



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 03:58 AM EST

PDB ID : 8TKH
EMDB ID : EMD-41351
Title : Human Type 3 IP3 Receptor - Labile Resting State 1 (+IP3/ATP)
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on : 2023-07-25
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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) : 2.39

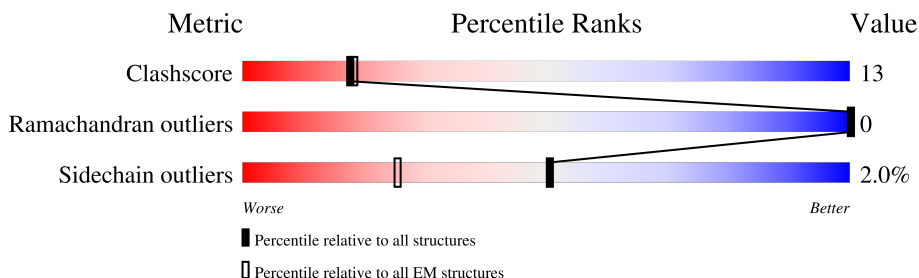
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	2671	
1	B	2671	
1	C	2671	
1	D	2671	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 145900 atoms, of which 72928 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.

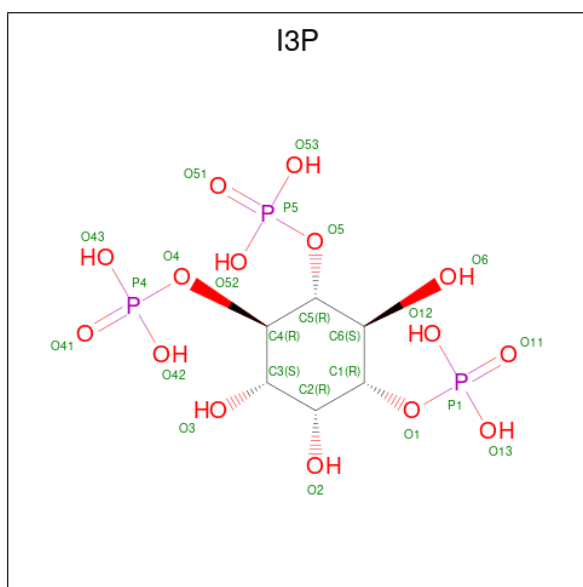
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2268	Total	C	H	N	O	S	0	0
			36398	11601	18211	3116	3355	115		
1	B	2268	Total	C	H	N	O	S	0	0
			36398	11601	18211	3116	3355	115		
1	C	2268	Total	C	H	N	O	S	0	0
			36398	11601	18211	3116	3355	115		
1	D	2268	Total	C	H	N	O	S	0	0
			36398	11601	18211	3116	3355	115		

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

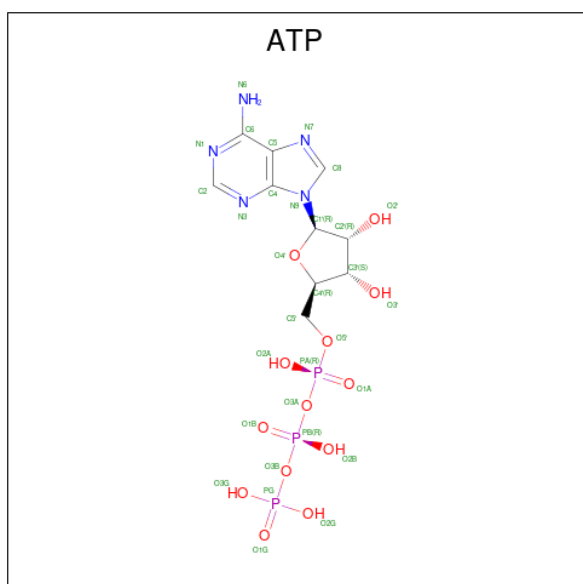
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- 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).

