32	0.48
1:A:4000:MET:HE2	1:A:4058:ILE:HG12	1.95	0.48
1:B:1093:GLU:HG2	1:B:1148:VAL:HG12	1.96	0.48
1:B:1833:SER:OG	1:B:1834:VAL:N	2.47	0.48
1:B:3065:VAL:O	1:B:3069:HIS:ND1	2.47	0.48
1:B:4767:TRP:O	1:B:4770:SER:OG	2.26	0.48
1:C:1220:GLN:NE2	1:D:3519:PRO:O	2.45	0.48
1:D:919:ASN:O	1:D:923:GLN:HG2	2.13	0.48
1:D:2355:ARG:HB3	1:D:2359:ARG:HH21	1.79	0.48
1:D:3645:PRO:HG2	1:D:3648:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:ILE:HB	1:A:930:LYS:HZ1	1.79	0.48
1:A:1217:CYS:SG	1:A:1218:GLY:N	2.86	0.48
1:A:1700:ASP:HB3	1:A:1703:LEU:HD12	1.96	0.48
1:A:1833:SER:OG	1:A:1834:VAL:N	2.47	0.48
1:A:3032:SER:N	1:A:3035:GLU:OE1	2.45	0.48
1:A:3319:ILE:HG13	1:A:3338:LEU:HD21	1.95	0.48
1:A:4059:LEU:HD21	1:A:4143:VAL:HG11	1.95	0.48
1:B:54:ASN:HD22	1:B:57:ASN:HD21	1.60	0.48
1:B:868:GLU:HA	1:B:871:ARG:HG3	1.95	0.48
1:B:4059:LEU:HD21	1:B:4143:VAL:HG11	1.96	0.48
1:B:4958:CYS:SG	1:B:4983:HIS:HD2	2.37	0.48
1:C:822:ARG:NH2	1:C:824:GLU:OE1	2.46	0.48
1:C:4003:LEU:HD21	1:C:4012:LEU:HB3	1.95	0.48
1:C:4115:SER:OG	1:C:4116:GLU:N	2.46	0.48
1:C:4878:ASP:OD1	1:C:4878:ASP:N	2.44	0.48
1:D:1018:ASN:OD1	1:D:1020:ARG:NE	2.46	0.48
1:D:1087:ARG:HB3	1:D:1223:PHE:CD1	2.49	0.48
1:D:1486:SER:O	1:D:1486:SER:OG	2.30	0.48
1:D:2098:VAL:HG11	1:D:2127:GLN:HG3	1.96	0.48
1:D:2506:LEU:HD12	1:D:2510:TYR:HB2	1.95	0.48
1:D:2657:LEU:N	1:D:2658:PRO:HD2	2.28	0.48
1:A:252:VAL:HB	1:A:257:ARG:HH12	1.78	0.48
1:A:571:SER:O	1:A:571:SER:OG	2.32	0.48
1:B:1520:VAL:HG12	1:B:1527:MET:HG2	1.96	0.48
1:B:2282:ASP:N	1:B:2282:ASP:OD1	2.46	0.48
1:B:2506:LEU:HD12	1:B:2510:TYR:HB2	1.95	0.48
1:B:4908:GLU:HG2	1:B:4908:GLU:O	2.12	0.48
1:C:1443:GLN:NE2	1:C:1444:GLU:O	2.44	0.48
1:C:1833:SER:OG	1:C:1834:VAL:N	2.47	0.48
1:C:3051:ARG:HG3	1:C:3052:HIS:H	1.79	0.48
1:D:1833:SER:OG	1:D:1834:VAL:N	2.47	0.48
1:A:3198:ALA:HB1	1:A:3280:TYR:HB2	1.95	0.47
1:A:4115:SER:OG	1:A:4116:GLU:N	2.46	0.47
1:A:4696:ASP:OD1	1:A:4696:ASP:N	2.38	0.47
1:B:277:GLY:HA2	1:B:315:CYS:SG	2.54	0.47
1:C:399:GLN:O	1:C:403:MET:HG3	2.14	0.47
1:C:2974:ILE:O	1:C:2978:GLU:N	2.43	0.47
1:C:3359:ILE:HD11	1:C:3434:LEU:HB2	1.96	0.47
1:D:892:THR:OG1	1:D:902:ARG:O	2.25	0.47
1:D:1289:LEU:HD12	1:D:1550:PRO:HG2	1.95	0.47
1:D:4059:LEU:HD21	1:D:4143:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:THR:HG21	2:G:68:LEU:HB2	1.95	0.47
1:B:224:HIS:HE2	1:B:386:ASP:HA	1.79	0.47
1:B:3395:ARG:HG2	1:B:3453:ARG:HH22	1.79	0.47
1:C:681:HIS:O	1:C:783:PHE:HA	2.14	0.47
1:C:861:ILE:O	1:C:930:LYS:NZ	2.44	0.47
1:C:1452:TRP:HE3	1:C:1548:LEU:HB3	1.79	0.47
1:C:2431:ASP:O	1:C:2435:ARG:HG2	2.14	0.47
1:D:689:THR:HB	1:D:778:PHE:HZ	1.79	0.47
1:D:1288:PHE:HE1	1:D:1598:GLN:HB2	1.79	0.47
1:A:299:LEU:HD22	1:A:357:LEU:HD11	1.95	0.47
1:A:359:TYR:HB2	1:A:383:HIS:HE1	1.78	0.47
1:A:2355:ARG:HB3	1:A:2359:ARG:HH21	1.79	0.47
1:A:3409:TYR:CE2	1:A:3510:ILE:HG23	2.48	0.47
1:B:416:LYS:C	1:B:416:LYS:HD3	2.34	0.47
1:B:3592:ILE:HA	1:B:3595:ARG:HE	1.79	0.47
1:C:571:SER:O	1:C:571:SER:OG	2.32	0.47
1:C:848:HIS:CE1	1:C:849:THR:HG23	2.49	0.47
1:C:1040:CYS:O	1:C:1044:ARG:HG2	2.13	0.47
1:C:1125:ASN:HB2	1:C:1132:TRP:HD1	1.79	0.47
1:D:3032:SER:N	1:D:3035:GLU:OE1	2.46	0.47
1:A:1644:GLU:OE1	1:A:1646:ARG:NE	2.43	0.47
1:A:2013:LYS:HE3	1:A:2031:LEU:HD23	1.95	0.47
1:B:1457:TYR:CZ	1:B:1459:GLN:HB2	2.48	0.47
1:B:2814:LYS:HD3	1:B:2814:LYS:HA	1.66	0.47
1:C:497:TYR:HA	1:C:503:PHE:CE2	2.50	0.47
1:C:877:ASN:O	1:C:880:GLU:HG3	2.14	0.47
1:C:1087:ARG:HB3	1:C:1223:PHE:CD1	2.49	0.47
1:C:2242:ILE:HG23	1:C:2246:ASN:HD22	1.80	0.47
1:C:2506:LEU:HD12	1:C:2510:TYR:HB2	1.95	0.47
1:C:3768:SER:HA	1:C:3771:HIS:ND1	2.30	0.47
2:F:53:GLN:HG2	2:F:54:GLU:N	2.29	0.47
2:H:53:GLN:HG2	2:H:54:GLU:N	2.28	0.47
1:A:2556:LEU:HD21	1:A:2597:LYS:HA	1.96	0.47
1:A:2963:LEU:HA	1:A:2966:TRP:HB2	1.96	0.47
1:B:595:ARG:NH2	1:B:1643:GLU:OE1	2.46	0.47
1:B:898:ASP:O	1:B:901:LYS:N	2.43	0.47
2:G:53:GLN:HG2	2:G:54:GLU:N	2.29	0.47
1:A:24:CYS:HB2	1:A:200:TRP:HA	1.96	0.47
1:A:1087:ARG:HB3	1:A:1223:PHE:CD1	2.49	0.47
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.96	0.47
1:B:1155:LEU:HD12	1:B:1155:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2094:LEU:O	1:B:2098:VAL:HG12	2.14	0.47
1:B:2983:SER:O	1:B:2983:SER:OG	2.30	0.47
1:C:630:GLU:HA	1:C:1642:PRO:HB2	1.96	0.47
1:C:3068:LEU:HA	1:C:3071:LEU:HB2	1.97	0.47
1:D:772:ASN:ND2	1:D:1471:ALA:H	2.10	0.47
1:D:1700:ASP:HB3	1:D:1703:LEU:HD12	1.96	0.47
1:D:2242:ILE:HG23	1:D:2246:ASN:HD22	1.80	0.47
1:A:224:HIS:HE2	1:A:386:ASP:HA	1.79	0.47
1:A:1011:GLN:NE2	1:A:1013:ILE:HG12	2.29	0.47
1:A:1277:TRP:CD1	1:A:1277:TRP:O	2.67	0.47
1:A:2257:LEU:HD21	1:A:2275:VAL:HG13	1.96	0.47
1:A:2310:CYS:HB3	1:A:2313:LEU:HD23	1.97	0.47
1:B:913:LEU:HB2	1:B:918:ARG:HG2	1.96	0.47
1:B:1217:CYS:SG	1:B:1218:GLY:N	2.87	0.47
1:B:2013:LYS:HE3	1:B:2031:LEU:HD23	1.96	0.47
1:B:2384:ILE:O	1:B:2388:GLU:HG2	2.13	0.47
1:B:2389:ASP:N	1:B:2390:PRO:HD3	2.30	0.47
1:B:3003:LEU:HD12	1:B:3004:PRO:CD	2.40	0.47
1:B:3037:GLU:O	1:B:3040:THR:OG1	2.27	0.47
1:B:3136:LEU:HA	1:B:3139:VAL:HG22	1.97	0.47
1:B:3263:TYR:O	1:B:3267:PRO:HD2	2.13	0.47
1:C:205:ILE:CG2	1:C:206:CYS:H	2.27	0.47
1:C:1000:ARG:HB3	1:C:1005:TRP:HB2	1.95	0.47
1:C:3842:LEU:O	1:C:3929:SER:OG	2.28	0.47
1:D:277:GLY:HA2	1:D:315:CYS:SG	2.55	0.47
1:D:877:ASN:O	1:D:880:GLU:HG3	2.15	0.47
1:D:1708:ARG:NH1	1:D:1836:PHE:O	2.47	0.47
1:D:2389:ASP:N	1:D:2390:PRO:HD3	2.30	0.47
1:D:4000:MET:HE2	1:D:4058:ILE:HG12	1.97	0.47
2:H:22:CYS:O	2:H:48:PHE:N	2.48	0.47
1:A:1452:TRP:HE1	1:A:1518:CYS:HB3	1.79	0.47
1:A:3842:LEU:O	1:A:3929:SER:OG	2.28	0.47
1:B:2310:CYS:HB3	1:B:2313:LEU:HD23	1.97	0.47
1:B:3768:SER:HA	1:B:3771:HIS:ND1	2.29	0.47
1:C:1018:ASN:OD1	1:C:1020:ARG:NH1	2.48	0.47
1:D:2431:ASP:O	1:D:2435:ARG:HG2	2.15	0.47
1:D:3768:SER:HA	1:D:3771:HIS:ND1	2.29	0.47
1:D:4159:ARG:HA	1:D:4162:ASN:HD21	1.80	0.47
1:A:772:ASN:ND2	1:A:1471:ALA:H	2.13	0.47
1:A:2431:ASP:O	1:A:2435:ARG:HG2	2.15	0.47
1:A:2500:ALA:HB1	1:A:2550:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3359:ILE:HD11	1:A:3434:LEU:HB2	1.97	0.47
1:A:4034:ASN:HD21	1:A:4153:HIS:CE1	2.33	0.47
1:B:399:GLN:O	1:B:403:MET:HG3	2.15	0.47
1:B:2440:MET:SD	1:B:2442:LEU:N	2.88	0.47
1:B:2963:LEU:HA	1:B:2966:TRP:HB2	1.97	0.47
1:C:895:PRO:HG2	1:C:896:VAL:HG23	1.96	0.47
1:C:1703:LEU:HD23	1:C:1704:PRO:HD2	1.95	0.47
1:D:2102:VAL:HG11	1:D:2124:LEU:HB2	1.97	0.47
2:E:38:SER:OG	2:E:41:ASP:OD2	2.32	0.47
1:B:1700:ASP:HB3	1:B:1703:LEU:HD12	1.97	0.47
1:C:813:GLU:HG3	1:C:1009:ALA:H	1.80	0.47
1:C:2389:ASP:N	1:C:2390:PRO:HD3	2.29	0.47
1:D:1125:ASN:HB2	1:D:1132:TRP:HD1	1.79	0.47
1:D:2310:CYS:HB3	1:D:2313:LEU:HD23	1.97	0.47
2:F:30:LEU:N	2:F:34:LYS:O	2.48	0.47
2:H:57:LYS:HB3	2:H:57:LYS:HE2	1.75	0.47
1:A:2094:LEU:O	1:A:2098:VAL:HG12	2.15	0.46
1:A:4958:CYS:SG	1:A:4983:HIS:HD2	2.37	0.46
1:B:1087:ARG:HB3	1:B:1223:PHE:CD1	2.50	0.46
1:B:3390:GLY:HA2	1:B:3393:LEU:HD12	1.96	0.46
1:C:224:HIS:HE2	1:C:386:ASP:HA	1.80	0.46
1:C:307:ALA:HB1	1:C:312:THR:HG21	1.96	0.46
1:C:498:THR:H	1:C:503:PHE:HE2	1.62	0.46
1:C:1708:ARG:NH1	1:C:1836:PHE:O	2.48	0.46
1:C:2968:ASP:O	1:C:2971:GLN:NE2	2.32	0.46
1:C:4059:LEU:HD21	1:C:4143:VAL:HG11	1.96	0.46
1:A:630:GLU:HA	1:A:1642:PRO:HB2	1.98	0.46
1:A:915:GLU:HA	1:A:918:ARG:HB2	1.97	0.46
1:B:664:PHE:HB3	1:B:746:CYS:HB3	1.96	0.46
1:B:1270:LEU:O	1:B:1564:PHE:N	2.42	0.46
1:C:1277:TRP:O	1:C:1277:TRP:HD1	1.98	0.46
1:D:2441:HIS:HA	1:D:2444:GLN:HB3	1.96	0.46
1:D:3051:ARG:HD2	1:D:3051:ARG:HA	1.74	0.46
1:D:3409:TYR:CE2	1:D:3510:ILE:HG23	2.48	0.46
1:A:861:ILE:HB	1:A:930:LYS:NZ	2.30	0.46
1:A:1930:LYS:HE3	1:A:1930:LYS:HB3	1.70	0.46
1:A:3133:THR:HG23	1:A:3134:VAL:HG13	1.96	0.46
1:A:3141:THR:O	1:A:3145:GLN:HG2	2.14	0.46
1:C:750:LEU:C	1:C:752:VAL:H	2.18	0.46
1:C:3032:SER:N	1:C:3035:GLU:OE1	2.46	0.46
1:C:3409:TYR:CE2	1:C:3510:ILE:HG23	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:595:ARG:NH2	1:D:1643:GLU:OE1	2.48	0.46
1:D:884:LEU:HG	1:D:959:TYR:HE2	1.81	0.46
1:D:4034:ASN:HD21	1:D:4153:HIS:CE1	2.34	0.46
1:D:4878:ASP:OD1	1:D:4878:ASP:N	2.44	0.46
1:A:755:ILE:HG13	1:A:771:PHE:CZ	2.50	0.46
1:B:977:LEU:HG	1:B:1044:ARG:NH1	2.30	0.46
1:B:3107:VAL:HA	1:B:3110:LEU:HB2	1.97	0.46
1:B:3999:MET:HE1	1:B:4003:LEU:HD22	1.97	0.46
1:C:2094:LEU:O	1:C:2098:VAL:HG12	2.14	0.46
1:D:18:ASP:OD1	1:D:19:GLU:N	2.49	0.46
1:D:502:HIS:CE1	1:D:1263:THR:HA	2.50	0.46
1:D:2614:ILE:O	1:D:2618:MET:N	2.49	0.46
1:A:1288:PHE:HE1	1:A:1598:GLN:HB2	1.79	0.46
1:A:1452:TRP:HE3	1:A:1548:LEU:HB3	1.81	0.46
1:A:2983:SER:O	1:A:2983:SER:OG	2.29	0.46
1:B:292:ALA:O	1:B:299:LEU:HD12	2.16	0.46
1:B:299:LEU:HD22	1:B:357:LEU:HD11	1.96	0.46
1:C:861:ILE:HB	1:C:930:LYS:NZ	2.29	0.46
1:C:924:MET:HA	1:C:927:GLU:OE2	2.15	0.46
1:C:977:LEU:HG	1:C:1044:ARG:HH21	1.81	0.46
1:C:1087:ARG:NE	1:C:1222:GLY:O	2.47	0.46
1:D:1077:ALA:HB3	1:D:1190:PRO:HD2	1.98	0.46
2:G:22:CYS:SG	2:G:48:PHE:HB3	2.55	0.46
2:H:30:LEU:N	2:H:34:LYS:O	2.47	0.46
1:A:181:HIS:CG	1:A:196:MET:HB2	2.50	0.46
1:A:205:ILE:CG2	1:A:206:CYS:H	2.27	0.46
1:A:1470:ARG:HD3	1:A:1470:ARG:HA	1.70	0.46
1:C:3065:VAL:O	1:C:3069:HIS:ND1	2.48	0.46
1:D:441:VAL:HG13	1:D:518:ILE:HD11	1.97	0.46
1:D:913:LEU:HB2	1:D:918:ARG:HG2	1.98	0.46
1:A:2389:ASP:N	1:A:2390:PRO:HD3	2.31	0.46
1:A:3696:ASP:CG	1:A:3697:PRO:HD3	2.35	0.46
1:B:284:HIS:CE1	1:B:286:THR:HB	2.50	0.46
1:C:591:ASP:OD1	1:C:1594:ARG:NH1	2.48	0.46
1:C:1470:ARG:HD3	1:C:1470:ARG:HA	1.71	0.46
1:C:2282:ASP:OD1	1:C:2282:ASP:N	2.47	0.46
1:D:830:ARG:NE	1:D:1612:PHE:HE2	2.13	0.46
1:D:886:ARG:NH2	1:D:889:GLN:OE1	2.44	0.46
1:D:2906:VAL:HG11	1:D:2911:LEU:HA	1.97	0.46
2:H:44:LYS:HD2	2:H:44:LYS:HA	1.80	0.46
1:A:3768:SER:HA	1:A:3771:HIS:ND1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4159:ARG:HA	1:A:4162:ASN:HD21	1.81	0.46
1:B:830:ARG:HH12	1:B:832:GLU:HG3	1.81	0.46
1:B:2242:ILE:HG23	1:B:2246:ASN:HD22	1.80	0.46
1:C:772:ASN:ND2	1:C:1471:ALA:H	2.13	0.46
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.96	0.46
1:C:1452:TRP:CE3	1:C:1548:LEU:HB3	2.51	0.46
1:C:1772:ARG:NH2	1:C:1952:GLN:OE1	2.48	0.46
1:C:2310:CYS:HB3	1:C:2313:LEU:HD23	1.98	0.46
1:C:3845:ASN:N	1:C:3845:ASN:OD1	2.49	0.46
1:C:4109:GLN:HA	1:C:4112:LEU:HD12	1.97	0.46
1:D:1155:LEU:H	1:D:1155:LEU:HD12	1.80	0.46
1:D:1217:CYS:SG	1:D:1218:GLY:N	2.88	0.46
1:D:2094:LEU:O	1:D:2098:VAL:HG12	2.16	0.46
1:D:2431:ASP:OD1	1:D:2435:ARG:NE	2.46	0.46
1:A:2150:GLU:HA	1:A:2153:MET:HB2	1.98	0.46
1:A:3068:LEU:HA	1:A:3071:LEU:HB2	1.98	0.46
1:A:3390:GLY:HA2	1:A:3393:LEU:HD12	1.98	0.46
1:B:2556:LEU:HD21	1:B:2597:LYS:HA	1.97	0.46
1:B:3845:ASN:N	1:B:3845:ASN:OD1	2.49	0.46
1:B:4034:ASN:HD21	1:B:4153:HIS:CE1	2.34	0.46
1:C:284:HIS:ND1	1:C:287:THR:OG1	2.33	0.46
1:C:416:LYS:C	1:C:416:LYS:HD3	2.37	0.46
1:C:718:GLY:HA3	1:C:737:LEU:HA	1.96	0.46
1:D:924:MET:HA	1:D:927:GLU:OE2	2.15	0.46
1:D:1093:GLU:HG2	1:D:1148:VAL:HG12	1.98	0.46
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.97	0.46
1:D:1454:THR:OG1	1:D:1455:PRO:HD2	2.15	0.46
1:D:2556:LEU:HD21	1:D:2597:LYS:HA	1.97	0.46
1:D:3438:VAL:HG11	1:D:3517:MET:HE1	1.98	0.46
2:H:14:THR:HG21	2:H:68:LEU:HB2	1.98	0.46
1:A:359:TYR:HB2	1:A:383:HIS:CE1	2.51	0.46
1:A:595:ARG:NH2	1:A:1643:GLU:OE1	2.49	0.46
1:A:954:LYS:HA	1:A:954:LYS:HD2	1.79	0.46
1:A:2950:SER:HB3	1:A:2954:ARG:HH21	1.80	0.46
1:B:630:GLU:HA	1:B:1642:PRO:CB	2.45	0.46
1:B:861:ILE:O	1:B:930:LYS:NZ	2.48	0.46
1:B:3329:ILE:HG12	1:B:3332:ALA:HB2	1.97	0.46
1:C:168:ASP:HB3	1:C:199:LEU:HB3	1.97	0.46
1:C:284:HIS:CE1	1:C:286:THR:HB	2.51	0.46
1:C:886:ARG:NH2	1:C:889:GLN:OE1	2.47	0.46
1:D:630:GLU:HA	1:D:1642:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1767:VAL:HG12	1:D:1767:VAL:O	2.16	0.46
1:D:3133:THR:HG23	1:D:3134:VAL:HG13	1.98	0.46
1:A:871:ARG:NH2	1:A:922:LEU:HD23	2.31	0.45
1:A:1220:GLN:NE2	1:B:3519:PRO:O	2.47	0.45
1:A:2154:SER:HB3	1:A:2188:ASN:HD21	1.81	0.45
1:A:2242:ILE:HG23	1:A:2246:ASN:HD22	1.81	0.45
1:A:2491:SER:O	1:A:2491:SER:OG	2.31	0.45
1:B:755:ILE:HG13	1:B:771:PHE:CZ	2.51	0.45
1:B:1534:LYS:HA	1:B:1534:LYS:HD2	1.82	0.45
1:B:1708:ARG:NH1	1:B:1836:PHE:O	2.48	0.45
1:B:2591:ARG:O	1:B:2594:SER:OG	2.30	0.45
1:B:3032:SER:N	1:B:3035:GLU:OE1	2.45	0.45
1:B:4162:ASN:HA	1:B:4165:GLU:HG2	1.98	0.45
1:B:4586:PRO:HB3	1:B:4628:VAL:HG21	1.98	0.45
1:C:24:CYS:SG	1:C:198:THR:OG1	2.74	0.45
1:C:502:HIS:CE1	1:C:1263:THR:HA	2.51	0.45
1:C:3526:ALA:HB2	1:C:3595:ARG:HH12	1.81	0.45
2:F:22:CYS:SG	2:F:48:PHE:HB3	2.55	0.45
1:A:1022:VAL:HG23	1:A:1027:LEU:HG	1.98	0.45
1:A:3323:ILE:HD11	1:A:3338:LEU:HD22	1.99	0.45
1:B:263:GLU:HB3	1:B:281:ARG:HB2	1.99	0.45
1:B:1077:ALA:HB3	1:B:1190:PRO:HD2	1.98	0.45
1:B:1868:PRO:O	1:B:1872:THR:OG1	2.25	0.45
1:C:531:ARG:HA	1:C:566:CYS:SG	2.56	0.45
1:C:2474:LEU:HA	1:C:2494:PHE:CD2	2.52	0.45
1:C:3971:GLY:O	1:C:3973:CYS:N	2.49	0.45
1:D:1008:SER:HB3	1:D:1017:ARG:HB3	1.98	0.45
1:A:102:LEU:HD12	1:A:161:GLU:O	2.16	0.45
1:A:1077:ALA:HB3	1:A:1190:PRO:HD2	1.98	0.45
1:A:1708:ARG:NH1	1:A:1836:PHE:O	2.48	0.45
1:A:1868:PRO:O	1:A:1872:THR:OG1	2.25	0.45
1:A:2384:ILE:O	1:A:2388:GLU:HG2	2.17	0.45
1:A:3999:MET:HE3	1:A:4003:LEU:HB2	1.97	0.45
1:B:899:ASP:HB2	1:B:902:ARG:CZ	2.46	0.45
1:B:4181:ILE:HG22	1:B:4182:GLU:H	1.81	0.45
1:C:2500:ALA:HB1	1:C:2550:LEU:HD22	1.97	0.45
1:D:68:THR:HG23	1:D:110:ARG:HB2	1.99	0.45
1:D:399:GLN:O	1:D:403:MET:HG3	2.15	0.45
1:D:1270:LEU:O	1:D:1564:PHE:N	2.37	0.45
1:A:531:ARG:HA	1:A:566:CYS:SG	2.56	0.45
1:A:591:ASP:OD1	1:A:1594:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2906:VAL:HG11	1:A:2911:LEU:HA	1.99	0.45
1:A:3208:PRO:HD2	1:A:3245:VAL:HG22	1.98	0.45
1:A:3245:VAL:HG12	1:A:3247:ASP:H	1.81	0.45
1:A:3804:ILE:HD12	1:A:3804:ILE:HA	1.87	0.45
1:B:1767:VAL:O	1:B:1767:VAL:HG12	2.17	0.45
1:C:1077:ALA:HB3	1:C:1190:PRO:HD2	1.99	0.45
1:C:1275:ARG:HG3	1:C:1276:THR:HG23	1.97	0.45
1:D:684:VAL:HG12	1:D:781:VAL:HG12	1.99	0.45
1:D:755:ILE:HG13	1:D:771:PHE:CZ	2.52	0.45
2:H:48:PHE:CE1	2:H:55:VAL:HG21	2.51	0.45
1:A:269:TRP:CD1	1:A:272:SER:HB2	2.52	0.45
1:A:284:HIS:CE1	1:A:286:THR:HB	2.52	0.45
1:A:1521:ASP:OD1	1:A:1524:THR:OG1	2.31	0.45
1:B:168:ASP:HB3	1:B:199:LEU:HB3	1.99	0.45
1:B:2614:ILE:O	1:B:2618:MET:N	2.49	0.45
1:C:269:TRP:NE1	1:C:333:GLY:O	2.50	0.45
1:C:441:VAL:HG13	1:C:518:ILE:HD11	1.97	0.45
1:C:1435:TYR:HE1	1:C:1452:TRP:CZ2	2.34	0.45
1:C:3107:VAL:HA	1:C:3110:LEU:HB2	1.97	0.45
1:D:2474:LEU:HA	1:D:2494:PHE:HD2	1.82	0.45
2:E:22:CYS:SG	2:E:48:PHE:HB3	2.57	0.45
1:A:430:PRO:HB2	1:A:509:GLU:HB2	1.99	0.45
1:A:899:ASP:HB2	1:A:902:ARG:CZ	2.47	0.45
1:A:1520:VAL:HG12	1:A:1527:MET:HG2	1.97	0.45
1:B:2974:ILE:O	1:B:2978:GLU:N	2.46	0.45
1:B:3068:LEU:H	1:B:3068:LEU:HD12	1.82	0.45
1:C:1562:ILE:HD12	1:C:1563:GLN:N	2.32	0.45
1:C:2191:PHE:HA	1:C:2198:MET:HE3	1.98	0.45
1:C:2983:SER:O	1:C:2983:SER:OG	2.29	0.45
1:C:3003:LEU:HD12	1:C:3004:PRO:CD	2.40	0.45
1:D:4181:ILE:HG22	1:D:4182:GLU:H	1.82	0.45
1:A:2442:LEU:HG	1:A:2443:ILE:HG12	1.98	0.45
1:A:3526:ALA:HB2	1:A:3595:ARG:HH12	1.82	0.45
1:B:875:ALA:HB1	1:B:910:PHE:CZ	2.51	0.45
1:B:959:TYR:HB3	1:B:967:PRO:HD2	1.98	0.45
1:B:1263:THR:N	1:B:1266:THR:O	2.47	0.45
1:C:263:GLU:HB3	1:C:281:ARG:HB2	1.98	0.45
1:C:977:LEU:CG	1:C:1044:ARG:HH21	2.30	0.45
1:D:871:ARG:HH22	1:D:922:LEU:HD13	1.80	0.45
1:D:894:GLY:HA3	1:D:903:LEU:HD22	1.98	0.45
1:D:986:ASP:HB3	1:D:1036:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1008:SER:HB2	1:D:1017:ARG:NH2	2.32	0.45
1:D:3319:ILE:HG13	1:D:3338:LEU:HD21	1.97	0.45
1:D:3524:MET:H	1:D:3524:MET:HG2	1.57	0.45
2:F:38:SER:OG	2:F:41:ASP:OD2	2.31	0.45
2:G:80:VAL:HG23	2:G:80:VAL:O	2.16	0.45
1:A:3995:VAL:O	1:A:3999:MET:HB2	2.17	0.45
1:A:4181:ILE:HG22	1:A:4182:GLU:H	1.81	0.45
1:B:269:TRP:NE1	1:B:333:GLY:O	2.49	0.45
1:C:479:GLN:O	1:C:479:GLN:NE2	2.50	0.45
1:C:961:MET:HE3	1:C:961:MET:H	1.82	0.45
1:C:1434:TYR:HA	1:C:1519:LEU:HD23	1.98	0.45
1:C:2442:LEU:HG	1:C:2443:ILE:HG12	1.99	0.45
1:C:3794:VAL:HG21	1:C:3835:LEU:HD11	1.99	0.45
1:C:4181:ILE:HG22	1:C:4182:GLU:H	1.82	0.45
1:D:430:PRO:HB2	1:D:509:GLU:HB2	1.98	0.45
1:D:531:ARG:HA	1:D:566:CYS:SG	2.56	0.45
2:F:48:PHE:CE1	2:F:55:VAL:HG21	2.51	0.45
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.84	0.45
1:A:681:HIS:NE2	1:A:683:ARG:HD2	2.32	0.45
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.97	0.45
1:A:3347:SER:O	1:A:3347:SER:OG	2.29	0.45
1:B:760:ASN:N	1:B:760:ASN:OD1	2.49	0.45
1:B:915:GLU:HA	1:B:918:ARG:HB2	1.98	0.45
1:B:924:MET:HA	1:B:927:GLU:OE2	2.16	0.45
1:B:1000:ARG:HB3	1:B:1005:TRP:HB2	1.98	0.45
1:C:417:GLY:O	1:C:420:SER:OG	2.35	0.45
1:C:2013:LYS:HE3	1:C:2031:LEU:HD23	1.97	0.45
1:D:1770:SER:OG	1:D:1956:GLU:OE2	2.28	0.45
1:D:4848:VAL:O	1:D:4852:THR:OG1	2.32	0.45
1:A:103:TYR:HB2	1:A:161:GLU:O	2.17	0.45
1:A:292:ALA:O	1:A:299:LEU:HD12	2.17	0.45
1:A:1172:ASP:OD1	1:A:1172:ASP:N	2.44	0.45
1:A:1767:VAL:O	1:A:1767:VAL:HG12	2.17	0.45
1:B:2474:LEU:HA	1:B:2494:PHE:CD2	2.50	0.45
1:C:1093:GLU:HG2	1:C:1148:VAL:HG12	1.99	0.45
1:C:1217:CYS:SG	1:C:1218:GLY:N	2.90	0.45
1:C:1767:VAL:O	1:C:1767:VAL:HG12	2.17	0.45
1:D:266:ARG:NH2	1:D:331:VAL:O	2.37	0.45
1:D:1037:ASP:O	1:D:1041:GLN:HG2	2.16	0.45
1:D:1769:THR:O	1:D:1769:THR:OG1	2.34	0.45
1:D:3398:PHE:HB3	1:D:3454:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3434:LEU:O	1:D:3438:VAL:HG12	2.17	0.45
2:E:17:LYS:NZ	2:E:18:LYS:O	2.46	0.45
1:A:417:GLY:O	1:A:420:SER:OG	2.35	0.44
1:A:721:LEU:HD21	1:A:768:PHE:CZ	2.53	0.44
1:A:3845:ASN:OD1	1:A:3845:ASN:N	2.49	0.44
1:B:925:SER:O	1:B:928:THR:OG1	2.32	0.44
1:B:2187:ASN:OD1	1:B:2187:ASN:N	2.43	0.44
1:B:2759:ALA:HB2	1:B:2806:ARG:HH22	1.83	0.44
1:B:3526:ALA:O	1:B:3528:THR:N	2.50	0.44
1:C:24:CYS:HB3	1:C:200:TRP:CE3	2.53	0.44
1:C:710:ASP:O	1:C:712:TYR:N	2.50	0.44
1:D:15:ARG:O	1:D:98:HIS:ND1	2.39	0.44
1:D:269:TRP:CD1	1:D:272:SER:HB2	2.53	0.44
1:D:649:PHE:HE2	1:D:845:CYS:HB2	1.82	0.44
1:D:2187:ASN:OD1	1:D:2187:ASN:N	2.44	0.44
2:G:57:LYS:HB3	2:G:57:LYS:HE2	1.78	0.44
1:A:3971:GLY:O	1:A:3973:CYS:N	2.50	0.44
1:B:1685:LEU:HD23	1:B:1718:ILE:HD11	1.99	0.44
1:C:277:GLY:HA2	1:C:315:CYS:SG	2.57	0.44
1:C:3398:PHE:HB3	1:C:3454:GLU:HG2	1.98	0.44
1:D:292:ALA:O	1:D:299:LEU:HD12	2.17	0.44
1:D:757:PHE:HB2	1:D:764:VAL:HG11	1.99	0.44
1:D:2325:PRO:HB3	1:D:2422:ILE:HA	2.00	0.44
1:D:3526:ALA:O	1:D:3528:THR:N	2.50	0.44
1:D:4109:GLN:HA	1:D:4112:LEU:HD12	2.00	0.44
1:A:830:ARG:HE	1:A:830:ARG:HB3	1.58	0.44
1:A:886:ARG:HB3	1:A:891:TRP:CD1	2.53	0.44
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.83	0.44
1:A:1452:TRP:CE3	1:A:1548:LEU:HB3	2.52	0.44
1:A:4189:ARG:NE	1:A:5032:TYR:OH	2.29	0.44
1:B:269:TRP:CD1	1:B:272:SER:HB2	2.52	0.44
1:B:531:ARG:HA	1:B:566:CYS:SG	2.56	0.44
1:B:2355:ARG:HB3	1:B:2359:ARG:HH21	1.82	0.44
1:B:2500:ALA:HB1	1:B:2550:LEU:HD22	1.99	0.44
1:C:3110:LEU:HD23	1:C:3110:LEU:HA	1.85	0.44
1:C:3695:PRO:HD2	1:C:3699:HIS:HB2	1.98	0.44
1:D:24:CYS:HB3	1:D:200:TRP:CE3	2.53	0.44
1:D:2474:LEU:HA	1:D:2494:PHE:CD2	2.52	0.44
1:D:2491:SER:O	1:D:2491:SER:OG	2.32	0.44
1:A:2003:GLN:HA	1:A:3652:MET:HE1	1.98	0.44
1:B:3842:LEU:O	1:B:3929:SER:OG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2614:ILE:O	1:C:2618:MET:N	2.50	0.44
1:C:2858:GLN:H	1:C:2858:GLN:HG3	1.67	0.44
1:C:4034:ASN:HD21	1:C:4153:HIS:CE1	2.35	0.44
1:B:710:ASP:O	1:B:712:TYR:N	2.50	0.44
1:B:1128:ARG:HD3	1:B:1130:GLN:NE2	2.33	0.44
1:B:4159:ARG:HA	1:B:4162:ASN:HD21	1.82	0.44
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.29	0.44
1:C:757:PHE:HB2	1:C:764:VAL:HG11	1.99	0.44
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.99	0.44
1:C:2325:PRO:HB3	1:C:2422:ILE:HA	2.00	0.44
1:C:3172:ILE:HG21	1:C:3194:LEU:HD21	1.99	0.44
1:D:477:LEU:HD12	1:D:477:LEU:HA	1.90	0.44
1:D:497:TYR:HA	1:D:503:PHE:CE2	2.52	0.44
1:D:1206:GLN:NE2	1:D:1230:MET:O	2.51	0.44
1:D:2500:ALA:HB1	1:D:2550:LEU:HD22	2.00	0.44
1:D:2974:ILE:O	1:D:2978:GLU:N	2.44	0.44
1:D:4003:LEU:HD21	1:D:4012:LEU:HB3	1.98	0.44
1:A:263:GLU:HB3	1:A:281:ARG:HB2	1.99	0.44
1:A:479:GLN:O	1:A:479:GLN:NE2	2.51	0.44
1:A:497:TYR:HA	1:A:503:PHE:CE2	2.53	0.44
1:A:686:TRP:NE1	1:A:746:CYS:SG	2.77	0.44
1:A:760:ASN:N	1:A:760:ASN:OD1	2.49	0.44
1:A:1000:ARG:HD2	1:A:1005:TRP:CG	2.52	0.44
1:A:2536:LEU:HA	1:A:2584:HIS:CE1	2.53	0.44
1:B:24:CYS:HB3	1:B:200:TRP:CE3	2.53	0.44
1:B:3579:LEU:HG	1:B:3581:GLY:H	1.82	0.44
1:C:1700:ASP:HB3	1:C:1703:LEU:HD12	1.99	0.44
1:C:4000:MET:HE2	1:C:4058:ILE:HG12	1.99	0.44
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.30	0.44
1:D:760:ASN:N	1:D:760:ASN:OD1	2.49	0.44
1:D:1454:THR:HG22	1:D:1491:ASN:HA	1.99	0.44
2:G:30:LEU:N	2:G:34:LYS:O	2.48	0.44
2:H:77:THR:HA	2:H:96:THR:HG22	2.00	0.44
1:A:1125:ASN:HB2	1:A:1132:TRP:HD1	1.83	0.44
1:A:1263:THR:N	1:A:1266:THR:O	2.41	0.44
1:A:3999:MET:HB3	1:A:3999:MET:HE2	1.78	0.44
1:A:4583:SER:HB3	1:A:4630:TYR:HE2	1.83	0.44
1:B:68:THR:HG23	1:B:110:ARG:HB2	2.00	0.44
1:B:3274:LEU:HG	1:B:3275:PRO:HD3	1.99	0.44
1:B:4109:GLN:HA	1:B:4112:LEU:HD12	2.00	0.44
1:B:4769:MET:SD	1:B:4769:MET:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:TRP:CD1	1:C:272:SER:HB2	2.52	0.44
1:C:3535:LEU:HD23	1:C:3535:LEU:H	1.83	0.44
1:D:102:LEU:HD12	1:D:161:GLU:O	2.17	0.44
1:D:830:ARG:NE	1:D:1612:PHE:CE2	2.83	0.44
1:D:954:LYS:HA	1:D:954:LYS:HD2	1.80	0.44
1:D:1644:GLU:OE1	1:D:1646:ARG:NE	2.42	0.44
1:D:3971:GLY:O	1:D:3973:CYS:N	2.50	0.44
2:G:38:SER:OG	2:G:41:ASP:OD2	2.35	0.44
1:A:158:SER:N	1:A:161:GLU:OE1	2.49	0.44
1:A:2614:ILE:O	1:A:2618:MET:N	2.51	0.44
1:A:4008:SER:OG	1:A:4009:GLN:OE1	2.24	0.44
1:C:68:THR:HG23	1:C:110:ARG:HB2	1.99	0.44
1:D:1040:CYS:O	1:D:1044:ARG:HG2	2.18	0.44
1:D:3526:ALA:HB2	1:D:3595:ARG:HH12	1.82	0.44
1:D:3845:ASN:OD1	1:D:3845:ASN:N	2.49	0.44
2:G:14:THR:OG1	2:G:68:LEU:N	2.51	0.44
1:A:1435:TYR:CZ	1:A:1550:PRO:HB3	2.53	0.44
1:A:4586:PRO:HB3	1:A:4628:VAL:HG21	1.98	0.44
1:B:30:LYS:HA	1:B:30:LYS:HD3	1.84	0.44
1:B:2368:LEU:HA	1:B:2374:SER:HB2	2.00	0.44
1:C:3289:PRO:HG2	1:C:3307:VAL:HG22	1.99	0.44
1:D:619:ASP:OD2	1:D:1680:ARG:NH2	2.50	0.44
1:D:2983:SER:O	1:D:2983:SER:OG	2.29	0.44
1:D:3359:ILE:HD11	1:D:3434:LEU:HB2	2.00	0.44
2:F:17:LYS:HD3	2:F:17:LYS:N	2.33	0.44
1:A:68:THR:HG23	1:A:110:ARG:HB2	2.00	0.43
1:A:277:GLY:HA2	1:A:315:CYS:SG	2.57	0.43
1:A:279:PRO:HA	1:A:314:PHE:O	2.18	0.43
1:A:757:PHE:HB2	1:A:764:VAL:HG11	1.99	0.43
1:A:1486:SER:O	1:A:1486:SER:OG	2.29	0.43
1:A:2258:LEU:HD12	1:A:2258:LEU:HA	1.87	0.43
1:B:2431:ASP:OD1	1:B:2435:ARG:NE	2.47	0.43
1:C:798:GLY:HA2	1:C:1623:ARG:HD3	1.99	0.43
1:C:1125:ASN:OD1	1:C:1126:GLY:N	2.51	0.43
1:C:2159:LEU:HD22	1:C:2201:LEU:HD21	2.00	0.43
1:D:269:TRP:NE1	1:D:333:GLY:O	2.51	0.43
1:D:448:LEU:HD23	1:D:448:LEU:HA	1.84	0.43
1:D:1805:GLU:OE2	1:D:1808:ARG:NH2	2.51	0.43
1:D:3940:LYS:HE2	1:D:3940:LYS:HB2	1.83	0.43
1:A:375:LYS:HB2	1:A:375:LYS:HE3	1.81	0.43
1:A:652:ARG:HG2	1:A:750:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3249:LEU:O	1:A:3253:ILE:HG12	2.18	0.43
1:A:3526:ALA:O	1:A:3528:THR:N	2.51	0.43
1:B:1018:ASN:HA	1:B:1019:PRO:HD3	1.78	0.43
1:B:3289:PRO:HG2	1:B:3307:VAL:HG22	2.00	0.43
1:C:651:GLY:H	1:C:776:LEU:HD23	1.83	0.43
1:C:1283:LEU:HD12	1:C:1283:LEU:HA	1.84	0.43
1:C:1652:GLU:OE1	1:C:1656:ARG:NH2	2.51	0.43
1:C:3327:LEU:HD12	1:C:3327:LEU:HA	1.82	0.43
1:D:263:GLU:HB3	1:D:281:ARG:HB2	1.99	0.43
1:D:1139:PHE:CE1	1:D:1169:LEU:HD11	2.53	0.43
2:H:22:CYS:SG	2:H:23:VAL:N	2.91	0.43
1:A:865:PRO:HA	1:A:868:GLU:HB2	2.00	0.43
1:A:1079:LYS:HG3	1:A:1107:PRO:HB3	2.00	0.43
1:A:1634:LEU:HD12	1:A:1634:LEU:HA	1.79	0.43
1:A:1805:GLU:OE2	1:A:1808:ARG:NH2	2.52	0.43
1:A:3424:LEU:HD23	1:A:3424:LEU:HA	1.86	0.43
1:A:3695:PRO:HD2	1:A:3699:HIS:HB2	1.99	0.43
1:A:4763:GLY:N	1:A:4766:THR:OG1	2.49	0.43
1:B:268:SER:OG	1:B:269:TRP:N	2.51	0.43
1:B:689:THR:HB	1:B:778:PHE:HZ	1.83	0.43
1:C:760:ASN:OD1	1:C:760:ASN:N	2.50	0.43
1:C:1442:GLY:HA3	1:C:1558:HIS:CD2	2.53	0.43
1:C:1461:ASP:HB3	1:C:1464:PHE:HB2	2.01	0.43
1:C:2536:LEU:HA	1:C:2584:HIS:CE1	2.53	0.43
1:C:2606:CYS:SG	1:C:2607:LEU:N	2.91	0.43
1:C:3051:ARG:HA	1:C:3051:ARG:HD2	1.73	0.43
1:D:919:ASN:O	1:D:922:LEU:HD12	2.18	0.43
1:D:1815:LEU:HD12	1:D:1815:LEU:HA	1.90	0.43
1:D:2368:LEU:HA	1:D:2374:SER:HB2	2.01	0.43
1:D:4583:SER:HB3	1:D:4630:TYR:HE2	1.83	0.43
1:A:2325:PRO:HB3	1:A:2422:ILE:HA	2.00	0.43
1:A:2476:ILE:HD12	1:A:2477:PRO:HD2	2.01	0.43
1:A:3232:LEU:HD12	1:A:3233:PRO:HD2	1.99	0.43
1:A:4187:SER:OG	1:A:4191:GLU:OE2	2.28	0.43
1:B:417:GLY:O	1:B:420:SER:OG	2.35	0.43
1:B:686:TRP:NE1	1:B:746:CYS:SG	2.75	0.43
1:B:757:PHE:HB2	1:B:764:VAL:HG11	1.99	0.43
1:B:960:MET:HG3	1:B:966:LYS:HG3	2.01	0.43
1:B:986:ASP:HB3	1:B:1036:ARG:HE	1.82	0.43
1:B:1000:ARG:HD2	1:B:1005:TRP:CG	2.53	0.43
1:B:1125:ASN:OD1	1:B:1126:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1436:SER:HA	1:B:1517:GLY:HA2	1.99	0.43
1:B:1457:TYR:O	1:B:1458:HIS:ND1	2.51	0.43
1:C:830:ARG:HH12	1:C:832:GLU:HG3	1.83	0.43
1:C:3677:LEU:HG	1:C:3697:PRO:HG2	2.00	0.43
1:C:3999:MET:HE2	1:C:4016:LEU:HD13	1.99	0.43
1:C:4162:ASN:HA	1:C:4165:GLU:HG2	2.00	0.43
1:D:681:HIS:O	1:D:783:PHE:HA	2.19	0.43
1:D:1842:LEU:HD23	1:D:1842:LEU:HA	1.89	0.43
1:D:2556:LEU:HD11	1:D:2597:LYS:HA	2.01	0.43
1:D:3842:LEU:O	1:D:3929:SER:OG	2.30	0.43
1:D:4845:ALA:O	1:D:4883:TYR:OH	2.34	0.43
1:A:1206:GLN:NE2	1:A:1230:MET:O	2.52	0.43
1:B:591:ASP:OD1	1:B:1594:ARG:NH1	2.51	0.43
1:B:718:GLY:HA3	1:B:737:LEU:HA	2.00	0.43
1:B:1141:ARG:NH2	1:B:1167:GLU:OE2	2.51	0.43
1:B:1805:GLU:OE2	1:B:1808:ARG:NH2	2.52	0.43
1:B:2159:LEU:HD22	1:B:2201:LEU:HD21	2.00	0.43
1:B:4189:ARG:NE	1:B:5032:TYR:OH	2.29	0.43
1:B:4583:SER:HB3	1:B:4630:TYR:HE2	1.83	0.43
1:B:4951:LYS:HE2	1:B:4951:LYS:HB2	1.88	0.43
1:C:103:TYR:HE1	1:C:152:PRO:HA	1.83	0.43
1:C:1125:ASN:HB2	1:C:1132:TRP:CD1	2.53	0.43
1:C:2759:ALA:HB2	1:C:2806:ARG:HH22	1.84	0.43
1:C:3103:ILE:HD11	1:C:3168:THR:HG22	2.00	0.43
1:C:4583:SER:HB3	1:C:4630:TYR:HE2	1.83	0.43
1:D:575:LEU:HD22	1:D:609:CYS:HB2	2.00	0.43
1:A:268:SER:OG	1:A:269:TRP:N	2.52	0.43
1:A:294:THR:HG23	1:A:297:GLN:H	1.83	0.43
1:A:1125:ASN:OD1	1:A:1126:GLY:N	2.51	0.43
1:A:2520:HIS:O	1:A:2524:VAL:HG23	2.19	0.43
1:B:224:HIS:HB2	1:B:388:LEU:HG	2.01	0.43
1:B:561:LEU:HD11	1:B:589:LEU:HD21	2.00	0.43
1:B:886:ARG:HB3	1:B:891:TRP:CD1	2.53	0.43
1:B:2313:LEU:HB3	1:B:2318:TYR:HD2	1.84	0.43
1:B:3524:MET:H	1:B:3524:MET:HG2	1.65	0.43
1:B:3971:GLY:O	1:B:3973:CYS:N	2.50	0.43
1:C:1805:GLU:OE2	1:C:1808:ARG:NH2	2.51	0.43
1:C:1947:CYS:HB3	1:C:2126:ARG:HH21	1.84	0.43
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.32	0.43
1:D:591:ASP:OD1	1:D:1594:ARG:NH1	2.52	0.43
1:D:977:LEU:H	1:D:1044:ARG:NH2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1442:GLY:HA3	1:D:1558:HIS:CD2	2.54	0.43
2:G:56:ILE:HG22	2:G:59:PHE:H	1.83	0.43
2:H:68:LEU:HD23	2:H:68:LEU:HA	1.80	0.43
1:A:871:ARG:HH12	1:A:926:GLY:CA	2.32	0.43
1:A:2212:VAL:HG22	1:A:2256:TYR:CZ	2.54	0.43
1:B:479:GLN:O	1:B:479:GLN:NE2	2.50	0.43
1:B:955:LEU:HD13	1:B:959:TYR:CG	2.53	0.43
1:B:1442:GLY:HA3	1:B:1558:HIS:CD2	2.54	0.43
1:B:2476:ILE:HD12	1:B:2477:PRO:HD2	2.01	0.43
1:C:649:PHE:HE2	1:C:845:CYS:HB2	1.83	0.43
1:C:2228:MET:HE3	1:C:2228:MET:HB3	1.91	0.43
1:D:294:THR:HG23	1:D:297:GLN:H	1.84	0.43
1:D:858:THR:OG1	1:D:930:LYS:HG3	2.18	0.43
1:D:881:LEU:HD12	1:D:881:LEU:HA	1.84	0.43
1:D:1006:SER:O	1:D:1017:ARG:NH1	2.51	0.43
1:D:3347:SER:O	1:D:3347:SER:OG	2.29	0.43
2:H:17:LYS:O	2:H:18:LYS:HG2	2.19	0.43
1:A:269:TRP:NE1	1:A:333:GLY:O	2.52	0.43
1:B:359:TYR:HB2	1:B:383:HIS:CE1	2.54	0.43
1:B:2556:LEU:HD11	1:B:2597:LYS:HA	2.01	0.43
1:B:3357:HIS:O	1:B:3361:THR:HG23	2.18	0.43
1:C:3232:LEU:HD12	1:C:3233:PRO:HD2	1.99	0.43
1:D:915:GLU:HA	1:D:918:ARG:HB2	2.00	0.43
1:D:1849:LEU:HD23	1:D:1849:LEU:HA	1.86	0.43
1:D:2159:LEU:HD22	1:D:2201:LEU:HD21	2.01	0.43
1:D:3447:LYS:HA	1:D:3447:LYS:HD2	1.75	0.43
1:D:4907:ASP:O	1:D:4908:GLU:HB3	2.19	0.43
1:A:858:THR:OG1	1:A:930:LYS:HG3	2.19	0.43
1:A:913:LEU:HB2	1:A:918:ARG:HG2	1.99	0.43
1:A:1277:TRP:O	1:A:1277:TRP:HD1	2.02	0.43
1:A:2310:CYS:O	1:A:2312:MET:N	2.52	0.43
1:A:2556:LEU:HD11	1:A:2597:LYS:HA	2.01	0.43
1:A:3235:SER:O	1:A:3235:SER:OG	2.35	0.43
1:B:2199:ARG:HG3	1:B:2246:ASN:OD1	2.19	0.43
1:B:2536:LEU:HA	1:B:2584:HIS:CE1	2.53	0.43
1:B:2856:ASN:OD1	1:B:2856:ASN:N	2.52	0.43
1:B:3398:PHE:HB3	1:B:3454:GLU:HG2	2.00	0.43
1:C:684:VAL:HG12	1:C:781:VAL:HG12	2.00	0.43
1:C:977:LEU:HB3	1:C:981:GLN:CB	2.48	0.43
1:C:1022:VAL:HG23	1:C:1027:LEU:HG	2.01	0.43
1:C:1288:PHE:HA	1:C:1551:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2021:CYS:SG	1:C:2023:LEU:HB3	2.59	0.43
1:D:268:SER:OG	1:D:269:TRP:N	2.52	0.43
1:D:402:ARG:HA	1:D:402:ARG:HD2	1.85	0.43
1:D:1634:LEU:HD12	1:D:1634:LEU:HA	1.79	0.43
1:D:1652:GLU:OE1	1:D:1656:ARG:NH2	2.52	0.43
1:D:3141:THR:O	1:D:3145:GLN:HG2	2.19	0.43
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.83	0.43
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.26	0.43
1:A:990:GLU:HG2	1:A:1024:TYR:CE2	2.53	0.43
1:A:3509:LEU:HD12	1:A:3509:LEU:HA	1.84	0.43
1:A:4109:GLN:HA	1:A:4112:LEU:HD12	2.00	0.43
1:A:4689:THR:OG1	1:A:4690:GLU:N	2.52	0.43
1:B:1770:SER:OG	1:B:1956:GLU:OE2	2.28	0.43
1:B:2283:ASN:HB3	1:B:2286:LEU:H	1.84	0.43
1:B:3172:ILE:HG21	1:B:3194:LEU:HD21	2.01	0.43
1:B:3263:TYR:O	1:B:3265:GLU:N	2.52	0.43
1:C:919:ASN:O	1:C:922:LEU:HD12	2.18	0.43
1:C:1272:LEU:HD11	1:C:1285:GLU:OE1	2.18	0.43
1:C:2556:LEU:HD11	1:C:2597:LYS:HA	2.01	0.43
1:C:2916:LYS:HA	1:C:2916:LYS:HD2	1.80	0.43
1:D:359:TYR:HB2	1:D:383:HIS:CE1	2.54	0.43
1:D:1028:ASP:O	1:D:1032:LYS:HG3	2.19	0.43
1:D:3274:LEU:HG	1:D:3275:PRO:HD3	2.01	0.43
1:D:3994:HIS:O	1:D:3998:HIS:ND1	2.50	0.43
1:A:971:ASP:O	1:A:974:HIS:NE2	2.51	0.42
1:A:981:GLN:HA	1:A:984:LEU:HD23	2.01	0.42
1:A:3519:PRO:O	1:D:1220:GLN:NE2	2.50	0.42
1:B:294:THR:HG23	1:B:297:GLN:H	1.84	0.42
1:B:2310:CYS:O	1:B:2312:MET:N	2.52	0.42
1:B:3359:ILE:HD11	1:B:3434:LEU:HB2	2.01	0.42
1:C:670:GLU:HA	1:C:740:PRO:HB3	2.01	0.42
1:C:2310:CYS:O	1:C:2312:MET:N	2.52	0.42
1:C:2355:ARG:HB3	1:C:2359:ARG:HH21	1.84	0.42
1:C:2454:ARG:HG2	1:C:2458:ARG:HH12	1.84	0.42
1:C:2476:ILE:HD12	1:C:2477:PRO:HD2	2.00	0.42
1:C:3447:LYS:HD2	1:C:3447:LYS:HA	1.74	0.42
1:C:3771:HIS:HD2	1:C:3815:LYS:HD2	1.84	0.42
1:D:29:LEU:HD12	1:D:30:LYS:N	2.34	0.42
1:D:479:GLN:O	1:D:479:GLN:NE2	2.50	0.42
1:D:1436:SER:HA	1:D:1517:GLY:HA2	2.01	0.42
1:D:2283:ASN:HB3	1:D:2286:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2606:CYS:SG	1:D:2607:LEU:N	2.92	0.42
1:D:3677:LEU:HG	1:D:3697:PRO:HG2	2.01	0.42
1:A:14:LEU:HD12	1:A:18:ASP:HB3	2.01	0.42
1:A:266:ARG:NH2	1:A:331:VAL:O	2.35	0.42
1:A:881:LEU:HD12	1:A:881:LEU:HA	1.78	0.42
1:A:1283:LEU:HD12	1:A:1283:LEU:HA	1.84	0.42
1:A:1442:GLY:HA3	1:A:1558:HIS:CD2	2.54	0.42
1:A:2035:HIS:CE1	1:A:3661:TRP:HB3	2.54	0.42
1:A:2149:VAL:O	1:A:2153:MET:N	2.49	0.42
1:A:2967:MET:H	1:A:2967:MET:HG2	1.60	0.42
1:A:3398:PHE:HB3	1:A:3454:GLU:HG2	2.00	0.42
1:B:497:TYR:HA	1:B:503:PHE:CE2	2.54	0.42
1:B:1079:LYS:HG3	1:B:1107:PRO:HB3	2.01	0.42
1:B:1459:GLN:HA	1:B:1459:GLN:OE1	2.19	0.42
1:B:4198:SER:HB3	1:B:4201:ASN:ND2	2.34	0.42
1:C:345:LEU:HD22	1:C:389:PHE:HB3	2.01	0.42
1:C:595:ARG:NH2	1:C:1643:GLU:OE1	2.50	0.42
1:C:655:GLY:HA3	1:C:852:VAL:HG12	2.01	0.42
1:C:1206:GLN:NE2	1:C:1230:MET:O	2.51	0.42
1:C:2283:ASN:HB3	1:C:2286:LEU:H	1.84	0.42
1:C:2431:ASP:OD1	1:C:2435:ARG:NE	2.49	0.42
1:C:2999:ALA:HA	1:C:3002:LEU:HG	2.00	0.42
1:C:4198:SER:HB3	1:C:4201:ASN:ND2	2.34	0.42
1:C:4897:ILE:HD12	1:C:4897:ILE:HA	1.89	0.42
1:D:2199:ARG:HG3	1:D:2246:ASN:OD1	2.19	0.42
1:D:4049:VAL:O	1:D:4052:SER:OG	2.35	0.42
1:D:4198:SER:HB3	1:D:4201:ASN:ND2	2.35	0.42
1:A:902:ARG:O	1:A:903:LEU:HD12	2.19	0.42
1:A:993:HIS:NE2	1:A:1027:LEU:HD11	2.34	0.42
1:A:2454:ARG:HG2	1:A:2458:ARG:HH12	1.85	0.42
1:A:3289:PRO:HG2	1:A:3307:VAL:HG22	2.00	0.42
1:A:3332:ALA:HB1	1:A:3334:TRP:CD1	2.54	0.42
1:B:12:GLN:HE21	1:B:14:LEU:HD11	1.84	0.42
1:B:1037:ASP:O	1:B:1041:GLN:HG2	2.18	0.42
1:B:1125:ASN:HB2	1:B:1132:TRP:HD1	1.84	0.42
1:B:2964:LEU:HA	1:B:2967:MET:HE2	2.02	0.42
1:C:273:HIS:HE1	1:C:334:MET:HG3	1.84	0.42
1:C:882:TRP:HZ3	1:C:921:ASN:ND2	2.17	0.42
1:C:899:ASP:HB2	1:C:902:ARG:CZ	2.49	0.42
1:C:1634:LEU:HD12	1:C:1634:LEU:HA	1.79	0.42
1:C:4689:THR:OG1	1:C:4690:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1434:TYR:HA	1:D:1519:LEU:HD23	2.01	0.42
1:D:2476:ILE:HD12	1:D:2477:PRO:HD2	2.00	0.42
1:D:3804:ILE:HD12	1:D:3804:ILE:HA	1.87	0.42
1:D:4184:MET:HB2	1:D:4190:ILE:HD13	2.02	0.42
1:A:345:LEU:HD22	1:A:389:PHE:HB3	2.00	0.42
1:A:710:ASP:O	1:A:712:TYR:N	2.52	0.42
1:A:1253:PRO:HB2	1:A:1254:HIS:CE1	2.54	0.42
1:A:3756:LYS:HE2	1:A:3756:LYS:HB3	1.86	0.42
1:B:725:HIS:O	1:B:725:HIS:ND1	2.52	0.42
1:C:887:ILE:HG13	1:C:891:TRP:O	2.20	0.42
1:C:1640:HIS:HA	1:C:1647:CYS:HA	2.01	0.42
1:C:2547:ALA:O	1:C:2551:ASN:ND2	2.52	0.42
1:C:3208:PRO:HD2	1:C:3245:VAL:HG22	2.02	0.42
1:D:871:ARG:HH11	1:D:926:GLY:HA3	1.83	0.42
1:D:1125:ASN:OD1	1:D:1126:GLY:N	2.52	0.42
1:D:1253:PRO:HB2	1:D:1254:HIS:CE1	2.54	0.42
1:D:1451:GLY:HA3	1:D:1494:MET:HG2	2.02	0.42
2:E:29:MET:HA	2:E:35:LYS:HA	2.01	0.42
1:A:670:GLU:HA	1:A:740:PRO:HB3	2.00	0.42
1:A:886:ARG:HB3	1:A:891:TRP:HD1	1.85	0.42
1:A:2103:VAL:HG13	1:A:3696:ASP:OD2	2.19	0.42
1:A:3806:ASN:HA	1:A:3890:LEU:HD21	2.01	0.42
1:A:4184:MET:HB2	1:A:4190:ILE:HD13	2.02	0.42
1:B:273:HIS:HE1	1:B:334:MET:HG3	1.84	0.42
1:B:345:LEU:HD22	1:B:389:PHE:HB3	2.01	0.42
1:B:954:LYS:HD2	1:B:954:LYS:HA	1.83	0.42
1:B:1263:THR:HG23	1:B:1265:ASP:H	1.85	0.42
1:B:1618:ARG:HG2	1:B:1627:ALA:HB3	2.01	0.42
1:B:1652:GLU:OE1	1:B:1656:ARG:NH2	2.53	0.42
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.85	0.42
1:C:2199:ARG:HG3	1:C:2246:ASN:OD1	2.19	0.42
1:C:4951:LYS:HE2	1:C:4951:LYS:HB2	1.88	0.42
1:D:710:ASP:O	1:D:712:TYR:N	2.52	0.42
1:D:887:ILE:HG13	1:D:891:TRP:O	2.19	0.42
1:D:977:LEU:HD12	1:D:1044:ARG:HH21	1.83	0.42
1:D:2858:GLN:H	1:D:2858:GLN:HG3	1.67	0.42
1:D:3263:TYR:O	1:D:3265:GLU:N	2.53	0.42
1:A:924:MET:HA	1:A:927:GLU:OE2	2.18	0.42
1:A:2313:LEU:HB3	1:A:2318:TYR:HD2	1.84	0.42
1:A:3107:VAL:HA	1:A:3110:LEU:HB2	2.02	0.42
1:B:266:ARG:NH2	1:B:331:VAL:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2035:HIS:CE1	1:B:3661:TRP:HB3	2.55	0.42
1:B:2442:LEU:HG	1:B:2443:ILE:HG12	2.01	0.42
1:C:1719:HIS:CE1	1:C:1800:PRO:HB2	2.55	0.42
1:C:2035:HIS:CE1	1:C:3661:TRP:HB3	2.55	0.42
1:C:3526:ALA:O	1:C:3528:THR:N	2.52	0.42
1:D:950:LEU:HD23	1:D:950:LEU:HA	1.84	0.42
1:D:3289:PRO:HG2	1:D:3307:VAL:HG22	2.00	0.42
1:D:3438:VAL:HG11	1:D:3517:MET:HE3	2.01	0.42
1:D:3771:HIS:HD2	1:D:3815:LYS:HD2	1.84	0.42