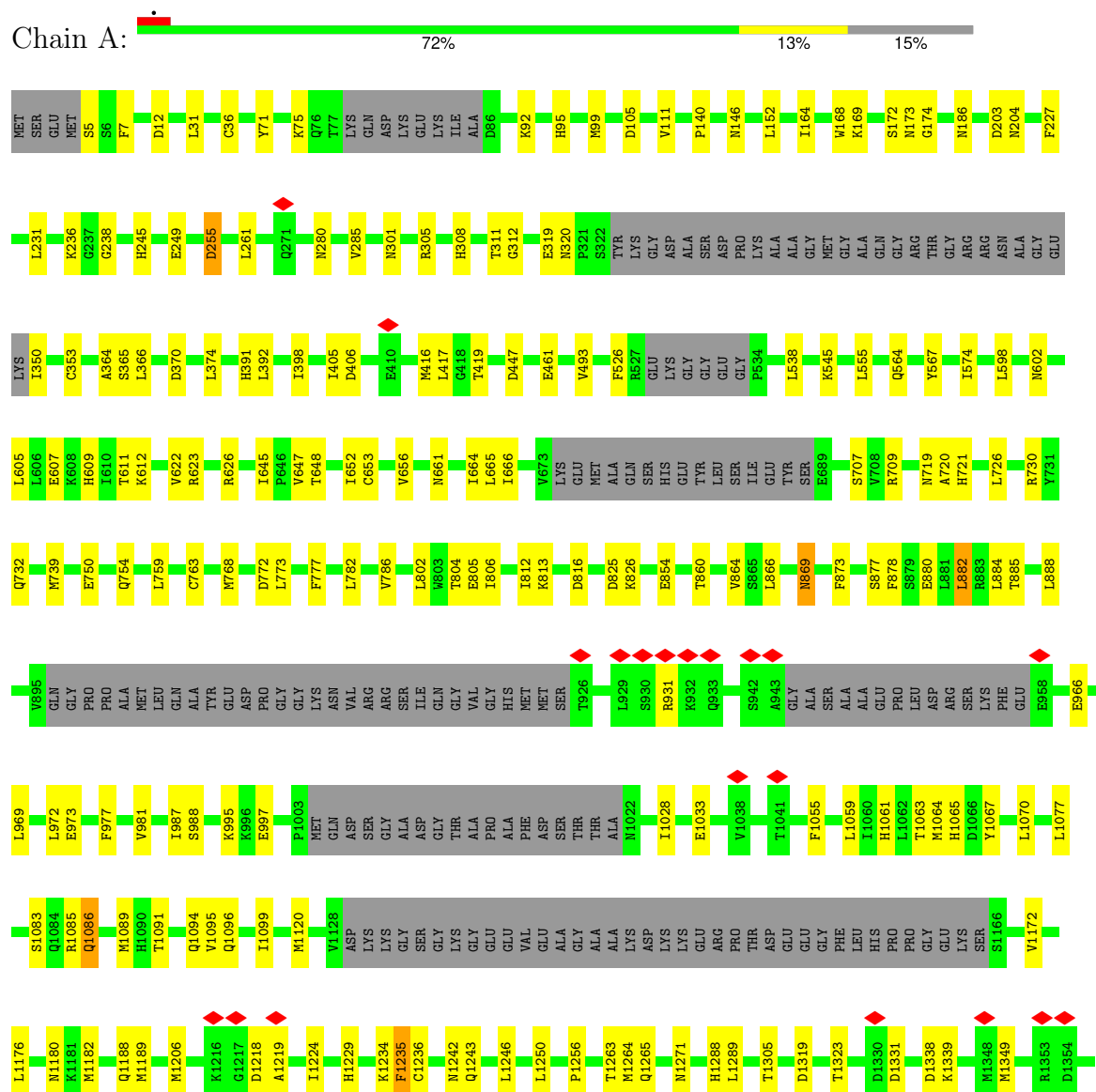


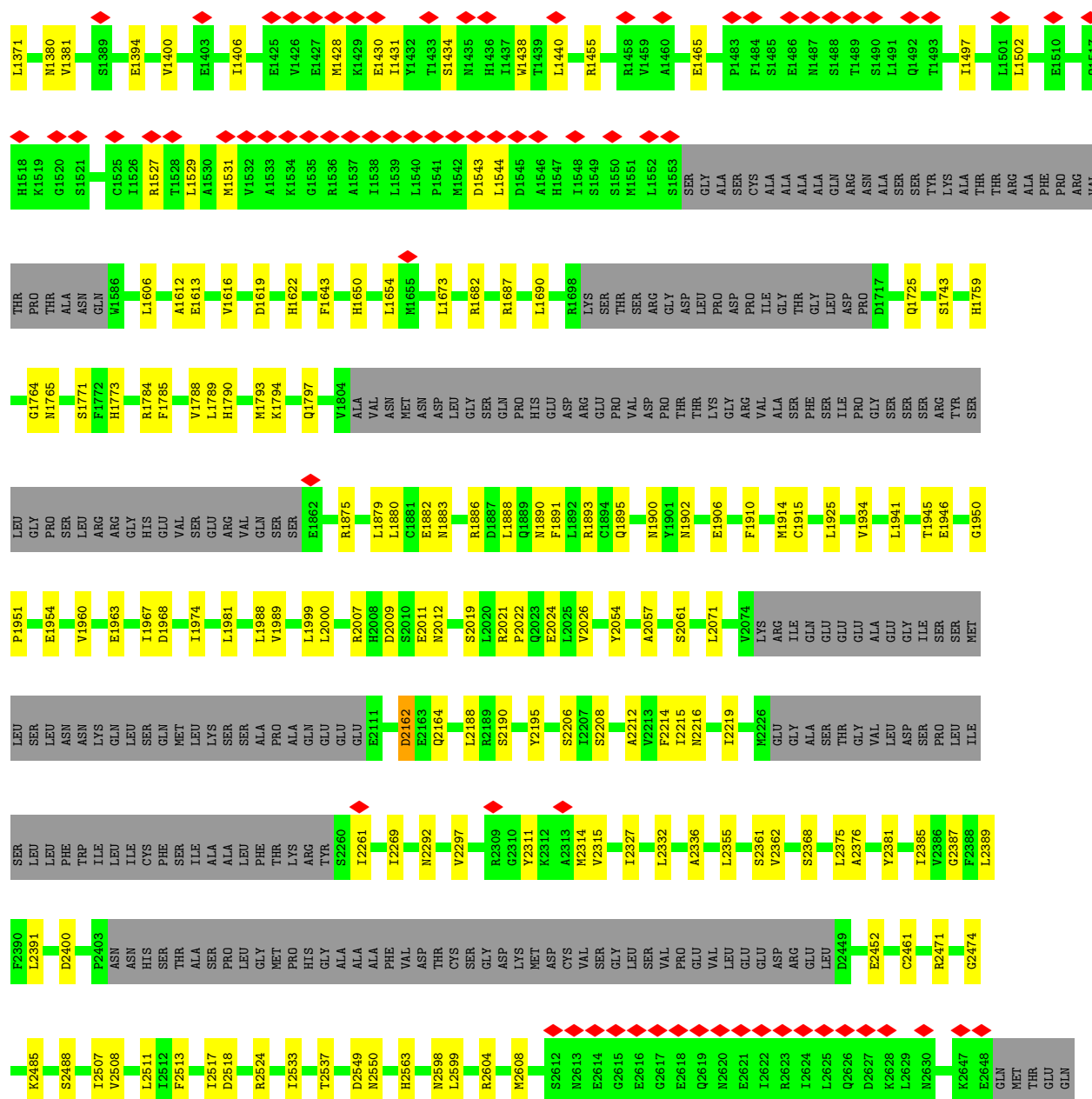
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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.