2:G:29:MET:HA	2:G:35:LYS:HA	2.02	0.42
1:A:255:HIS:ND1	1:A:480:GLU:OE2	2.52	0.42
1:A:575:LEU:HD22	1:A:609:CYS:HB2	2.02	0.42
1:A:1436:SER:HA	1:A:1517:GLY:HA2	2.01	0.42
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.00	0.42
1:A:2974:ILE:O	1:A:2978:GLU:N	2.44	0.42
1:A:3771:HIS:HD2	1:A:3815:LYS:HD2	1.84	0.42
1:A:4907:ASP:O	1:A:4908:GLU:HB3	2.19	0.42
1:B:1288:PHE:CE1	1:B:1598:GLN:HB2	2.54	0.42
1:B:2021:CYS:SG	1:B:2023:LEU:HB3	2.60	0.42
1:B:2606:CYS:SG	1:B:2607:LEU:N	2.92	0.42
1:C:233:ILE:HG22	1:C:234:SER:N	2.35	0.42
1:C:268:SER:OG	1:C:269:TRP:N	2.51	0.42
1:C:575:LEU:HD22	1:C:609:CYS:HB2	2.02	0.42
1:C:952:LYS:HG2	1:C:953:THR:H	1.84	0.42
1:C:993:HIS:NE2	1:C:1027:LEU:HD11	2.35	0.42
1:C:1079:LYS:HG3	1:C:1107:PRO:HB3	2.00	0.42
1:C:1101:ARG:HB3	1:C:1123:VAL:HG21	2.00	0.42
1:C:1618:ARG:HG2	1:C:1627:ALA:HB3	2.01	0.42
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.84	0.42
1:C:3396:ASP:OD1	1:C:3397:GLU:N	2.53	0.42
1:C:4159:ARG:HA	1:C:4162:ASN:HD21	1.84	0.42
1:D:981:GLN:O	1:D:984:LEU:HG	2.19	0.42
1:D:990:GLU:HG2	1:D:1024:TYR:CZ	2.55	0.42
1:D:2212:VAL:HG22	1:D:2256:TYR:CZ	2.55	0.42
1:D:3068:LEU:H	1:D:3068:LEU:HD12	1.84	0.42
1:D:3136:LEU:HA	1:D:3139:VAL:HG22	2.01	0.42
1:D:4586:PRO:HA	1:D:4587:PRO:HD3	1.91	0.42
1:A:875:ALA:HB1	1:A:910:PHE:CZ	2.55	0.42
1:A:1275:ARG:HG3	1:A:1276:THR:HG23	2.01	0.42
1:A:2159:LEU:HD22	1:A:2201:LEU:HD21	2.02	0.42
1:A:2236:LEU:HD22	1:A:2250:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2759:ALA:HB2	1:A:2806:ARG:HH22	1.84	0.42
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.85	0.42
1:A:3447:LYS:HA	1:A:3447:LYS:HD2	1.75	0.42
1:B:575:LEU:HD22	1:B:609:CYS:HB2	2.01	0.42
1:B:1470:ARG:HA	1:B:1470:ARG:HD3	1.70	0.42
1:B:4845:ALA:O	1:B:4883:TYR:OH	2.36	0.42
1:C:33:LEU:HG	1:C:53:SER:OG	2.20	0.42
1:C:2212:VAL:HG22	1:C:2256:TYR:CZ	2.55	0.42
1:C:3272:ILE:HG13	1:C:3273:THR:HG22	2.02	0.42
1:C:3509:LEU:HD12	1:C:3509:LEU:HA	1.84	0.42
1:D:829:TYR:HE2	1:D:1608:MET:HG2	1.85	0.42
1:D:875:ALA:HB1	1:D:910:PHE:CZ	2.55	0.42
1:D:1275:ARG:HG3	1:D:1276:THR:HG23	2.01	0.42
1:D:2035:HIS:CE1	1:D:3661:TRP:HB3	2.55	0.42
1:D:2360:LYS:HE3	1:D:2360:LYS:HB2	1.95	0.42
1:D:3696:ASP:CG	1:D:3697:PRO:HD3	2.39	0.42
2:E:57:LYS:HB3	2:E:57:LYS:HE2	1.76	0.42
2:H:29:MET:HA	2:H:35:LYS:HA	2.02	0.42
1:A:17:ASP:HB2	1:A:98:HIS:HE1	1.84	0.42
1:A:723:THR:HG21	1:A:768:PHE:HE2	1.85	0.42
1:A:1618:ARG:HG2	1:A:1627:ALA:HB3	2.01	0.42
1:A:2199:ARG:HG3	1:A:2246:ASN:OD1	2.20	0.42
1:A:2283:ASN:HB3	1:A:2286:LEU:H	1.84	0.42
1:B:233:ILE:HG22	1:B:234:SER:N	2.35	0.42
1:B:681:HIS:O	1:B:783:PHE:HA	2.20	0.42
1:B:3323:ILE:HD11	1:B:3338:LEU:HD22	2.01	0.42
1:B:4008:SER:OG	1:B:4009:GLN:OE1	2.27	0.42
1:C:892:THR:OG1	1:C:902:ARG:O	2.28	0.42
1:C:1000:ARG:HD2	1:C:1000:ARG:HA	1.81	0.42
1:C:1849:LEU:HD23	1:C:1849:LEU:HA	1.87	0.42
1:C:2313:LEU:HB3	1:C:2318:TYR:HD2	1.84	0.42
1:C:3674:ILE:HG13	1:C:3732:SER:HB2	2.02	0.42
1:C:4049:VAL:O	1:C:4052:SER:OG	2.32	0.42
1:D:299:LEU:HD12	1:D:299:LEU:HA	1.81	0.42
1:D:1947:CYS:HB3	1:D:2126:ARG:HH21	1.84	0.42
1:D:2741:GLU:HB3	1:D:2744:ASN:HB2	2.01	0.42
1:D:2963:LEU:HA	1:D:2966:TRP:HB2	2.01	0.42
1:D:3323:ILE:HD11	1:D:3338:LEU:HD22	2.01	0.42
1:D:3714:SER:O	1:D:3714:SER:OG	2.37	0.42
1:A:33:LEU:HG	1:A:53:SER:OG	2.20	0.42
1:A:233:ILE:HG22	1:A:234:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:PHE:HA	1:A:1551:ALA:HA	2.02	0.42
1:A:1947:CYS:HB3	1:A:2126:ARG:HH21	1.85	0.42
1:A:2021:CYS:SG	1:A:2023:LEU:HB3	2.60	0.42
1:A:3777:GLU:H	1:A:3777:GLU:HG2	1.64	0.42
1:B:913:LEU:H	1:B:913:LEU:HD12	1.85	0.42
1:B:1275:ARG:HG3	1:B:1276:THR:HG23	2.01	0.42
1:B:2454:ARG:HG2	1:B:2458:ARG:HH12	1.84	0.42
1:B:3771:HIS:HD2	1:B:3815:LYS:HD2	1.84	0.42
1:C:107:ILE:HG22	1:C:148:TRP:HB2	2.01	0.42
1:C:224:HIS:HB2	1:C:388:LEU:HG	2.02	0.42
1:C:915:GLU:HA	1:C:918:ARG:HB2	2.01	0.42
1:C:2930:LEU:HB2	1:C:2935:TYR:HB3	2.02	0.42
1:C:3940:LYS:HB2	1:C:3940:LYS:HE2	1.83	0.42
1:D:22:LEU:HB3	1:D:200:TRP:CE3	2.55	0.42
1:D:33:LEU:HG	1:D:53:SER:OG	2.20	0.42
1:D:1008:SER:HB2	1:D:1017:ARG:CZ	2.50	0.42
1:D:1079:LYS:HG3	1:D:1107:PRO:HB3	2.01	0.42
1:D:1536:SER:OG	1:D:1537:ASN:N	2.53	0.42
1:D:2310:CYS:O	1:D:2312:MET:N	2.52	0.42
1:D:4767:TRP:O	1:D:4770:SER:OG	2.35	0.42
1:A:920:TYR:HD1	1:A:923:GLN:HE21	1.68	0.41
1:A:2858:GLN:H	1:A:2858:GLN:HG3	1.67	0.41
1:A:3172:ILE:HG21	1:A:3194:LEU:HD21	2.01	0.41
1:B:880:GLU:HG3	1:B:968:ALA:H	1.84	0.41
1:B:1220:GLN:HG3	1:C:3519:PRO:HB3	2.02	0.41
1:B:1644:GLU:OE1	1:B:1646:ARG:NE	2.42	0.41
1:B:4170:ILE:HD13	1:B:4170:ILE:HA	1.94	0.41
1:C:867:LEU:O	1:C:870:ILE:HG22	2.19	0.41
1:C:1435:TYR:CZ	1:C:1550:PRO:HB3	2.55	0.41
1:C:2179:ILE:HD11	1:C:2228:MET:HG2	2.02	0.41
1:C:3677:LEU:HG	1:C:3697:PRO:CG	2.50	0.41
1:C:4845:ALA:O	1:C:4883:TYR:OH	2.35	0.41
1:D:72:SER:H	1:D:99:ARG:HH12	1.68	0.41
1:D:2905:LEU:HD23	1:D:2905:LEU:H	1.83	0.41
2:E:48:PHE:HE1	2:E:55:VAL:HG21	1.84	0.41
1:A:24:CYS:HB3	1:A:200:TRP:CE3	2.54	0.41
1:A:655:GLY:HA3	1:A:852:VAL:HG12	2.01	0.41
1:A:952:LYS:HG2	1:A:953:THR:H	1.85	0.41
1:A:1028:ASP:O	1:A:1032:LYS:HG3	2.20	0.41
1:A:1640:HIS:HA	1:A:1647:CYS:HA	2.02	0.41
1:A:1652:GLU:OE1	1:A:1656:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1849:LEU:HD23	1:A:1849:LEU:HA	1.87	0.41
1:A:2179:ILE:HD11	1:A:2228:MET:HG2	2.02	0.41
1:A:3983:SER:OG	1:A:3984:ARG:N	2.54	0.41
1:B:1253:PRO:HB2	1:B:1254:HIS:CE1	2.54	0.41
1:B:3051:ARG:HD2	1:B:3051:ARG:HA	1.62	0.41
1:B:3806:ASN:HA	1:B:3890:LEU:HD21	2.01	0.41
1:B:4907:ASP:O	1:B:4908:GLU:HB3	2.19	0.41
1:B:4957:LYS:HB3	1:B:4957:LYS:HE2	1.88	0.41
1:C:833:GLY:HA3	1:C:838:HIS:ND1	2.35	0.41
1:C:1037:ASP:O	1:C:1041:GLN:HG2	2.20	0.41
1:C:1927:LEU:HD22	1:C:2097:LEU:HD11	2.02	0.41
1:C:3994:HIS:O	1:C:3998:HIS:ND1	2.49	0.41
1:D:833:GLY:N	1:D:836:GLY:O	2.52	0.41
1:D:955:LEU:HD13	1:D:959:TYR:CG	2.55	0.41
1:D:987:ARG:O	1:D:991:ASN:ND2	2.43	0.41
1:D:2520:HIS:O	1:D:2524:VAL:HG23	2.20	0.41
1:D:3103:ILE:HD11	1:D:3168:THR:HG22	2.02	0.41
1:D:3416:VAL:HG21	1:D:3517:MET:SD	2.60	0.41
2:G:44:LYS:HA	2:G:44:LYS:HD2	1.81	0.41
1:A:955:LEU:HD13	1:A:959:TYR:CG	2.54	0.41
1:A:1139:PHE:CE1	1:A:1169:LEU:HD11	2.55	0.41
1:A:2236:LEU:HD23	1:A:2236:LEU:HA	1.90	0.41
1:A:4951:LYS:HE2	1:A:4951:LYS:HB2	1.88	0.41
1:B:255:HIS:ND1	1:B:480:GLU:OE2	2.54	0.41
1:B:774:ASP:O	1:B:848:HIS:ND1	2.52	0.41
1:B:1634:LEU:HD12	1:B:1634:LEU:HA	1.79	0.41
1:C:619:ASP:OD2	1:C:1680:ARG:NH2	2.48	0.41
1:C:682:LEU:HD12	1:C:787:VAL:HG12	2.00	0.41
1:C:2906:VAL:HG11	1:C:2911:LEU:HA	2.03	0.41
1:C:3777:GLU:H	1:C:3777:GLU:HG2	1.64	0.41
1:D:393:CYS:HB2	1:D:397:GLU:HG3	2.03	0.41
1:D:881:LEU:HD23	1:D:1041:GLN:HG3	2.02	0.41
1:D:913:LEU:H	1:D:913:LEU:HD12	1.84	0.41
1:D:1521:ASP:OD1	1:D:1524:THR:OG1	2.32	0.41
1:A:778:PHE:HB2	1:A:780:VAL:HG13	2.01	0.41
1:B:1521:ASP:OD1	1:B:1524:THR:OG1	2.33	0.41
1:B:2541:PHE:HD1	1:B:2541:PHE:HA	1.81	0.41
1:B:3940:LYS:HB2	1:B:3940:LYS:HE2	1.83	0.41
1:C:12:GLN:HB2	1:C:165:VAL:HG13	2.03	0.41
1:C:255:HIS:ND1	1:C:480:GLU:OE2	2.54	0.41
1:C:711:LEU:HD12	1:C:1470:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2524:VAL:HA	1:C:2527:LEU:HD23	2.02	0.41
1:D:284:HIS:CE1	1:D:286:THR:HB	2.55	0.41
1:D:884:LEU:O	1:D:887:ILE:HG22	2.21	0.41
1:D:1288:PHE:HA	1:D:1551:ALA:HA	2.03	0.41
1:D:3110:LEU:HD12	1:D:3175:LEU:HD11	2.02	0.41
1:D:3592:ILE:HA	1:D:3595:ARG:NE	2.34	0.41
1:D:4689:THR:OG1	1:D:4690:GLU:N	2.53	0.41
1:A:537:CYS:O	1:A:541:SER:OG	2.39	0.41
1:A:1284:VAL:HG22	1:A:1555:LEU:HD13	2.02	0.41
1:A:1434:TYR:HB2	1:A:1572:ILE:HG21	2.02	0.41
1:A:2458:ARG:NH2	1:A:2509:VAL:O	2.54	0.41
1:A:3416:VAL:HG21	1:A:3517:MET:SD	2.60	0.41
1:B:393:CYS:HB2	1:B:397:GLU:HG3	2.03	0.41
1:B:830:ARG:HE	1:B:830:ARG:HB3	1.67	0.41
1:B:987:ARG:O	1:B:991:ASN:ND2	2.46	0.41
1:B:1139:PHE:CE1	1:B:1169:LEU:HD11	2.55	0.41
1:B:1206:GLN:NE2	1:B:1230:MET:O	2.52	0.41
1:C:689:THR:HB	1:C:778:PHE:HZ	1.84	0.41
1:C:874:LEU:HD13	1:C:929:LEU:HD21	2.02	0.41
1:D:224:HIS:HB2	1:D:388:LEU:HG	2.02	0.41
1:D:996:TRP:C	1:D:996:TRP:CD1	2.93	0.41
1:D:3040:THR:HG21	1:D:3080:VAL:HG21	2.01	0.41
1:D:3509:LEU:HD12	1:D:3509:LEU:HA	1.85	0.41
1:D:3832:ILE:HD13	1:D:3832:ILE:HA	1.97	0.41
1:A:14:LEU:HD22	1:A:202:MET:HE2	2.01	0.41
1:A:4897:ILE:HD12	1:A:4897:ILE:HA	1.91	0.41
1:B:72:SER:H	1:B:99:ARG:HH12	1.69	0.41
1:B:902:ARG:O	1:B:903:LEU:HD12	2.20	0.41
1:B:2547:ALA:O	1:B:2551:ASN:ND2	2.54	0.41
1:B:3714:SER:O	1:B:3714:SER:OG	2.36	0.41
1:B:3891:LEU:HD22	1:B:3899:PHE:CE2	2.56	0.41
1:B:4689:THR:OG1	1:B:4690:GLU:N	2.53	0.41
1:C:402:ARG:HA	1:C:402:ARG:HD2	1.85	0.41
1:C:913:LEU:H	1:C:913:LEU:HD12	1.85	0.41
1:C:3068:LEU:HD12	1:C:3068:LEU:H	1.85	0.41
1:C:3430:ASN:OD1	1:C:3430:ASN:N	2.54	0.41
1:D:345:LEU:HD22	1:D:389:PHE:HB3	2.01	0.41
1:D:1851:MET:HB2	1:D:1853:ILE:HG13	2.03	0.41
1:D:2454:ARG:HG2	1:D:2458:ARG:HH12	1.85	0.41
1:D:3107:VAL:HA	1:D:3110:LEU:HB2	2.03	0.41
1:D:3327:LEU:HA	1:D:3327:LEU:HD12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3359:ILE:HD13	1:D:3359:ILE:HA	1.93	0.41
1:A:206:CYS:N	1:A:271:GLY:HA3	2.36	0.41
1:A:247:TYR:OH	1:A:388:LEU:HD11	2.20	0.41
1:A:650:VAL:HG12	1:A:777:PHE:HB2	2.02	0.41
1:A:800:PHE:HD2	1:A:804:PRO:HG3	1.86	0.41
1:A:2741:GLU:HB3	1:A:2744:ASN:HB2	2.02	0.41
1:B:1288:PHE:HA	1:B:1551:ALA:HA	2.03	0.41
1:B:2179:ILE:HD11	1:B:2228:MET:HG2	2.02	0.41
1:B:2999:ALA:HA	1:B:3002:LEU:HG	2.03	0.41
1:B:4686:LEU:HD23	1:B:4687:TYR:CE1	2.55	0.41
1:C:630:GLU:HA	1:C:1642:PRO:CB	2.51	0.41
1:C:955:LEU:HD13	1:C:959:TYR:CG	2.55	0.41
1:D:839:LEU:O	1:D:1200:GLY:N	2.46	0.41
1:D:2536:LEU:HA	1:D:2584:HIS:CE1	2.55	0.41
1:D:2547:ALA:O	1:D:2551:ASN:ND2	2.54	0.41
1:D:3606:LEU:HD12	1:D:3606:LEU:HA	1.93	0.41
1:A:293:LEU:HD22	1:A:378:LEU:HD13	2.02	0.41
1:A:927:GLU:O	1:A:931:THR:HG23	2.21	0.41
1:A:1207:ASP:O	1:A:1210:SER:N	2.52	0.41
1:A:2102:VAL:HG11	1:A:2124:LEU:HB2	2.03	0.41
1:A:2606:CYS:SG	1:A:2607:LEU:N	2.91	0.41
1:A:4182:GLU:OE2	1:A:4192:ARG:NH1	2.54	0.41
1:B:12:GLN:HB2	1:B:165:VAL:HG13	2.03	0.41
1:B:29:LEU:HD12	1:B:30:LYS:N	2.36	0.41
1:B:205:ILE:HG22	1:B:206:CYS:N	2.30	0.41
1:B:4859:PHE:HB3	1:B:4862:PHE:HD2	1.86	0.41
1:C:622:THR:O	1:C:627:PRO:HD3	2.21	0.41
1:C:1253:PRO:HB2	1:C:1254:HIS:CE1	2.55	0.41
1:C:1536:SER:OG	1:C:1537:ASN:N	2.53	0.41
1:D:959:TYR:HB3	1:D:967:PRO:HD2	2.03	0.41
1:D:1618:ARG:HG2	1:D:1627:ALA:HB3	2.02	0.41
1:D:2313:LEU:HB3	1:D:2318:TYR:HD2	1.84	0.41
1:D:2759:ALA:HB2	1:D:2806:ARG:HH22	1.85	0.41
1:D:3891:LEU:HG	1:D:3899:PHE:CE2	2.55	0.41
1:D:4859:PHE:HB3	1:D:4862:PHE:HD2	1.86	0.41
2:G:82:TYR:HB3	2:G:86:GLY:HA2	2.03	0.41
1:A:29:LEU:HD12	1:A:30:LYS:N	2.35	0.41
1:A:320:LYS:HB3	1:A:356:TRP:CD1	2.56	0.41
1:A:2023:LEU:HG	1:A:2024:PRO:HD2	2.02	0.41
1:A:3263:TYR:O	1:A:3265:GLU:N	2.54	0.41
1:A:3272:ILE:HG13	1:A:3273:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4790:LEU:HD23	1:A:4790:LEU:HA	1.92	0.41
1:A:4801:LEU:HD12	1:A:4801:LEU:HA	1.94	0.41
1:B:707:VAL:HG12	1:B:782:SER:HB3	2.02	0.41
1:B:1434:TYR:HA	1:B:1519:LEU:HD23	2.01	0.41
1:B:1536:SER:OG	1:B:1537:ASN:N	2.53	0.41
1:B:2228:MET:HE3	1:B:2228:MET:HB3	1.98	0.41
1:B:3606:LEU:HD12	1:B:3606:LEU:HA	1.93	0.41
1:B:4184:MET:HB2	1:B:4190:ILE:HD13	2.02	0.41
1:B:4763:GLY:N	1:B:4766:THR:OG1	2.40	0.41
1:C:393:CYS:HB2	1:C:397:GLU:HG3	2.03	0.41
1:C:772:ASN:ND2	1:C:1470:ARG:HA	2.35	0.41
1:C:784:SER:OG	1:C:785:ALA:N	2.53	0.41
1:C:1041:GLN:O	1:C:1044:ARG:HB2	2.21	0.41
1:C:1668:ARG:HE	1:C:1668:ARG:HB2	1.58	0.41
1:C:1847:THR:O	1:C:1851:MET:HG3	2.21	0.41
1:C:2368:LEU:HA	1:C:2374:SER:HB2	2.02	0.41
1:C:3592:ILE:HA	1:C:3595:ARG:NE	2.34	0.41
1:D:866:HIS:HA	1:D:869:ARG:HD3	2.03	0.41
1:D:952:LYS:HG2	1:D:953:THR:H	1.85	0.41
1:D:2106:ALA:HB3	1:D:3696:ASP:OD1	2.21	0.41
1:D:2179:ILE:HD11	1:D:2228:MET:HG2	2.02	0.41
1:D:2789:PRO:O	1:D:2792:ARG:NH1	2.53	0.41
1:D:4897:ILE:HD12	1:D:4897:ILE:HA	1.92	0.41
2:E:26:TYR:CE1	2:E:39:SER:HB3	2.55	0.41
2:F:29:MET:HA	2:F:35:LYS:HA	2.02	0.41
1:A:206:CYS:SG	1:A:207:SER:N	2.94	0.41
1:A:1536:SER:OG	1:A:1537:ASN:N	2.53	0.41
1:A:4049:VAL:O	1:A:4052:SER:OG	2.34	0.41
1:B:375:LYS:HE3	1:B:375:LYS:HB2	1.81	0.41
1:B:674:PHE:N	1:B:680:THR:OG1	2.54	0.41
1:B:886:ARG:HB3	1:B:891:TRP:HD1	1.86	0.41
1:C:206:CYS:SG	1:C:207:SER:N	2.93	0.41
1:C:247:TYR:OH	1:C:388:LEU:HD11	2.20	0.41
1:C:860:GLN:HG2	1:C:860:GLN:O	2.21	0.41
1:C:1101:ARG:HB2	1:C:1193:SER:HB3	2.03	0.41
1:D:49:LEU:HD21	1:D:191:VAL:HG23	2.03	0.41
1:D:255:HIS:ND1	1:D:480:GLU:OE2	2.53	0.41
1:D:655:GLY:HA3	1:D:852:VAL:HG12	2.03	0.41
1:D:1277:TRP:O	1:D:1277:TRP:HD1	2.04	0.41
1:D:4577:LEU:HD23	1:D:4577:LEU:HA	1.95	0.41
1:A:273:HIS:HE1	1:A:334:MET:HG3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1477:GLY:HA2	1:A:1482:ASN:O	2.21	0.40
1:A:1847:THR:O	1:A:1851:MET:HG3	2.21	0.40
1:A:2098:VAL:CG1	1:A:2127:GLN:HG3	2.51	0.40
1:B:299:LEU:HD12	1:B:299:LEU:HA	1.81	0.40
1:B:650:VAL:HG12	1:B:777:PHE:HB2	2.03	0.40
1:B:1815:LEU:HD12	1:B:1815:LEU:HA	1.89	0.40
1:B:3424:LEU:HA	1:B:3424:LEU:HD23	1.87	0.40
1:C:835:ARG:HH12	1:C:1212:ARG:HG3	1.87	0.40
1:C:952:LYS:HE2	1:C:952:LYS:HB3	1.97	0.40
1:C:1457:TYR:O	1:C:1458:HIS:ND1	2.54	0.40
1:C:1830:VAL:HB	1:C:1837:GLN:HG3	2.04	0.40
1:C:3832:ILE:HD13	1:C:3832:ILE:HA	1.97	0.40
1:C:4859:PHE:HB3	1:C:4862:PHE:HD2	1.86	0.40
1:D:17:ASP:HB2	1:D:98:HIS:HE1	1.86	0.40
1:D:320:LYS:HB3	1:D:356:TRP:CD1	2.56	0.40
1:A:4859:PHE:HB3	1:A:4862:PHE:HD2	1.85	0.40
1:B:996:TRP:CD1	1:B:996:TRP:C	2.94	0.40
1:B:1640:HIS:HA	1:B:1647:CYS:HA	2.04	0.40
1:B:2905:LEU:H	1:B:2905:LEU:HD23	1.86	0.40
1:C:262:LEU:HD13	1:C:274:LEU:HD22	2.04	0.40
1:C:901:LYS:HE3	1:C:903:LEU:HD12	2.03	0.40
1:C:954:LYS:HA	1:C:954:LYS:HD2	1.85	0.40
1:C:1434:TYR:HB2	1:C:1572:ILE:HG21	2.02	0.40
1:C:3507:THR:HB	1:C:3508:SER:H	1.74	0.40
1:D:869:ARG:NH2	1:D:941:MET:HE1	2.36	0.40
1:D:3103:ILE:H	1:D:3103:ILE:HG12	1.76	0.40
1:D:4170:ILE:HD13	1:D:4170:ILE:HA	1.94	0.40
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.34	0.40
2:E:82:TYR:HB3	2:E:86:GLY:HA2	2.04	0.40
1:A:810:PRO:HD2	1:A:813:GLU:OE1	2.21	0.40
1:B:670:GLU:HA	1:B:740:PRO:HB3	2.02	0.40
1:B:2360:LYS:HE3	1:B:2360:LYS:HB2	1.93	0.40
1:C:650:VAL:HG12	1:C:777:PHE:HB2	2.04	0.40
1:C:1519:LEU:HD23	1:C:1519:LEU:HA	1.95	0.40
1:C:1534:LYS:HD2	1:C:1534:LYS:HA	1.82	0.40
1:D:830:ARG:CZ	1:D:1612:PHE:CE2	3.04	0.40
1:D:918:ARG:O	1:D:922:LEU:HG	2.22	0.40
1:A:214:VAL:HG11	1:A:339:ILE:HG13	2.04	0.40
1:A:2359:ARG:HE	1:A:2359:ARG:HB2	1.77	0.40
1:A:2497:ASP:HA	1:A:2547:ALA:HB2	2.03	0.40
1:A:2547:ALA:O	1:A:2551:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2905:LEU:H	1:A:2905:LEU:HD23	1.87	0.40
1:B:784:SER:OG	1:B:785:ALA:N	2.54	0.40
1:B:863:LEU:H	1:B:863:LEU:HD23	1.87	0.40
1:B:887:ILE:HG13	1:B:891:TRP:O	2.21	0.40
1:B:961:MET:HE2	1:B:962:SER:N	2.37	0.40
1:B:2102:VAL:HG11	1:B:2124:LEU:HB2	2.03	0.40
1:B:3090:ALA:O	1:B:3094:SER:N	2.46	0.40
1:B:3180:ASN:OD1	1:B:3180:ASN:N	2.54	0.40
1:B:4958:CYS:C	1:B:4960:ILE:H	2.25	0.40
1:C:869:ARG:NH2	1:C:941:MET:HE1	2.37	0.40
1:C:1008:SER:HB2	1:C:1017:ARG:CZ	2.51	0.40
1:D:682:LEU:HD12	1:D:787:VAL:HG12	2.04	0.40
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.87	0.40
1:D:4771:ILE:HD13	1:D:4771:ILE:HA	1.90	0.40
2:F:44:LYS:HA	2:F:44:LYS:HD2	1.79	0.40
1:A:393:CYS:HB2	1:A:397:GLU:HG3	2.04	0.40
1:A:648:ILE:HG12	1:A:648:ILE:O	2.21	0.40
1:A:1093:GLU:HG2	1:A:1148:VAL:HG12	2.02	0.40
1:A:2368:LEU:HA	1:A:2374:SER:HB2	2.04	0.40
1:B:33:LEU:HG	1:B:53:SER:OG	2.20	0.40
1:B:1847:THR:O	1:B:1851:MET:HG3	2.22	0.40
1:B:1947:CYS:HB3	1:B:2126:ARG:HH21	1.86	0.40
1:B:2023:LEU:HG	1:B:2024:PRO:HD2	2.03	0.40
1:B:2212:VAL:HG22	1:B:2256:TYR:CZ	2.56	0.40
1:B:2440:MET:SD	1:B:2442:LEU:HB3	2.61	0.40
1:C:707:VAL:HG12	1:C:782:SER:HB3	2.03	0.40
1:C:1180:ARG:NE	1:C:1180:ARG:HA	2.36	0.40
1:C:1477:GLY:HA2	1:C:1482:ASN:O	2.22	0.40
1:C:3804:ILE:HD12	1:C:3804:ILE:HA	1.87	0.40
1:D:158:SER:N	1:D:161:GLU:OE1	2.54	0.40
1:D:359:TYR:HB2	1:D:383:HIS:HE1	1.86	0.40
1:D:972:LEU:HD22	1:D:1044:ARG:HB3	2.03	0.40
1:D:1562:ILE:HD13	1:D:1562:ILE:HA	1.94	0.40
1:D:4055:VAL:HG11	1:D:4163:PHE:HZ	1.87	0.40
2:F:26:TYR:CE1	2:F:39:SER:HB3	2.56	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	4214/5037 (84%)	3883 (92%)	329 (8%)	2 (0%)	100	100
1	B	4214/5037 (84%)	3873 (92%)	340 (8%)	1 (0%)	100	100
1	C	4214/5037 (84%)	3878 (92%)	334 (8%)	2 (0%)	100	100
1	D	4214/5037 (84%)	3886 (92%)	327 (8%)	1 (0%)	100	100
2	E	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
2	F	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	G	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	H	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
All	All	17276/20576 (84%)	15878 (92%)	1392 (8%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	862	VAL
1	C	899	ASP
1	A	1023	PRO
1	C	1023	PRO
1	D	1023	PRO
1	B	1023	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	3334/4276 (78%)	3266 (98%)	68 (2%)	50	72
1	B	3334/4276 (78%)	3244 (97%)	90 (3%)	40	65
1	C	3334/4276 (78%)	3260 (98%)	74 (2%)	47	70
1	D	3334/4276 (78%)	3259 (98%)	75 (2%)	47	70
2	E	80/88 (91%)	78 (98%)	2 (2%)	42	67
2	F	80/88 (91%)	79 (99%)	1 (1%)	65	79
2	G	80/88 (91%)	79 (99%)	1 (1%)	65	79
2	H	80/88 (91%)	79 (99%)	1 (1%)	65	79
All	All	13656/17456 (78%)	13344 (98%)	312 (2%)	46	69

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TYR
1	A	164	ARG
1	A	178	ARG
1	A	195	PHE
1	A	247	TYR
1	A	261	ARG
1	A	275	ARG
1	A	421	PHE
1	A	493	ARG
1	A	503	PHE
1	A	506	TYR
1	A	720	HIS
1	A	771	PHE
1	A	812	HIS
1	A	830	ARG
1	A	866	HIS
1	A	904	HIS
1	A	913	LEU
1	A	919	ASN
1	A	1006	SER
1	A	1089	TYR
1	A	1112	ASP
1	A	1143	TRP
1	A	1288	PHE
1	A	1421	ARG
1	A	1423	ASP
1	A	1563	GLN

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Mol	Chain	Res	Type
1	A	1579	MET
1	A	1647	CYS
1	A	1814	MET
1	A	1865	MET
1	A	1929	MET
1	A	2014	ASP
1	A	2128	TYR
1	A	2170	MET
1	A	2211	MET
1	A	2331	TYR
1	A	2440	MET
1	A	2494	PHE
1	A	2519	LEU
1	A	2633	LEU
1	A	2939	ARG
1	A	2957	PHE
1	A	2966	TRP
1	A	2971	GLN
1	A	3003	LEU
1	A	3010	PHE
1	A	3030	HIS
1	A	3068	LEU
1	A	3193	CYS
1	A	3213	TYR
1	A	3277	LEU
1	A	3358	PHE
1	A	3444	TYR
1	A	3540	TYR
1	A	3727	ASP
1	A	3899	PHE
1	A	3924	LEU
1	A	3977	GLN
1	A	3999	MET
1	A	4039	MET
1	A	4087	LEU
1	A	4156	HIS
1	A	4166	LEU
1	A	4571	PHE
1	A	4743	MET
1	A	4807	PHE
1	A	4912	TYR
1	B	103	TYR