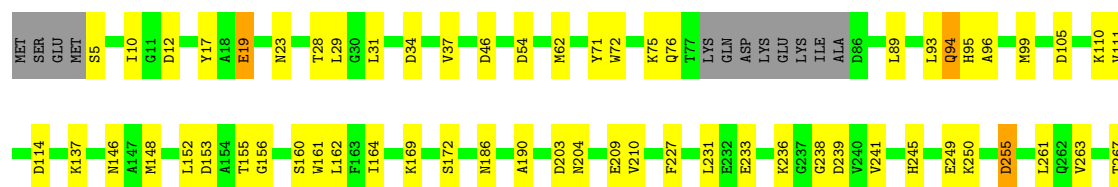
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

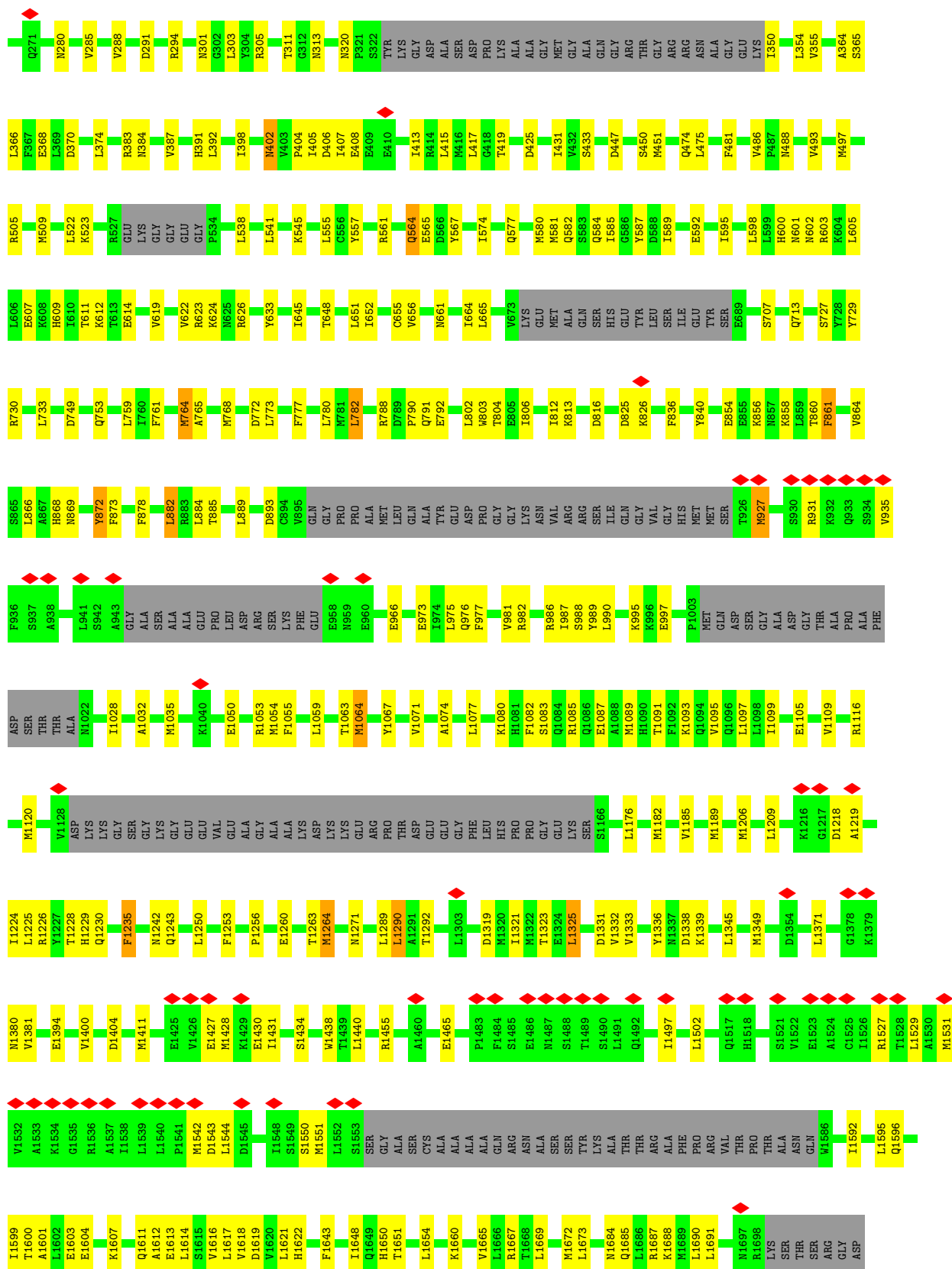


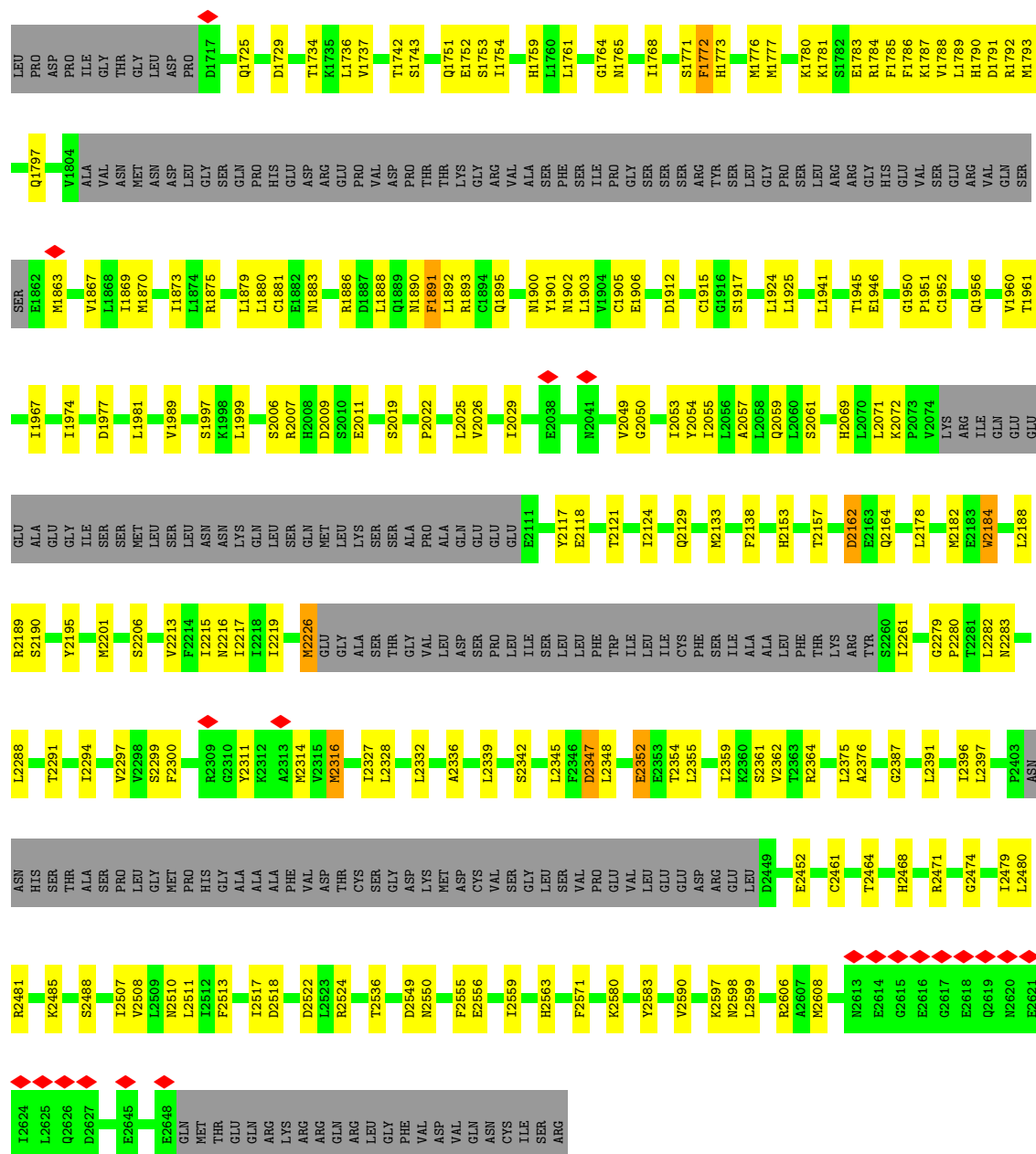


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

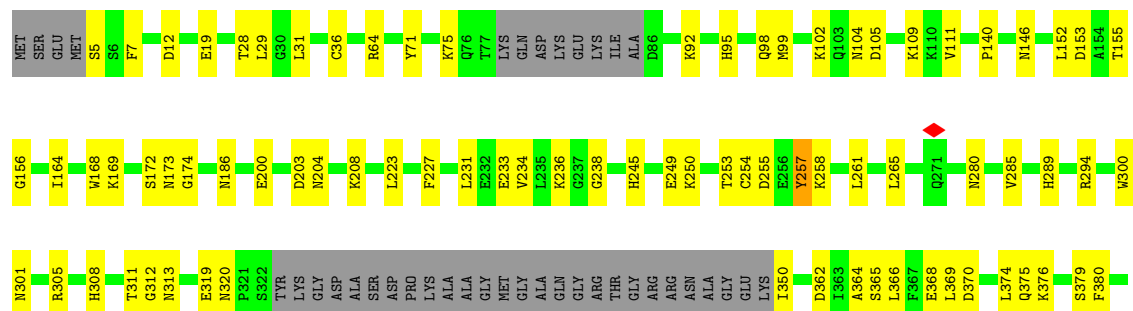
Chain B: 64% 20% 15%



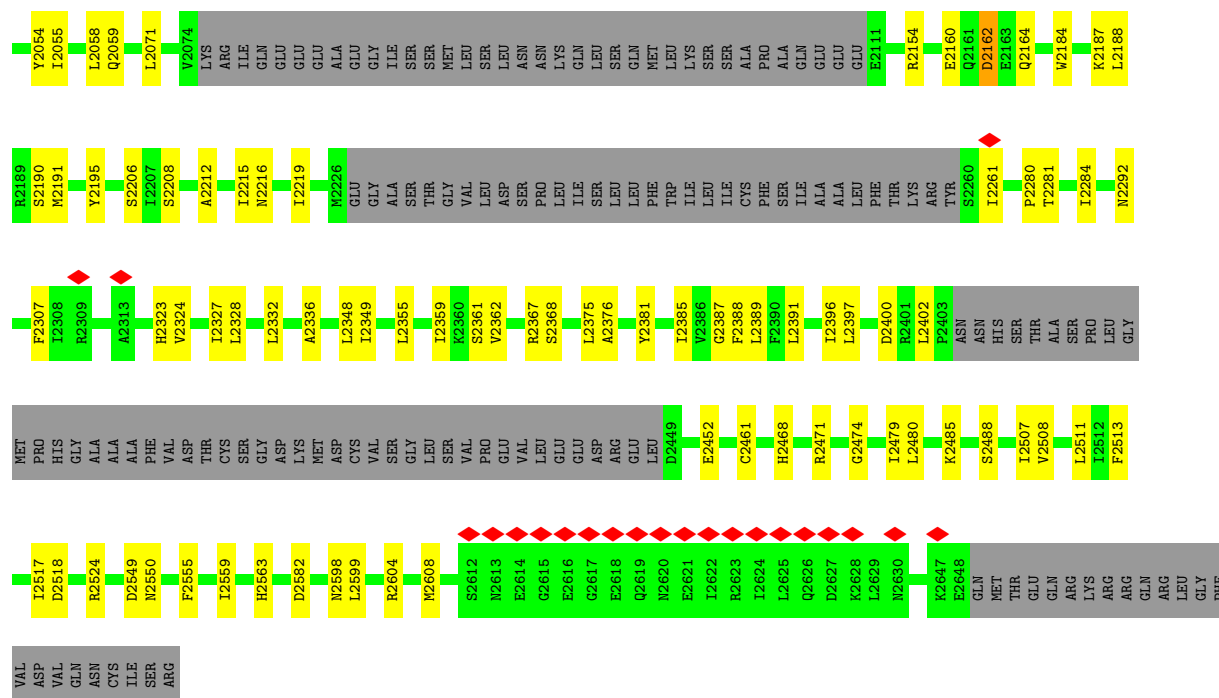




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

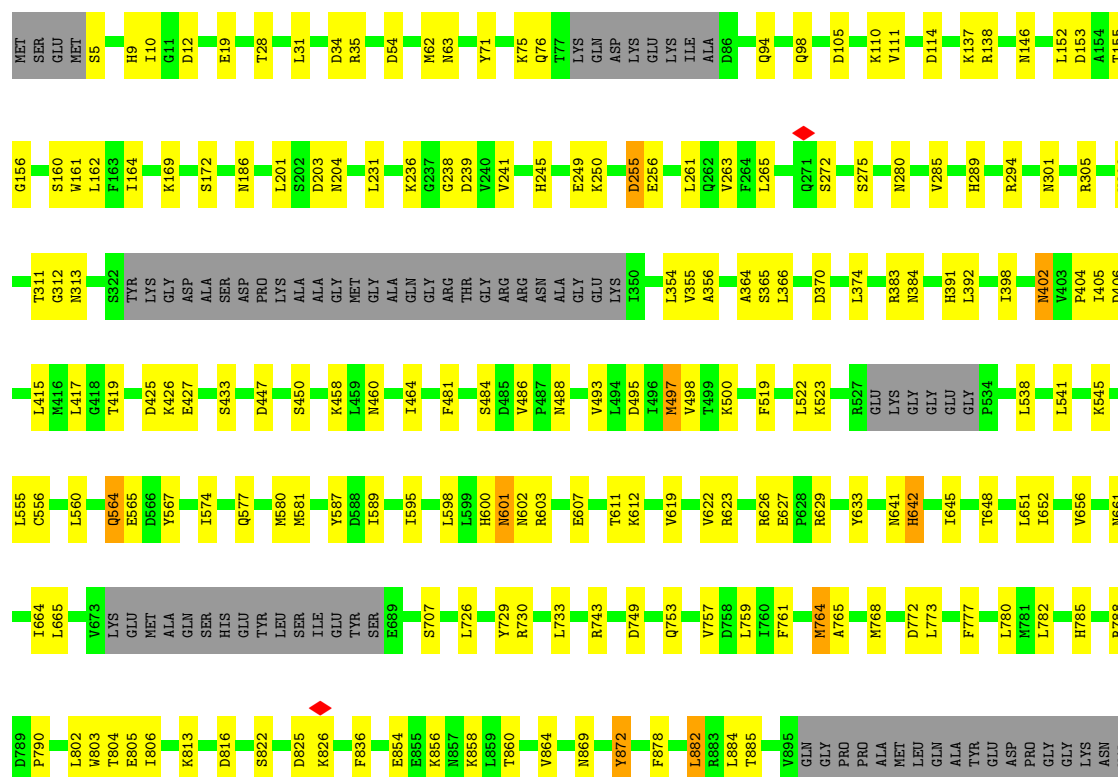






• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D: 65% 19% 15%



GLU	GLU	GLU	E2111	Y2117	E2118	T2121	I2124	M2133	F2138	F2146	H2153	T2157	D2162	E2163	Q2164	L2178	M2182	E2183	W2184	Q2185	T2187	L2188	R2189	S2190	Y2195	M2201	S2206	F2209	M2216	I2219	Y2223	M2226	GLU	GLY	ALA	SER	THR	GLY	VAL													
L1908	L1908	R2021	F1910	Q2023	L1911	D1912	L1913	M1914	C1915	G1916	S1917	L1922	G1923	L1924	L1925	G1926	L1927	Y1928	L1941	T1945	E1946	G1950	P1951	C1952	H1953	E1954	N1955	Q1956	T1957	C1958	I1959	V1960	T1961	T1971	T1974	L1975	N1976	D1977	L1981	V1989	L1999	L2003	S2006	R2007	H2008	D2009	E2014	S2019				