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Mol	Chain	Res	Type
1	B	131	LEU
1	B	164	ARG
1	B	178	ARG
1	B	195	PHE
1	B	247	TYR
1	B	261	ARG
1	B	275	ARG
1	B	421	PHE
1	B	493	ARG
1	B	503	PHE
1	B	506	TYR
1	B	579	GLN
1	B	659	TYR
1	B	674	PHE
1	B	714	TYR
1	B	721	LEU
1	B	771	PHE
1	B	811	CYS
1	B	812	HIS
1	B	830	ARG
1	B	866	HIS
1	B	899	ASP
1	B	904	HIS
1	B	911	HIS
1	B	913	LEU
1	B	919	ASN
1	B	961	MET
1	B	1011	GLN
1	B	1038	SER
1	B	1089	TYR
1	B	1112	ASP
1	B	1143	TRP
1	B	1155	LEU
1	B	1219	LEU
1	B	1288	PHE
1	B	1421	ARG
1	B	1435	TYR
1	B	1492	CYS
1	B	1494	MET
1	B	1506	GLN
1	B	1553	PHE
1	B	1563	GLN

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Mol	Chain	Res	Type
1	B	1579	MET
1	B	1647	CYS
1	B	1814	MET
1	B	1865	MET
1	B	1929	MET
1	B	2014	ASP
1	B	2109	ASP
1	B	2186	MET
1	B	2211	MET
1	B	2232	CYS
1	B	2331	TYR
1	B	2440	MET
1	B	2494	PHE
1	B	2519	LEU
1	B	2633	LEU
1	B	2863	SER
1	B	2939	ARG
1	B	2966	TRP
1	B	2971	GLN
1	B	3003	LEU
1	B	3010	PHE
1	B	3030	HIS
1	B	3068	LEU
1	B	3131	TYR
1	B	3213	TYR
1	B	3268	HIS
1	B	3277	LEU
1	B	3444	TYR
1	B	3525	CYS
1	B	3540	TYR
1	B	3576	TYR
1	B	3652	MET
1	B	3679	LYS
1	B	3720	TYR
1	B	3727	ASP
1	B	3899	PHE
1	B	3999	MET
1	B	4039	MET
1	B	4087	LEU
1	B	4156	HIS
1	B	4571	PHE
1	B	4704	LEU

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Mol	Chain	Res	Type
1	B	4743	MET
1	B	4768	LEU
1	B	4769	MET
1	B	4807	PHE
1	B	4912	TYR
1	C	164	ARG
1	C	178	ARG
1	C	247	TYR
1	C	261	ARG
1	C	275	ARG
1	C	315	CYS
1	C	493	ARG
1	C	503	PHE
1	C	506	TYR
1	C	652	ARG
1	C	771	PHE
1	C	812	HIS
1	C	820	ARG
1	C	830	ARG
1	C	866	HIS
1	C	904	HIS
1	C	913	LEU
1	C	919	ASN
1	C	922	LEU
1	C	961	MET
1	C	984	LEU
1	C	1006	SER
1	C	1011	GLN
1	C	1038	SER
1	C	1089	TYR
1	C	1139	PHE
1	C	1143	TRP
1	C	1155	LEU
1	C	1288	PHE
1	C	1421	ARG
1	C	1553	PHE
1	C	1579	MET
1	C	1647	CYS
1	C	1814	MET
1	C	1929	MET
1	C	2014	ASP
1	C	2109	ASP

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Mol	Chain	Res	Type
1	C	2192	TYR
1	C	2211	MET
1	C	2232	CYS
1	C	2331	TYR
1	C	2494	PHE
1	C	2519	LEU
1	C	2568	LEU
1	C	2633	LEU
1	C	2939	ARG
1	C	2966	TRP
1	C	2971	GLN
1	C	3003	LEU
1	C	3010	PHE
1	C	3030	HIS
1	C	3068	LEU
1	C	3131	TYR
1	C	3213	TYR
1	C	3223	SER
1	C	3268	HIS
1	C	3277	LEU
1	C	3358	PHE
1	C	3398	PHE
1	C	3444	TYR
1	C	3540	TYR
1	C	3679	LYS
1	C	3720	TYR
1	C	3727	ASP
1	C	3899	PHE
1	C	3924	LEU
1	C	3977	GLN
1	C	4068	LEU
1	C	4087	LEU
1	C	4156	HIS
1	C	4571	PHE
1	C	4704	LEU
1	C	4743	MET
1	C	4807	PHE
1	D	103	TYR
1	D	164	ARG
1	D	178	ARG
1	D	247	TYR
1	D	261	ARG

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Mol	Chain	Res	Type
1	D	275	ARG
1	D	315	CYS
1	D	421	PHE
1	D	493	ARG
1	D	503	PHE
1	D	506	TYR
1	D	579	GLN
1	D	630	GLU
1	D	674	PHE
1	D	771	PHE
1	D	778	PHE
1	D	811	CYS
1	D	812	HIS
1	D	871	ARG
1	D	904	HIS
1	D	911	HIS
1	D	913	LEU
1	D	919	ASN
1	D	922	LEU
1	D	961	MET
1	D	996	TRP
1	D	1089	TYR
1	D	1112	ASP
1	D	1143	TRP
1	D	1155	LEU
1	D	1288	PHE
1	D	1421	ARG
1	D	1423	ASP
1	D	1435	TYR
1	D	1489	CYS
1	D	1492	CYS
1	D	1579	MET
1	D	1647	CYS
1	D	1648	MET
1	D	1814	MET
1	D	1865	MET
1	D	1929	MET
1	D	2014	ASP
1	D	2109	ASP
1	D	2211	MET
1	D	2232	CYS
1	D	2331	TYR

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Mol	Chain	Res	Type
1	D	2423	MET
1	D	2494	PHE
1	D	2519	LEU
1	D	2633	LEU
1	D	2939	ARG
1	D	2966	TRP
1	D	2971	GLN
1	D	3003	LEU
1	D	3010	PHE
1	D	3030	HIS
1	D	3068	LEU
1	D	3213	TYR
1	D	3268	HIS
1	D	3277	LEU
1	D	3444	TYR
1	D	3540	TYR
1	D	3652	MET
1	D	3899	PHE
1	D	3999	MET
1	D	4039	MET
1	D	4087	LEU
1	D	4156	HIS
1	D	4166	LEU
1	D	4571	PHE
1	D	4704	LEU
1	D	4743	MET
1	D	4768	LEU
1	D	4807	PHE
2	E	15	PHE
2	E	79	ASP
2	F	18	LYS
2	G	40	ARG
2	H	22	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	181	HIS
1	A	772	ASN
1	A	1011	GLN
1	A	1130	GLN

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Mol	Chain	Res	Type
1	A	1563	GLN
1	A	1696	HIS
1	A	2005	GLN
1	A	2112	GLN
1	A	2176	ASN
1	A	2188	ASN
1	A	2246	ASN
1	A	2247	GLN
1	A	2663	ASN
1	A	3013	HIS
1	A	3837	GLN
1	A	4162	ASN
1	A	4650	HIS
1	A	4700	GLN
1	B	772	ASN
1	B	1130	GLN
1	B	1545	ASN
1	B	1563	GLN
1	B	2005	GLN
1	B	2112	GLN
1	B	2188	ASN
1	B	2246	ASN
1	B	2247	GLN
1	B	2663	ASN
1	B	3013	HIS
1	B	3837	GLN
1	B	3882	GLN
1	B	4162	ASN
1	B	4650	HIS
1	B	4700	GLN
1	B	4983	HIS
1	C	12	GLN
1	C	23	GLN
1	C	181	HIS
1	C	772	ASN
1	C	1130	GLN
1	C	2005	GLN
1	C	2112	GLN
1	C	2176	ASN
1	C	2188	ASN
1	C	2246	ASN
1	C	2247	GLN

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Mol	Chain	Res	Type
1	C	2663	ASN
1	C	3013	HIS
1	C	3837	GLN
1	C	4162	ASN
1	C	4650	HIS
1	D	23	GLN
1	D	772	ASN
1	D	838	HIS
1	D	1011	GLN
1	D	1130	GLN
1	D	2005	GLN
1	D	2112	GLN
1	D	2176	ASN
1	D	2188	ASN
1	D	2246	ASN
1	D	2247	GLN
1	D	2663	ASN
1	D	3013	HIS
1	D	3837	GLN
1	D	4162	ASN
1	D	4650	HIS
1	D	4700	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	B	5102	-	28,33,33	0.66	0	34,52,52	0.58	1 (2%)
5	U1C	C	5103	-	23,25,25	6.21	12 (52%)	26,35,35	3.18	9 (34%)
4	ATP	C	5102	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
5	U1C	B	5103	-	23,25,25	6.19	12 (52%)	26,35,35	3.20	9 (34%)
5	U1C	D	5103	-	23,25,25	6.20	12 (52%)	26,35,35	3.19	9 (34%)
4	ATP	A	5102	-	28,33,33	0.65	0	34,52,52	0.58	1 (2%)
4	ATP	D	5102	-	28,33,33	0.65	0	34,52,52	0.58	1 (2%)
5	U1C	A	5103	-	23,25,25	6.21	12 (52%)	26,35,35	3.20	9 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	5102	-	-	9/18/38/38	0/3/3/3
5	U1C	C	5103	-	-	1/7/25/25	0/3/3/3
4	ATP	C	5102	-	-	9/18/38/38	0/3/3/3
5	U1C	B	5103	-	-	1/7/25/25	0/3/3/3
5	U1C	D	5103	-	-	1/7/25/25	0/3/3/3
4	ATP	A	5102	-	-	9/18/38/38	0/3/3/3
4	ATP	D	5102	-	-	9/18/38/38	0/3/3/3
5	U1C	A	5103	-	-	1/7/25/25	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5103	U1C	C1-N2	-18.77	1.32	1.45
5	A	5103	U1C	C1-N2	-18.76	1.32	1.45
5	D	5103	U1C	C1-N2	-18.64	1.32	1.45
5	B	5103	U1C	C1-N2	-18.59	1.32	1.45
5	B	5103	U1C	C1-C2	-10.54	1.39	1.51
5	D	5103	U1C	C1-C2	-10.54	1.39	1.51
5	C	5103	U1C	C1-C2	-10.51	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5103	U1C	C1-C2	-10.49	1.39	1.51
5	B	5103	U1C	O4-N4	10.46	1.40	1.22
5	A	5103	U1C	O4-N4	10.42	1.40	1.22
5	C	5103	U1C	O4-N4	10.41	1.40	1.22
5	D	5103	U1C	O4-N4	10.41	1.40	1.22
5	A	5103	U1C	O2-C3	9.84	1.40	1.23
5	B	5103	U1C	O2-C3	9.81	1.40	1.23
5	C	5103	U1C	O2-C3	9.81	1.40	1.23
5	D	5103	U1C	O2-C3	9.80	1.40	1.23
5	A	5103	U1C	O1-C2	8.68	1.40	1.23
5	B	5103	U1C	O1-C2	8.67	1.40	1.23
5	D	5103	U1C	O1-C2	8.67	1.40	1.23
5	C	5103	U1C	O1-C2	8.61	1.40	1.23
5	B	5103	U1C	C4-N3	6.66	1.45	1.27
5	C	5103	U1C	C4-N3	6.66	1.45	1.27
5	D	5103	U1C	C4-N3	6.66	1.45	1.27
5	A	5103	U1C	C4-N3	6.66	1.45	1.27
5	D	5103	U1C	C3-N2	-5.27	1.32	1.37
5	B	5103	U1C	C3-N2	-5.24	1.32	1.37
5	C	5103	U1C	C3-N2	-5.23	1.32	1.37
5	A	5103	U1C	C3-N2	-5.22	1.32	1.37
5	B	5103	U1C	C5-C4	4.23	1.53	1.45
5	A	5103	U1C	C5-C4	4.22	1.53	1.45
5	A	5103	U1C	C9-C8	4.19	1.53	1.46
5	D	5103	U1C	C5-C4	4.19	1.53	1.45
5	C	5103	U1C	C9-C8	4.17	1.53	1.46
5	B	5103	U1C	C9-C8	4.15	1.53	1.46
5	C	5103	U1C	C5-C4	4.15	1.53	1.45
5	D	5103	U1C	C9-C8	4.13	1.53	1.46
5	D	5103	U1C	N2-N3	3.86	1.41	1.37
5	C	5103	U1C	N2-N3	3.81	1.41	1.37
5	A	5103	U1C	N2-N3	3.79	1.41	1.37
5	B	5103	U1C	N2-N3	3.77	1.41	1.37
5	A	5103	U1C	C3-N1	-3.29	1.32	1.38
5	C	5103	U1C	C3-N1	-3.25	1.32	1.38
5	B	5103	U1C	C3-N1	-3.22	1.32	1.38
5	D	5103	U1C	C3-N1	-3.22	1.32	1.38
5	A	5103	U1C	C2-N1	-2.94	1.32	1.37
5	B	5103	U1C	C2-N1	-2.90	1.32	1.37
5	D	5103	U1C	C2-N1	-2.90	1.32	1.37
5	C	5103	U1C	C2-N1	-2.85	1.32	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5103	U1C	C2-C1-N2	8.41	106.93	101.45
5	B	5103	U1C	C2-C1-N2	8.40	106.92	101.45
5	A	5103	U1C	C2-C1-N2	8.38	106.91	101.45
5	D	5103	U1C	C2-C1-N2	8.37	106.90	101.45
5	B	5103	U1C	C1-N2-C3	-7.36	108.27	112.31
5	A	5103	U1C	C1-N2-C3	-7.32	108.29	112.31
5	D	5103	U1C	C1-N2-C3	-7.29	108.31	112.31
5	A	5103	U1C	C3-N2-N3	7.24	125.89	119.83
5	C	5103	U1C	C1-N2-C3	-7.24	108.33	112.31
5	B	5103	U1C	C3-N2-N3	7.17	125.83	119.83
5	D	5103	U1C	C3-N2-N3	7.15	125.80	119.83
5	C	5103	U1C	C3-N2-N3	7.13	125.79	119.83
5	B	5103	U1C	C2-N1-C3	-4.84	108.22	112.47
5	D	5103	U1C	C2-N1-C3	-4.84	108.22	112.47
5	C	5103	U1C	C2-N1-C3	-4.81	108.25	112.47
5	A	5103	U1C	C2-N1-C3	-4.75	108.30	112.47
5	A	5103	U1C	C5-C4-N3	-4.32	110.43	118.74
5	C	5103	U1C	C5-C4-N3	-4.27	110.52	118.74
5	D	5103	U1C	C5-C4-N3	-4.27	110.52	118.74
5	B	5103	U1C	C5-C4-N3	-4.27	110.52	118.74
5	B	5103	U1C	N1-C3-N2	3.65	109.63	106.12
5	D	5103	U1C	N1-C3-N2	3.63	109.61	106.12
5	A	5103	U1C	N1-C3-N2	3.62	109.59	106.12
5	C	5103	U1C	N1-C3-N2	3.61	109.58	106.12
5	C	5103	U1C	C7-C8-C9	-3.43	125.57	128.77
5	D	5103	U1C	C7-C8-C9	-3.42	125.57	128.77
5	B	5103	U1C	C7-C8-C9	-3.42	125.58	128.77
5	A	5103	U1C	C7-C8-C9	-3.40	125.59	128.77
5	A	5103	U1C	O2-C3-N2	-2.69	125.13	127.67
5	B	5103	U1C	O2-C3-N2	-2.64	125.18	127.67
5	C	5103	U1C	O2-C3-N2	-2.60	125.22	127.67
5	D	5103	U1C	O2-C3-N2	-2.60	125.22	127.67
5	A	5103	U1C	C1-N2-N3	-2.54	125.82	127.64
5	C	5103	U1C	C1-N2-N3	-2.46	125.88	127.64
5	D	5103	U1C	C1-N2-N3	-2.45	125.89	127.64
5	B	5103	U1C	C1-N2-N3	-2.43	125.90	127.64
4	C	5102	ATP	C5-C6-N6	2.34	123.88	120.31
4	A	5102	ATP	C5-C6-N6	2.32	123.85	120.31
4	B	5102	ATP	C5-C6-N6	2.29	123.81	120.31
4	D	5102	ATP	C5-C6-N6	2.29	123.80	120.31

There are no chirality outliers.

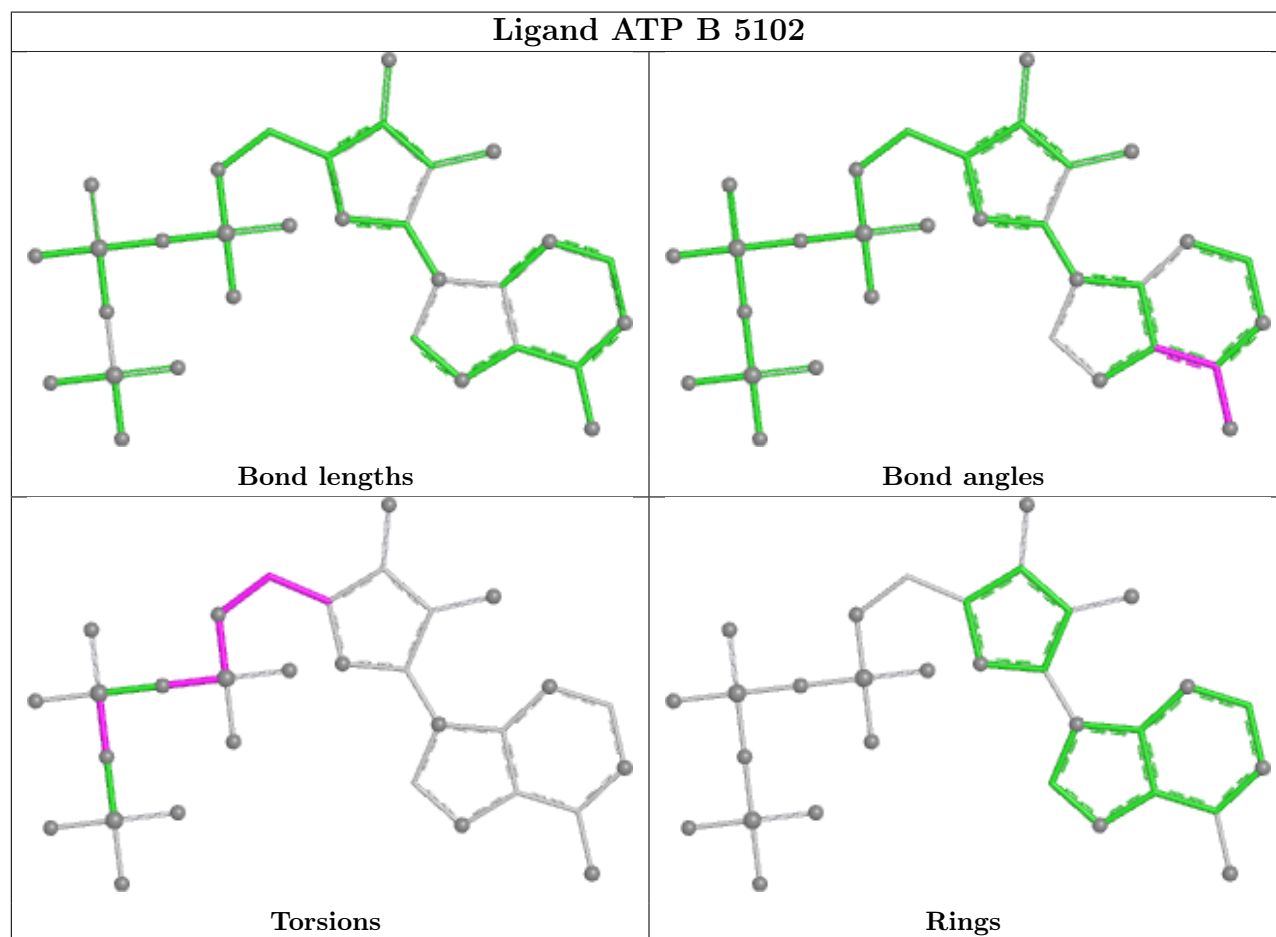
All (40) torsion outliers are listed below:

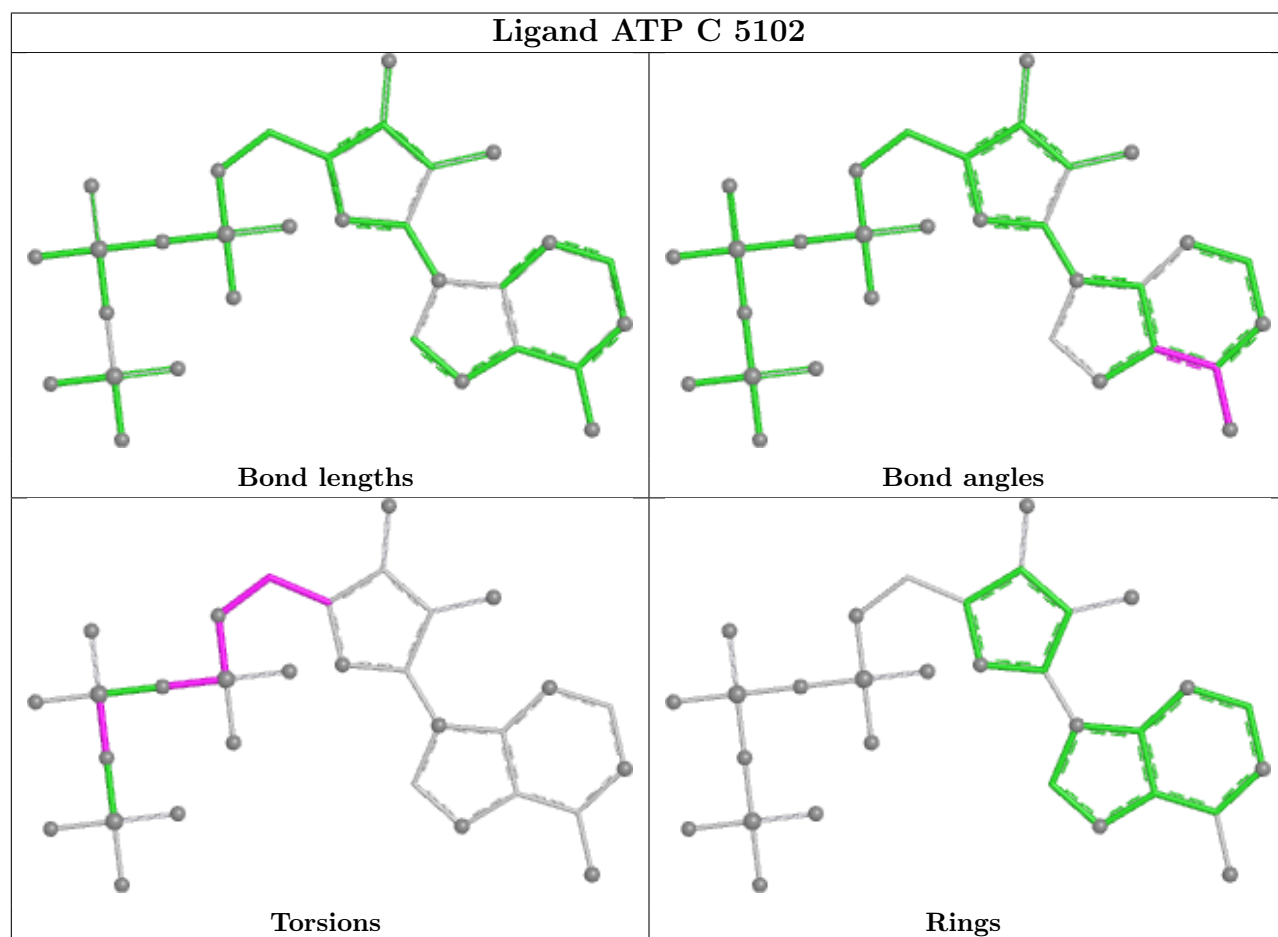
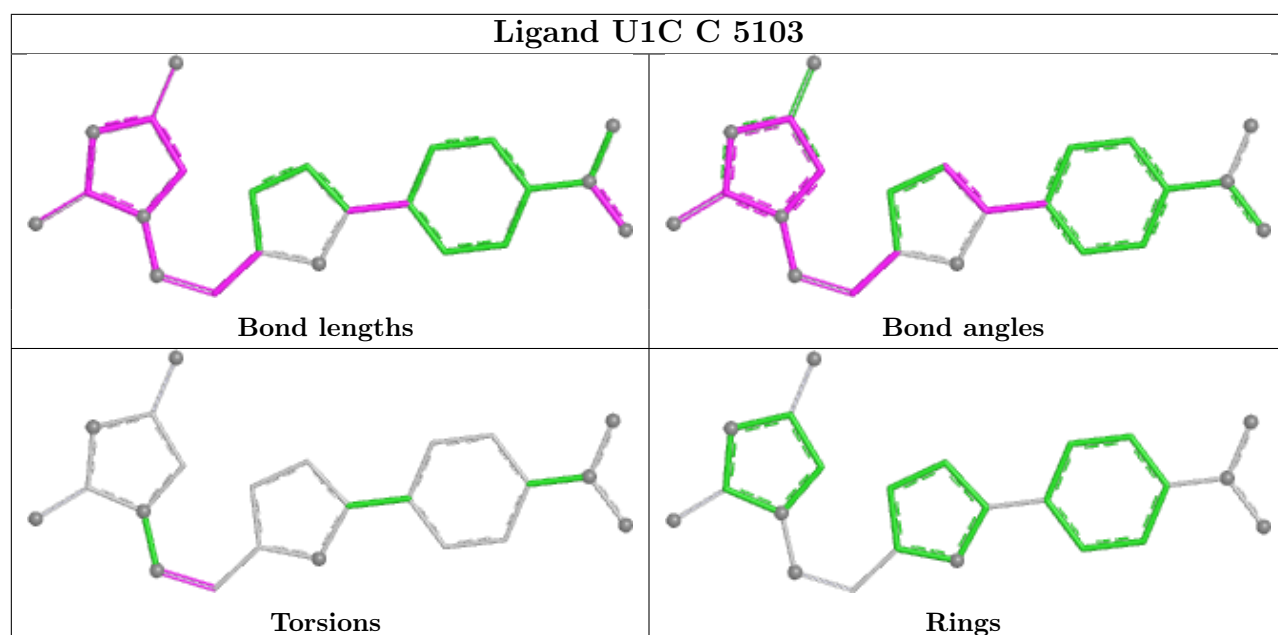
Mol	Chain	Res	Type	Atoms
4	A	5102	ATP	C5'-O5'-PA-O1A
4	A	5102	ATP	C5'-O5'-PA-O2A
4	A	5102	ATP	C5'-O5'-PA-O3A
4	A	5102	ATP	O4'-C4'-C5'-O5'
4	B	5102	ATP	C5'-O5'-PA-O1A
4	B	5102	ATP	C5'-O5'-PA-O2A
4	B	5102	ATP	C5'-O5'-PA-O3A
4	B	5102	ATP	O4'-C4'-C5'-O5'
4	C	5102	ATP	C5'-O5'-PA-O1A
4	C	5102	ATP	C5'-O5'-PA-O2A
4	C	5102	ATP	C5'-O5'-PA-O3A
4	C	5102	ATP	O4'-C4'-C5'-O5'
4	D	5102	ATP	C5'-O5'-PA-O1A
4	D	5102	ATP	C5'-O5'-PA-O2A
4	D	5102	ATP	C5'-O5'-PA-O3A
4	D	5102	ATP	O4'-C4'-C5'-O5'
5	A	5103	U1C	C5-C4-N3-N2
5	B	5103	U1C	C5-C4-N3-N2
5	C	5103	U1C	C5-C4-N3-N2
5	D	5103	U1C	C5-C4-N3-N2
4	A	5102	ATP	C3'-C4'-C5'-O5'
4	B	5102	ATP	C3'-C4'-C5'-O5'
4	C	5102	ATP	C3'-C4'-C5'-O5'
4	D	5102	ATP	C3'-C4'-C5'-O5'
4	A	5102	ATP	PB-O3A-PA-O2A
4	B	5102	ATP	PB-O3A-PA-O2A
4	C	5102	ATP	PB-O3A-PA-O2A
4	D	5102	ATP	PB-O3A-PA-O2A
4	A	5102	ATP	C4'-C5'-O5'-PA
4	B	5102	ATP	C4'-C5'-O5'-PA
4	C	5102	ATP	C4'-C5'-O5'-PA
4	D	5102	ATP	C4'-C5'-O5'-PA
4	A	5102	ATP	PG-O3B-PB-O2B
4	B	5102	ATP	PG-O3B-PB-O2B
4	C	5102	ATP	PG-O3B-PB-O2B
4	D	5102	ATP	PG-O3B-PB-O2B
4	A	5102	ATP	PB-O3A-PA-O1A
4	B	5102	ATP	PB-O3A-PA-O1A
4	C	5102	ATP	PB-O3A-PA-O1A
4	D	5102	ATP	PB-O3A-PA-O1A