L2020	R2021	P2022	Q2023	E2024	L2025	V2026	Y2033	E2038	N2041	S2042	E2043	R2047	Y2054	A2057	S2061	L2071	V2074	LYS	ARG	ILE	GLN	GLU	ALA	GLU	GLU	GLY	ILE	SER	SER	LEU	SER	LEU	ASN	ASN	LYS	GLN	SER	GLN	MET	LEU	LYS	SER	ALA	PRO	GLY	ALA	GLN					
VAL	ALA	SER	PHE	SER	ILE	PRO	GLY	SER	SER	ARG	TYR	SER	LEU	GLY	SER	LEU	ARG	ARG	GLY	HIS	GLU	VAL	SER	SER	SER	SER	ILE	M1862	M1863	R1875	L1879	L1880	C1881	E1882	R1886	D1887	L1888	Q1889	N1890	F1891	L1892	C1894	Q1895	N1900	Y1901	N1902	C1905	Y1907				
I1754	H1759	L1760	L1761	M1765	I1768	S1771	F1772	H1773	M1776	M1777	S1778	R1784	F1785	N1786	V1787	L1788	L1789	H1790	D1791	R1792	M1793	K1794	Q1797	Q1798	E1799	V1804	ALA	VAL	ASN	MET	ASN	ASP	LEU	GLY	SER	GLN	PRO	HIS	GLU	ASP	ARG	PRO	VAL	ASP	PRO	THR	LYS	THR	ARG			
I1663	K1664	V1665	L1666	R1667	M1672	L1673	N1684	L1685	L1686	R1687	K1688	M1689	L1690	L1691	Y1694	L1695	Q1696	N1697	R1698	LYS	SER	THR	ARG	GLY	ASP	PRO	PRO	ILE	GLY	THR	GLY	THR	GLY	THR	F1643	L1644	L1647	T1648	Q1649	H1650	T1651	K1652	D1653	L1654	E1659	K1660	S1753					
TYR	LYS	ALA	THR	ARG	ALA	PHE	PRO	VAL	THR	PRO	THR	ALA	ASN	GLN	W1586	I1592	L1595	L1596	I1599	E1603	E1604	L1605	A1612	E1613	V1616	L1617	V1618	D1619	V1620	L1621	H1622	V1623	L1626	F1643	L1644	L1647	T1648	Q1649	H1650	T1651	K1652	D1653	L1654	E1659	K1660	S1753						
Q1492	I1497	L1502	E1510	Q1516	Q1517	H1518	S1521	V1522	E1523	A1524	C1525	I1526	R1527	M1528	L1529	A1530	M1531	V1532	A1533	Q1535	R1536	A1537	I1538	L1539	L1540	P1541	M1542	D1543	L1544	D1545	A1546	H1547	I1548	S1549	M1550	M1551	L1552	S1553	SER	GLY	ALA	SER	CYS	ALA	ALA	ALA	GLN	GLN	ASN	ALA	SER	SER
M1206	L1209	L1210	G1211	I1212	K1216	G1217	A1219	I1224	T1228	H1229	G1230	F1231	K1234	F1235	C1236	N1242	Q1243	L1246	L1250	F1253	P1256	E1260	T1263	M1264	N1271	H1288	L1289	L1290	A1291	T1292	D1319	M1320	I1321	M1322	F1324	L1325	D1331	D1338	K1339													
M1089	H1090	T1091	F1092	K1093	Q1094	Y1095	Q1096	L1097	V1128	ASP	LYS	GLY	SER	ALA	THR	ALA	ALA	ASP	LYS	LYS	ARG	THR	ASP	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	GLU	LYS	SER	S1186	L1176	M1182	M1189	K1192	Q1193	L1197											
1987	S988	Y989	L990	K995	K996	E997	P1003	MET	GLN	ASP	SER	GLY	ALA	ASP	THR	ALA	ALA	THR	ALA	N1022	I1028	A1032	K1040	T1041	F1055	L1056	L1059	T1063	M1064	Y1067	V1071	L1077	K1080	H1081	F1082	S1083	Q1084	R1085	D1086	E1087	A1088											