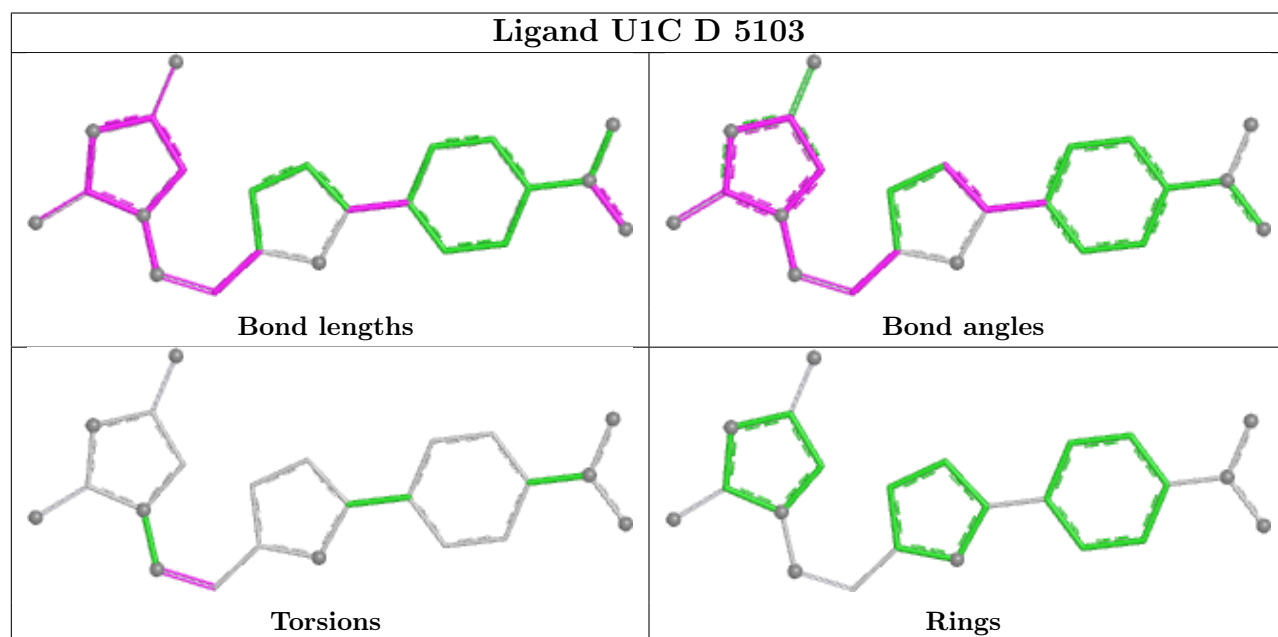
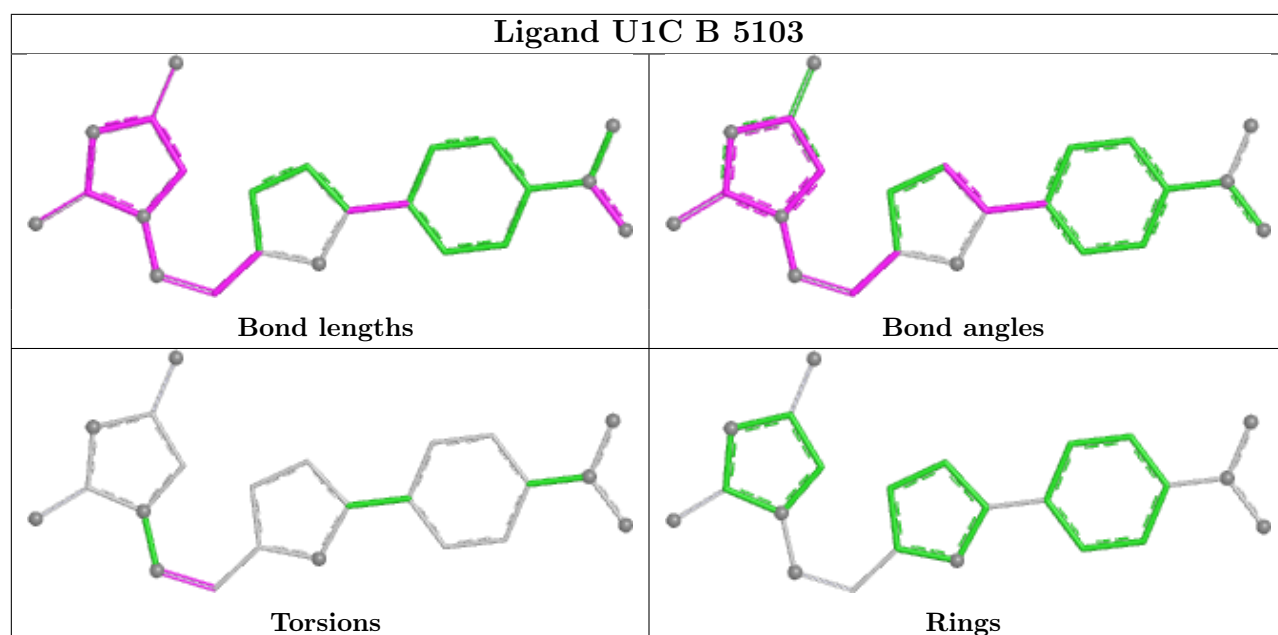
There are no ring outliers.

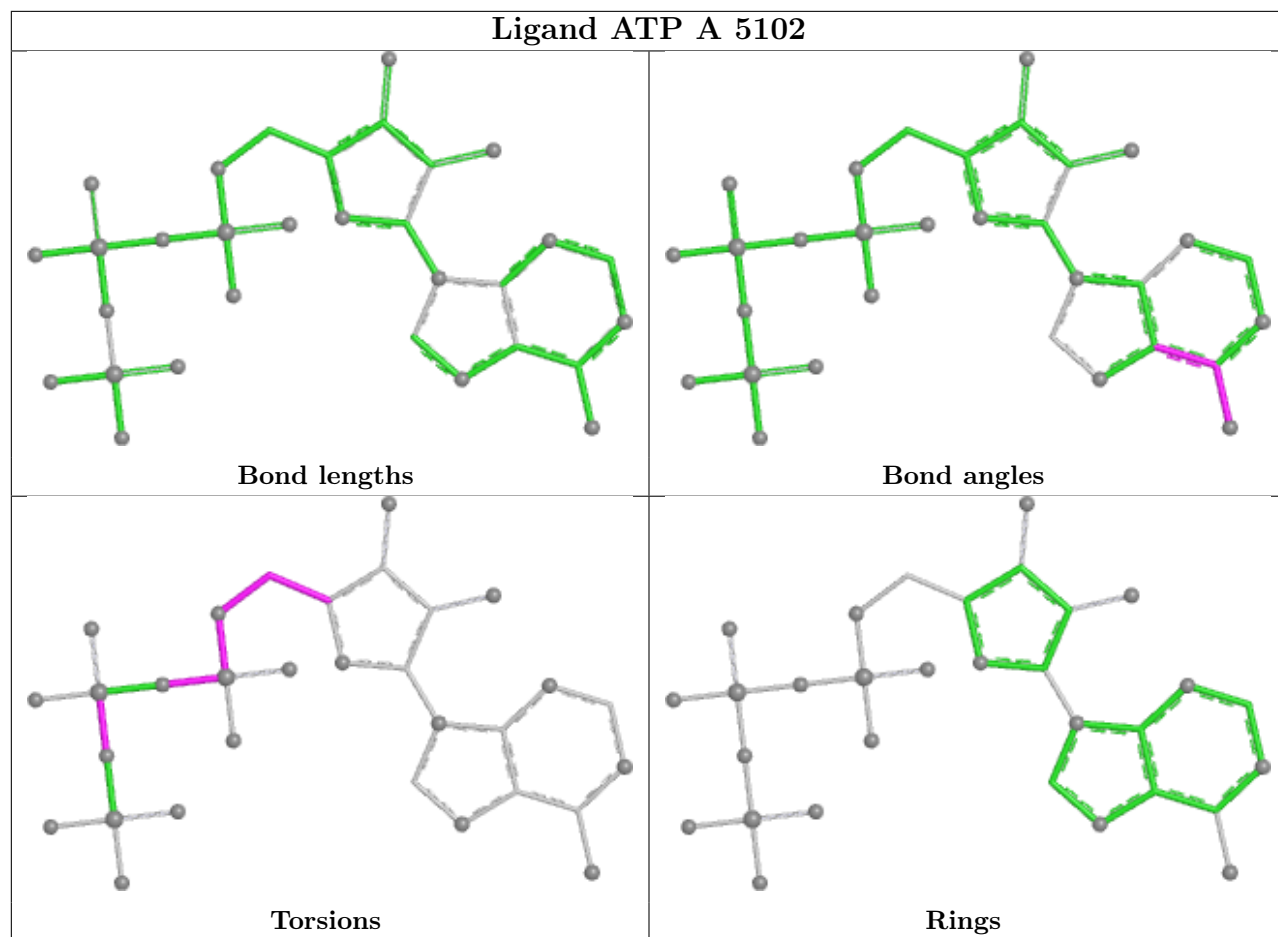
No monomer is involved in short contacts.

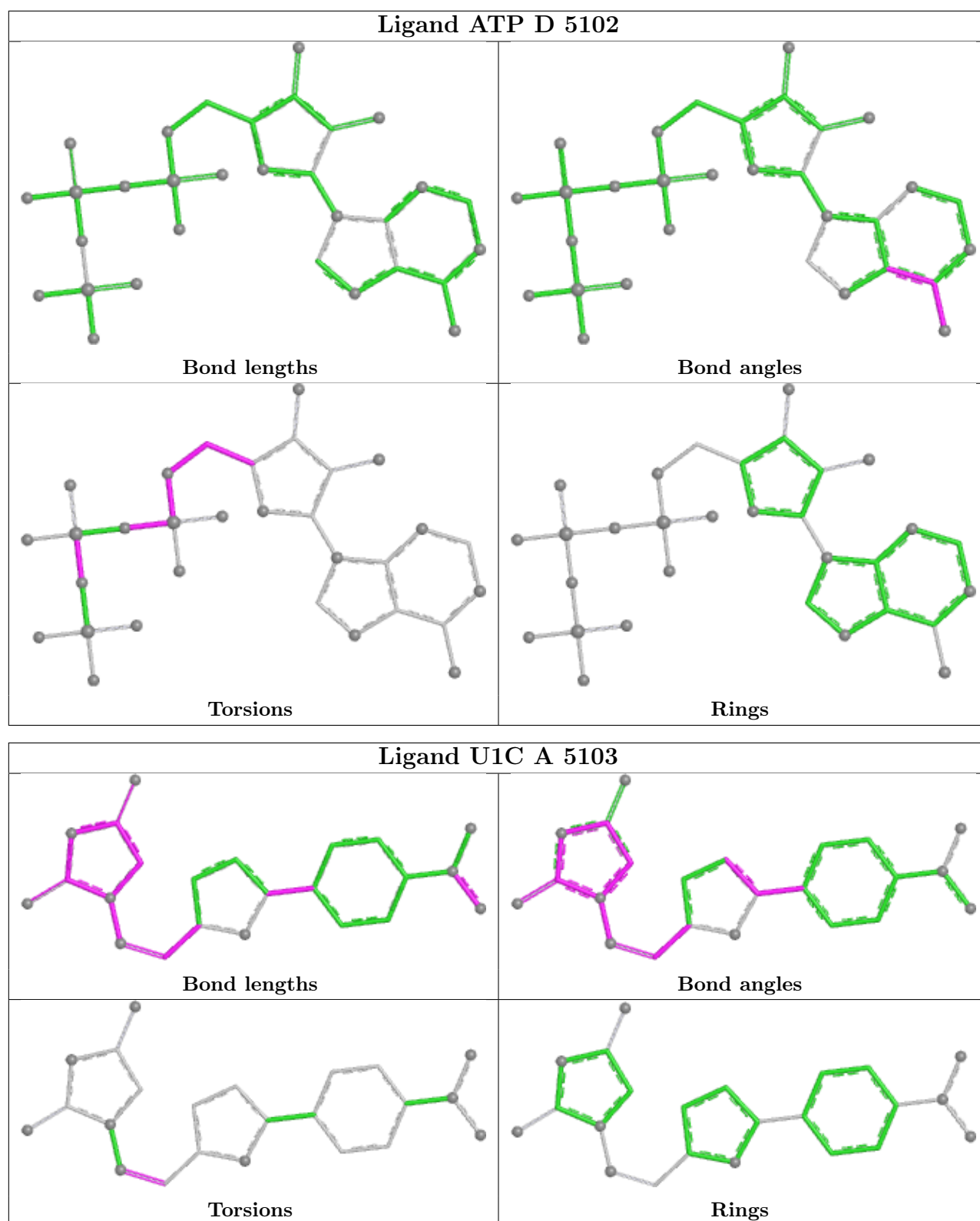
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

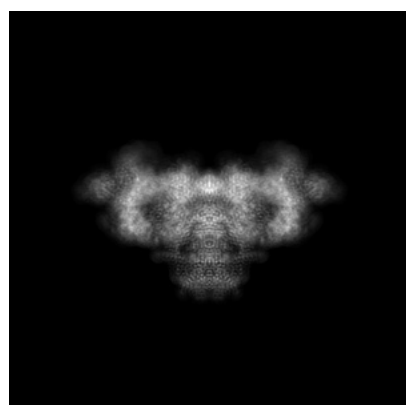
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45584. These allow visual inspection of the internal detail of the map and identification of artifacts.

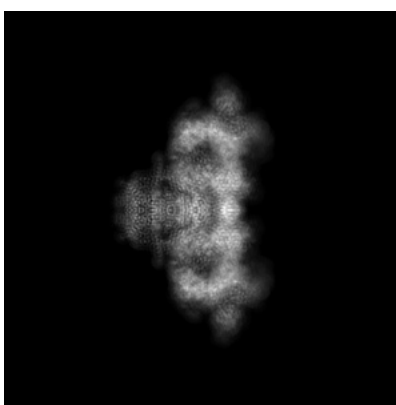
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

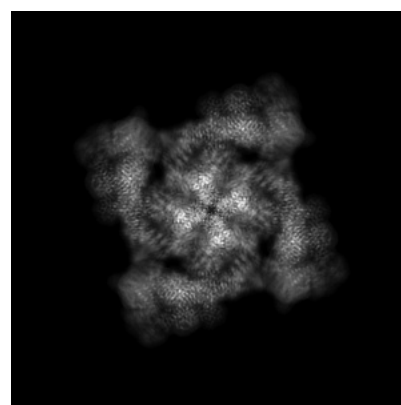
6.1.1 Primary map



X



Y

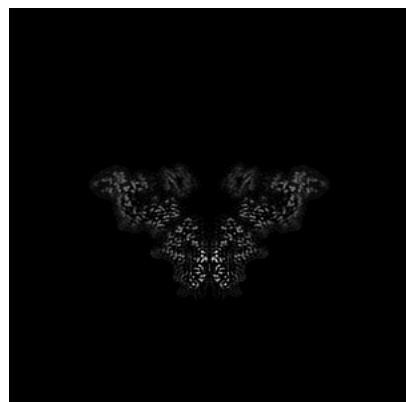


Z

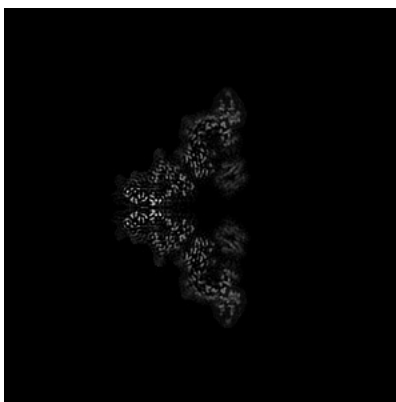
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

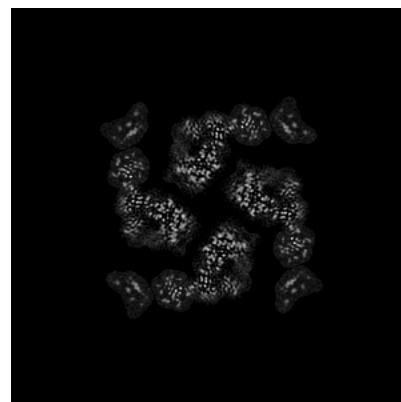
6.2.1 Primary map



X Index: 232



Y Index: 232

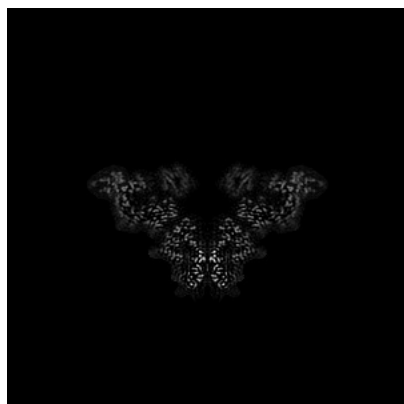


Z Index: 232

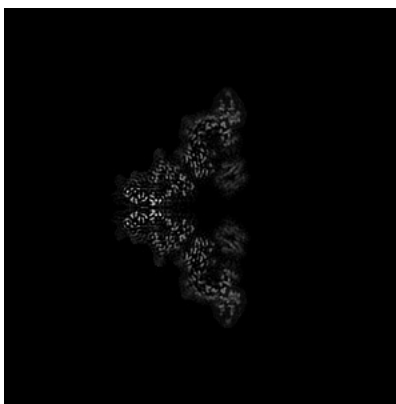
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

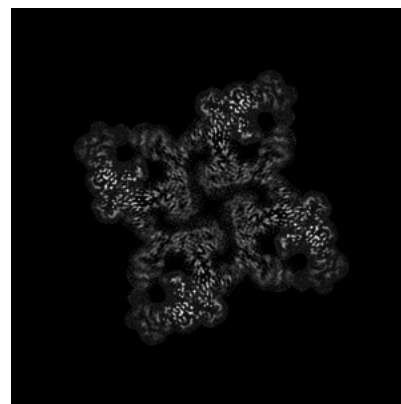
6.3.1 Primary map



X Index: 232



Y Index: 232

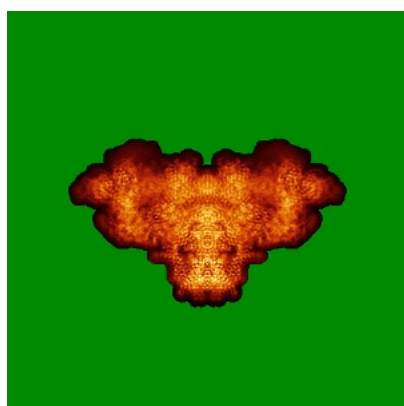


Z Index: 261

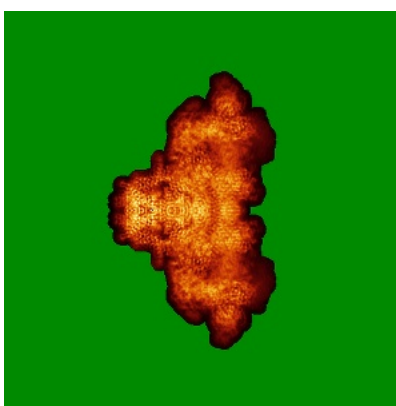
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