ARG	ARG	SER	ILE	GLN	GLY	VAL	GLY	HIS	MET	MET	SER	T926	M927	V928	L929	S930	R931	K932	Q933	S934	V935	F936	S937	A938	L941	S942	A943	GLY	ALA	SER	ALA	ALA	GLU	PRO	LEU	ASP	ARG	SER	PHE	GLU	E958	N959	E960	V963	V964	T967	K968	Q976	F977	V981	R982	R986



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91326	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.965	Depositor
Minimum map value	-0.388	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.16	Depositor
Map size (\AA)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.826, 0.826, 0.826	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, I3P, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.24	0/18521	0.45	0/25031
1	B	0.24	0/18521	0.45	0/25031
1	C	0.24	0/18521	0.45	0/25031
1	D	0.24	0/18521	0.45	0/25031
All	All	0.24	0/74084	0.45	0/100124

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18187	18211	18208	292	0
1	B	18187	18211	18209	657	0
1	C	18187	18211	18208	536	0
1	D	18187	18211	18210	612	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	0	0
3	C	24	9	9	0	0
3	D	24	9	9	0	0
4	A	31	12	12	1	0
4	B	31	12	12	1	0
4	C	31	12	12	1	0
4	D	31	12	12	1	0
All	All	72972	72928	72919	1931	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 13.

All (1931) 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:1691:LEU:CD1	1:D:1695:LEU:HD12	1.48	1.44
1:A:2452:GLU:OE1	1:D:2485:LYS:CE	1.71	1.37
1:D:62:MET:CE	1:D:161:TRP:CZ3	2.04	1.37
1:B:2025:LEU:CD1	1:B:2053:ILE:HD11	1.54	1.36
1:B:99:MET:SD	1:C:1922:LEU:HD13	1.65	1.34
1:B:1050:GLU:OE1	1:B:1053:ARG:CZ	1.75	1.34
1:B:99:MET:HE1	1:C:1922:LEU:CG	1.58	1.34
1:A:545:LYS:HD3	1:B:1394:GLU:OE1	1.28	1.30
1:A:2452:GLU:OE1	1:D:2485:LYS:HE3	1.18	1.30
1:B:1777:MET:SD	1:B:1891:PHE:CE1	2.24	1.30
1:B:99:MET:CE	1:C:1922:LEU:CG	2.11	1.27
1:B:1250:LEU:HD11	1:B:1264:MET:CE	1.65	1.26
1:D:1659:GLU:OE1	1:D:1749:ILE:CD1	1.81	1.26
1:A:2452:GLU:OE1	1:D:2485:LYS:CD	1.82	1.26
1:C:1055:PHE:O	1:C:1059:LEU:HD12	1.33	1.26
1:B:2485:LYS:CD	1:C:2452:GLU:OE2	1.83	1.24
1:C:2187:LYS:HE3	1:C:2191:MET:CE	1.66	1.24
1:B:2485:LYS:HD3	1:C:2452:GLU:OE2	1.37	1.23
1:D:1542:MET:SD	1:D:1543:ASP:N	2.13	1.22
1:C:1056:LEU:HD21	1:C:1081:HIS:CD2	1.74	1.21
1:B:1902:ASN:ND2	1:B:1905:CYS:SG	2.13	1.20
1:B:1902:ASN:OD1	1:B:1905:CYS:SG	2.00	1.20
1:C:545:LYS:HD3	1:D:1394:GLU:OE1	1.38	1.19
1:C:1953:HIS:ND1	1:C:2007:ARG:NH1	1.91	1.19
1:B:1050:GLU:OE1	1:B:1053:ARG:NE	1.75	1.18
1:C:1250:LEU:HD11	1:C:1264:MET:CE	1.74	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2479:ILE:CD1	1:C:2480:LEU:HD23	1.73	1.17
1:B:1050:GLU:OE1	1:B:1053:ARG:NH2	1.78	1.17
1:C:2187:LYS:HE3	1:C:2191:MET:HE3	1.19	1.16
1:A:2513:PHE:HD2	1:B:2513:PHE:CZ	1.65	1.15
1:C:768:MET:HA	1:C:768:MET:HE3	1.22	1.15
1:D:1667:ARG:NH1	1:D:1752:GLU:OE2	1.79	1.15
1:B:99:MET:SD	1:C:1922:LEU:CD1	2.29	1.14
1:C:394:THR:HG22	1:C:396:THR:HG23	1.27	1.14
1:D:764:MET:SD	1:D:836:PHE:CE1	2.41	1.13
1:C:2513:PHE:HD2	1:D:2513:PHE:CZ	1.66	1.13
1:A:2513:PHE:CD2	1:B:2513:PHE:CZ	2.35	1.13
1:D:764:MET:SD	1:D:836:PHE:CD1	2.42	1.13
1:B:764:MET:SD	1:B:836:PHE:CD1	2.42	1.12
1:B:2025:LEU:HD11	1:B:2053:ILE:CD1	1.78	1.12
1:A:353:CYS:SG	1:A:416:MET:HE3	1.89	1.12
1:B:764:MET:SD	1:B:836:PHE:CE1	2.41	1.12
1:C:2513:PHE:CD2	1:D:2513:PHE:CZ	2.36	1.12
1:C:1056:LEU:HD21	1:C:1081:HIS:HD2	1.01	1.11
1:B:62:MET:HE2	1:B:161:TRP:CE3	1.86	1.10
1:A:353:CYS:SG	1:A:416:MET:CE	2.41	1.09
1:A:1288:HIS:NE2	1:D:138:ARG:NH2	2.00	1.09
1:B:729:TYR:O	1:B:733:LEU:HD23	1.53	1.09
1:D:768:MET:HA	1:D:768:MET:HE3	1.18	1.09
1:D:1659:GLU:OE1	1:D:1749:ILE:HD11	1.45	1.09
1:A:1934:VAL:HG11	1:A:1988:LEU:HD13	1.34	1.08
1:C:2479:ILE:HD11	1:C:2480:LEU:HD23	1.35	1.08
1:D:62:MET:HE2	1:D:161:TRP:CE3	1.87	1.08
1:D:1684:ASN:O	1:D:1688:LYS:HG2	1.52	1.08
1:A:1288:HIS:CD2	1:D:138:ARG:NH2	2.22	1.07
1:B:1250:LEU:CD1	1:B:1264:MET:CE	2.32	1.07
1:B:2201:MET:SD	1:B:2300:PHE:HA	1.94	1.07
1:D:1652:LYS:HD2	1:D:1652:LYS:O	1.51	1.07
1:B:768:MET:HE3	1:B:768:MET:HA	1.21	1.07
1:B:1786:PHE:CD2	1:B:1895:GLN:NE2	2.21	1.07
1:B:1607:LYS:O	1:B:1611:GLN:OE1	1.71	1.06
1:D:1660:LYS:HE2	1:D:1660:LYS:HA	1.23	1.06
1:D:927:MET:O	1:D:927:MET:SD	2.14	1.06
1:D:2007:ARG:HG3	1:D:2009:ASP:OD1	1.55	1.06
1:B:1209:LEU:HD23	1:B:1228:THR:HG21	1.37	1.05