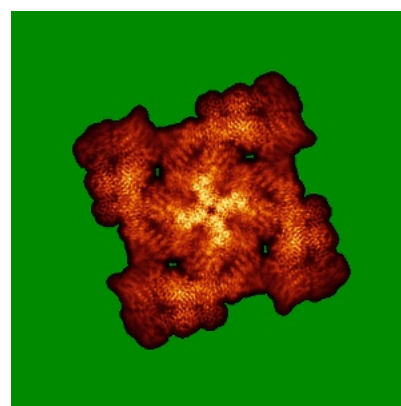
6.4.1 Primary map



X



Y

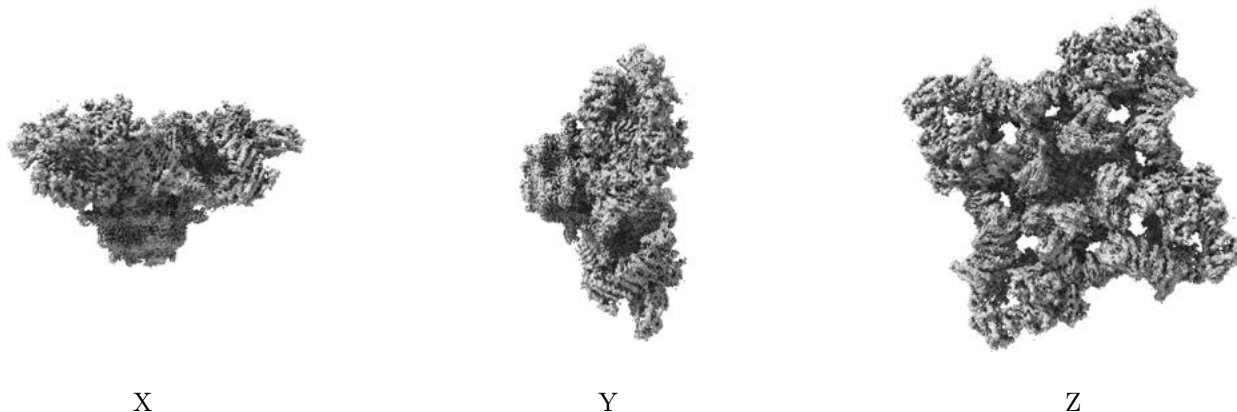


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

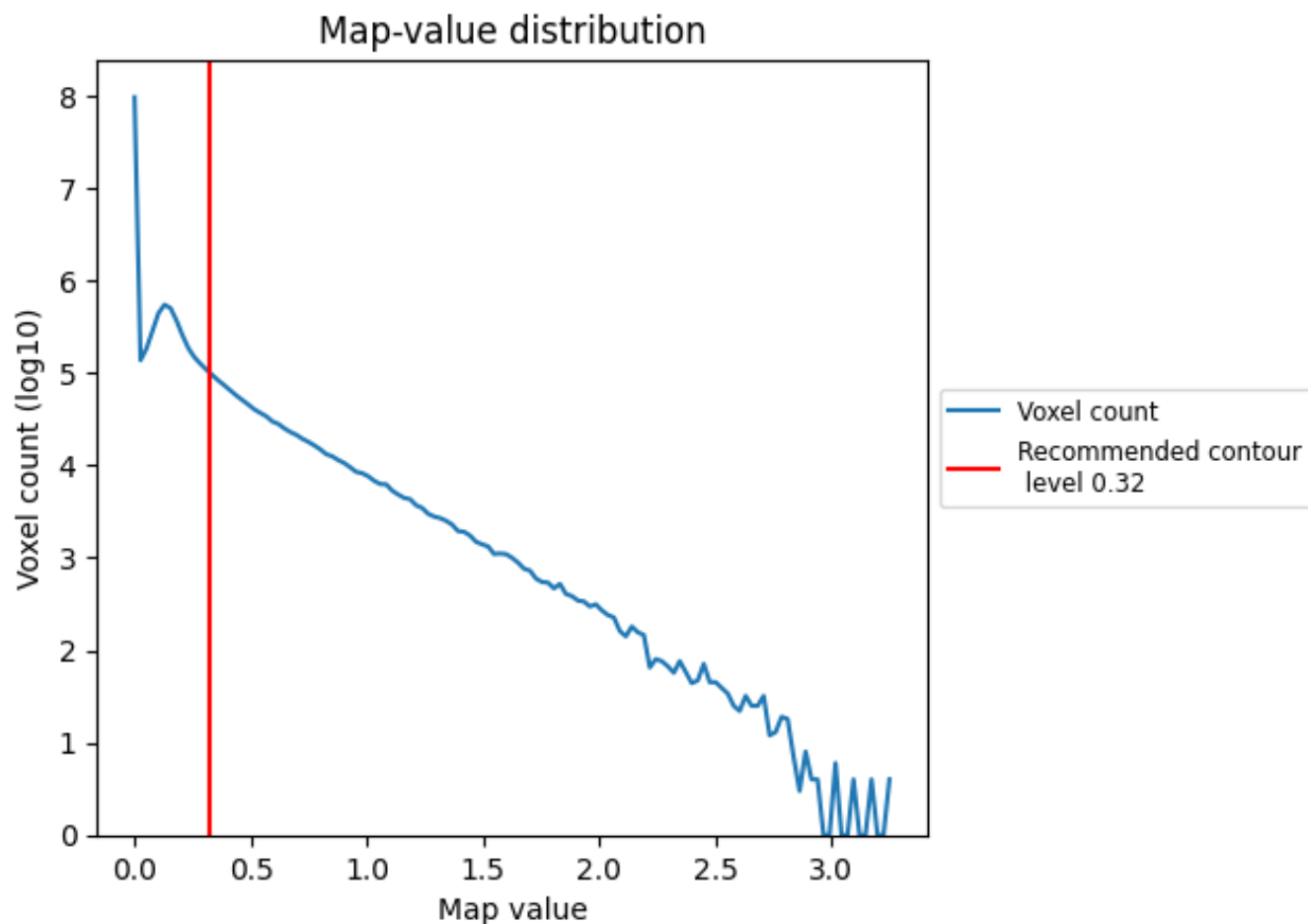
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

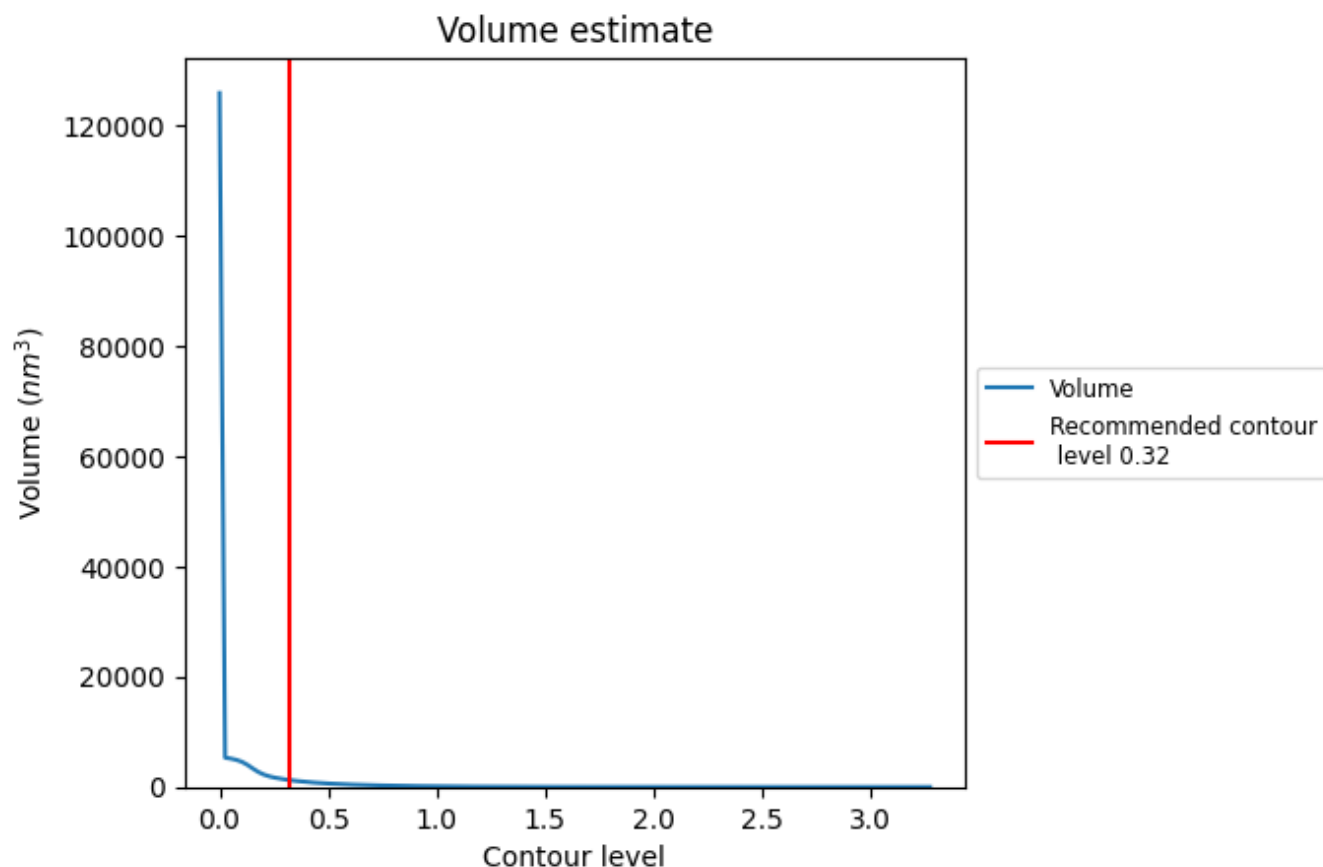
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

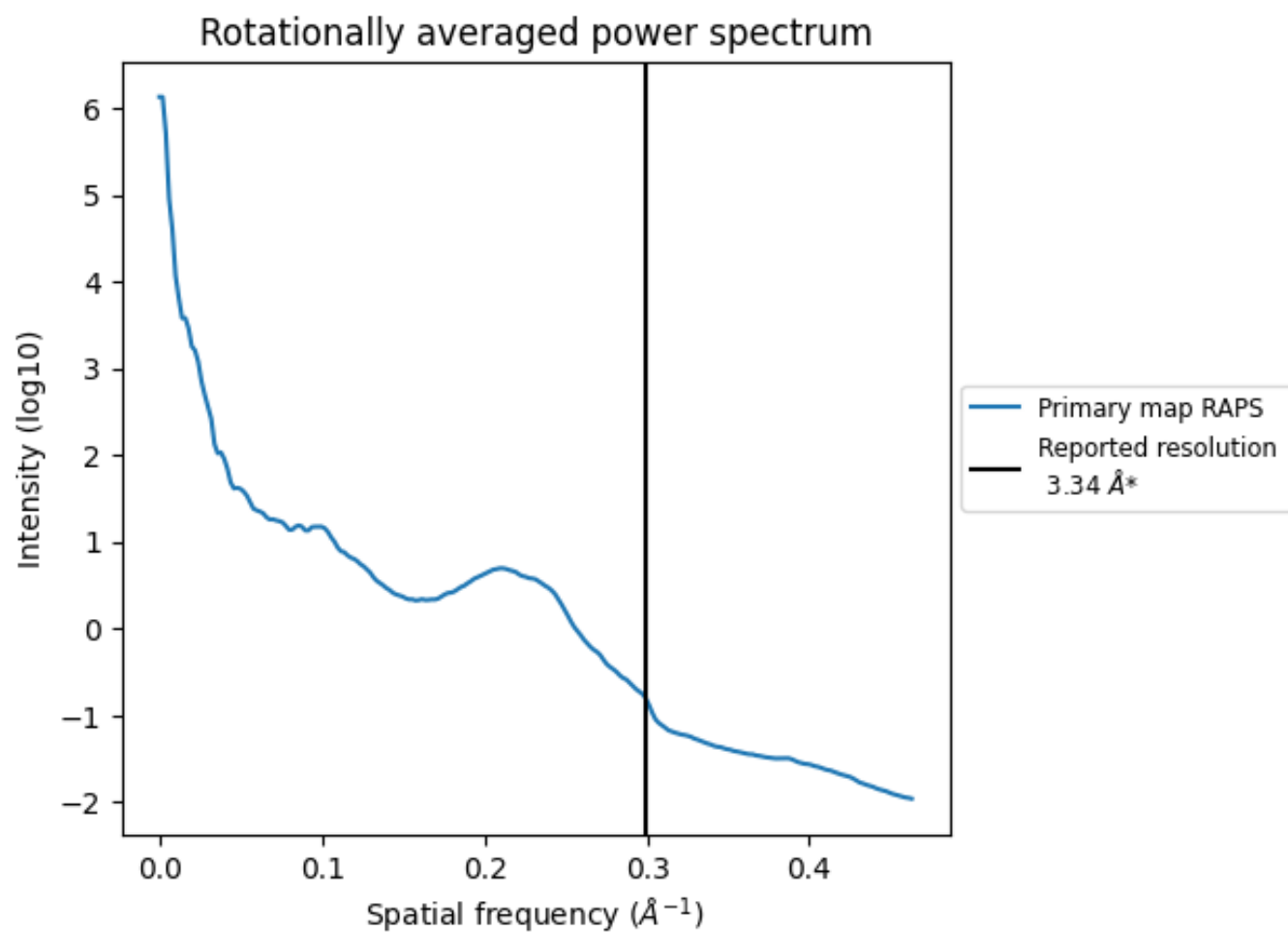
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1262 nm^3 ; this corresponds to an approximate mass of 1140 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

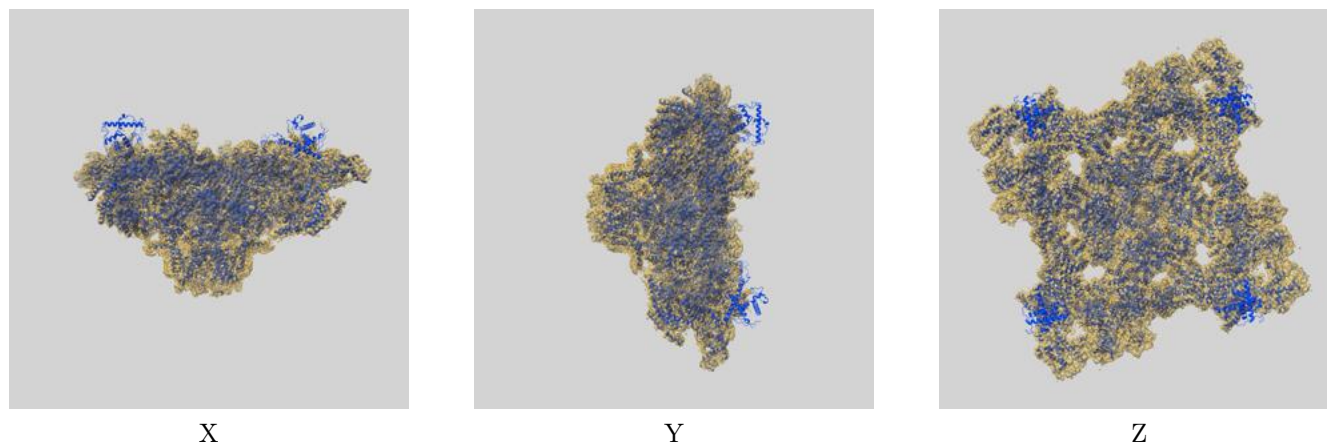
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

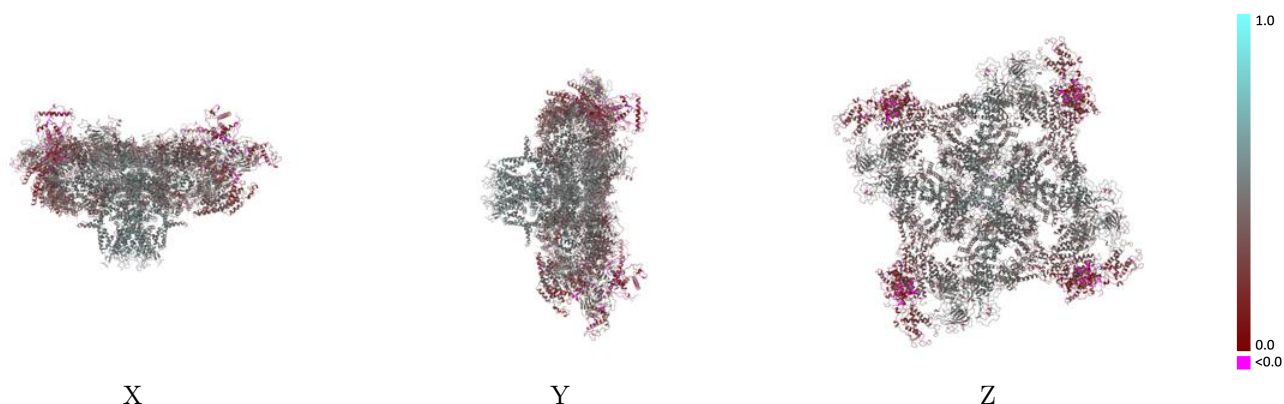
This section contains information regarding the fit between EMDB map EMD-45584 and PDB model 9CGP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



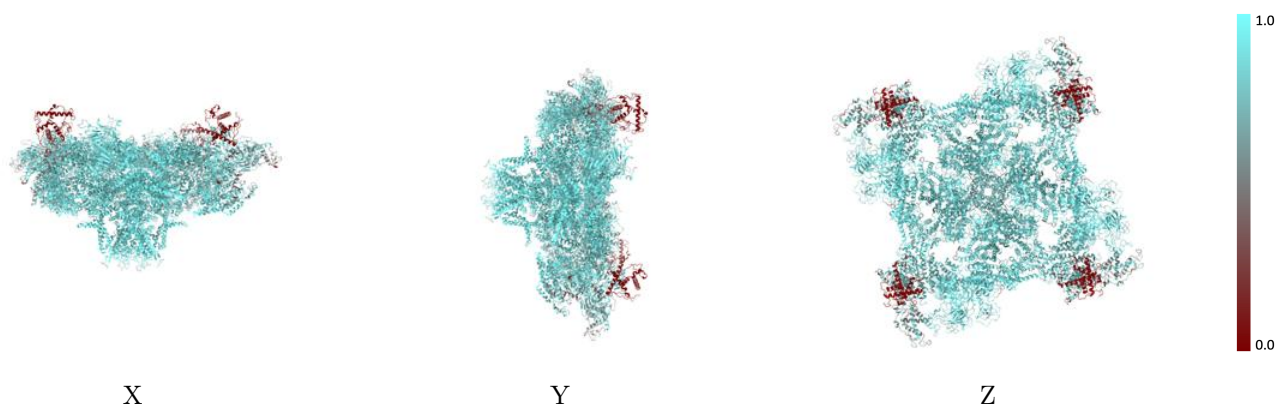
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



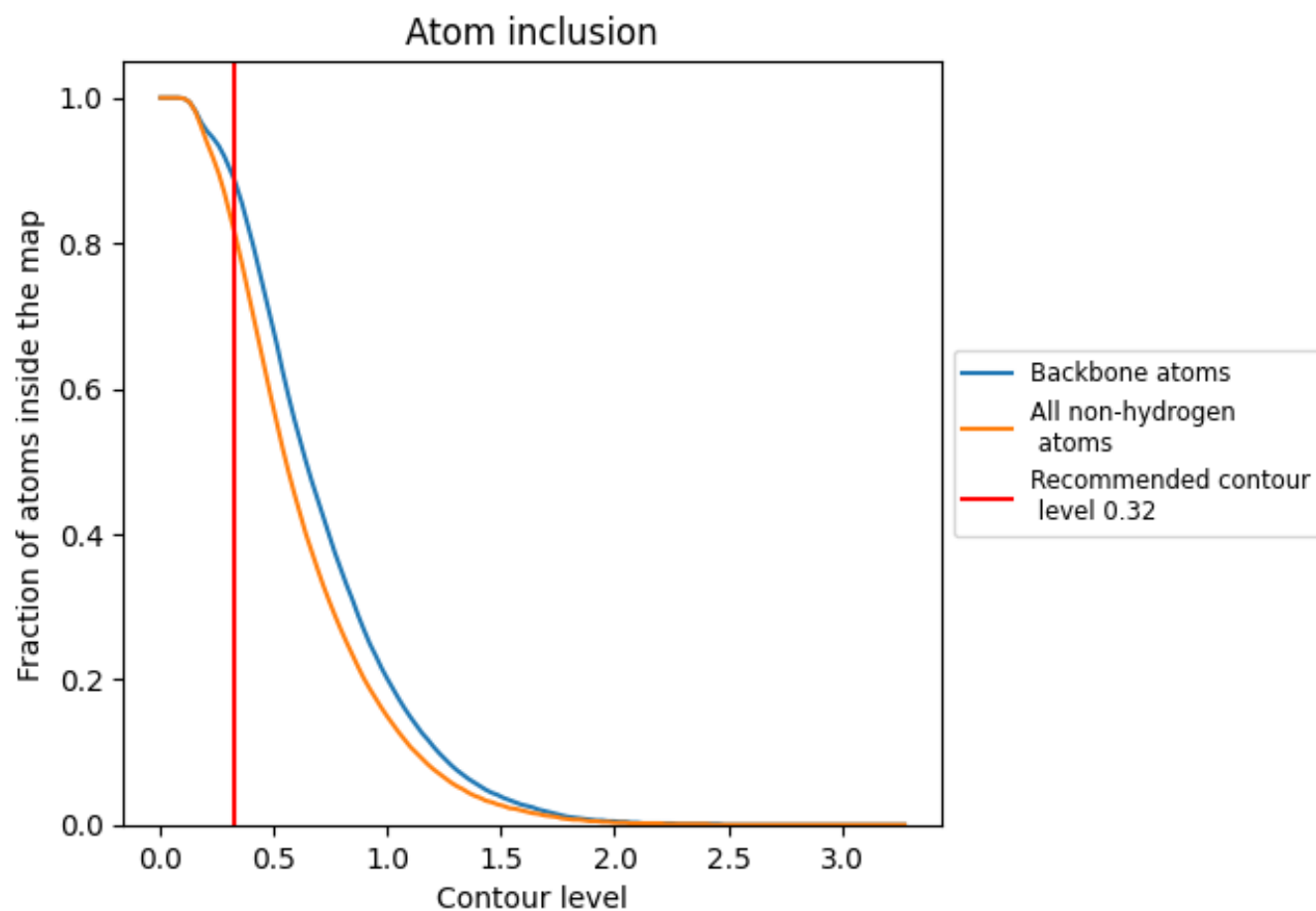
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8220	<div></div> 0.4080
A	<div></div> 0.8210	<div></div> 0.4070
B	<div></div> 0.8220	<div></div> 0.4080
C	<div></div> 0.8210	<div></div> 0.4070
D	<div></div> 0.8230	<div></div> 0.4080
E	<div></div> 0.8530	<div></div> 0.4190
F	<div></div> 0.8480	<div></div> 0.4210
G	<div></div> 0.8490	<div></div> 0.4200
H	<div></div> 0.8490	<div></div> 0.4230