1:B:1902:ASN:CG	1:B:1905:CYS:SG	2.35	1.05
1:D:62:MET:CE	1:D:161:TRP:CH2	2.40	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:MET:HE2	1:D:161:TRP:CZ3	1.78	1.05
1:D:1691:LEU:HD11	1:D:1695:LEU:CD1	1.84	1.05
1:B:2216:ASN:ND2	1:B:2345:LEU:HG	1.71	1.05
1:C:768:MET:HA	1:C:768:MET:CE	1.85	1.05
1:D:62:MET:HE1	1:D:161:TRP:CZ3	1.85	1.05
1:D:768:MET:HA	1:D:768:MET:CE	1.87	1.04
1:B:768:MET:HA	1:B:768:MET:CE	1.84	1.04
1:D:2279:GLY:O	1:D:2283:ASN:OD1	1.75	1.04
1:B:2007:ARG:HG3	1:B:2009:ASP:OD1	1.55	1.03
1:B:2215:ILE:O	1:B:2219:ILE:HD12	1.59	1.03
1:B:2213:VAL:O	1:B:2217:ILE:HG13	1.57	1.03
1:C:2187:LYS:CE	1:C:2191:MET:HE3	1.89	1.02
1:B:2279:GLY:O	1:B:2283:ASN:OD1	1.75	1.02
1:B:1783:GLU:N	1:B:1783:GLU:OE2	1.91	1.02
1:B:1687:ARG:O	1:B:1691:LEU:HG	1.56	1.01
1:C:1250:LEU:HD11	1:C:1264:MET:SD	2.01	1.01
1:C:2513:PHE:CD2	1:D:2513:PHE:HZ	1.79	1.00
1:C:2400:ASP:OD1	1:C:2400:ASP:O	1.77	1.00
1:D:761:PHE:O	1:D:764:MET:HE3	1.61	1.00
1:C:1953:HIS:CE1	1:C:2007:ARG:HH11	1.80	0.99
1:C:554:ARG:HG2	1:C:590:LEU:CD1	1.92	0.99
1:C:1055:PHE:O	1:C:1059:LEU:CD1	2.11	0.99
1:D:54:ASP:OD1	1:D:54:ASP:O	1.81	0.99
1:B:1250:LEU:CD1	1:B:1264:MET:HE2	1.89	0.99
1:C:2187:LYS:HD2	1:C:2187:LYS:O	1.63	0.99
1:B:603:ARG:O	1:B:607:GLU:HG3	1.62	0.98
1:D:62:MET:HE1	1:D:161:TRP:CH2	1.96	0.98
1:D:497:MET:SD	1:D:497:MET:O	2.21	0.98
1:A:1934:VAL:HG11	1:A:1988:LEU:CD1	1.93	0.98
1:B:62:MET:CE	1:B:161:TRP:CZ3	2.45	0.98
1:B:1780:LYS:O	1:B:1783:GLU:OE1	1.81	0.98
1:C:1362:LEU:O	1:C:1366:ILE:HG13	1.62	0.98
1:D:603:ARG:O	1:D:607:GLU:HG3	1.61	0.98
1:A:2452:GLU:CD	1:D:2485:LYS:HE3	1.84	0.98
1:A:2513:PHE:CD2	1:B:2513:PHE:HZ	1.77	0.98
1:B:1787:LYS:NZ	1:B:1791:ASP:OD2	1.96	0.98
1:B:54:ASP:OD1	1:B:54:ASP:O	1.82	0.97
1:C:2388:PHE:HE2	1:D:2223:TYR:HE1	1.11	0.97
1:A:2518:ASP:OD1	1:B:2524:ARG:HD3	1.63	0.97
1:C:2518:ASP:OD1	1:D:2524:ARG:HD3	1.64	0.97
1:B:889:LEU:CD1	1:B:975:LEU:HD21	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1786:PHE:CD2	1:C:1895:GLN:NE2	2.34	0.96
1:D:110:LYS:O	1:D:110:LYS:HD3	1.64	0.96
1:D:1956:GLN:O	1:D:1960:VAL:HG12	1.64	0.96
1:C:1954:GLU:OE2	1:C:1954:GLU:N	1.99	0.96
1:B:1209:LEU:CD2	1:B:1228:THR:HG21	1.96	0.96
1:B:1777:MET:SD	1:B:1891:PHE:CZ	2.59	0.95
1:B:619:VAL:HG21	1:B:655:CYS:SG	2.06	0.95
1:C:2007:ARG:HG3	1:C:2009:ASP:OD1	1.66	0.95
1:B:62:MET:HE2	1:B:161:TRP:CZ3	2.01	0.95
1:D:1193:GLN:O	1:D:1197:LEU:HG	1.66	0.95
1:B:856:LYS:O	1:B:860:THR:HG23	1.65	0.95
1:C:1250:LEU:HD11	1:C:1264:MET:HE3	1.49	0.95
1:C:1041:THR:O	1:C:1044:MET:SD	2.25	0.94
1:B:538:LEU:HD22	1:B:587:TYR:CD1	2.02	0.94
1:C:893:ASP:OD1	1:C:1054:MET:CE	2.16	0.94
1:B:889:LEU:HD11	1:B:975:LEU:HD21	1.47	0.94
1:B:1772:PHE:HD2	1:B:1776:MET:CE	1.80	0.94
1:B:761:PHE:O	1:B:764:MET:HE3	1.68	0.94
1:D:1664:LYS:HA	1:D:1664:LYS:HE3	1.48	0.94
1:D:1691:LEU:CD1	1:D:1695:LEU:CD1	2.43	0.93
1:A:1288:HIS:CD2	1:D:138:ARG:CZ	2.52	0.93
1:B:2178:LEU:O	1:B:2182:MET:HG3	1.68	0.93
1:D:2178:LEU:O	1:D:2182:MET:HG3	1.69	0.92
1:C:394:THR:HG22	1:C:396:THR:CG2	1.98	0.92
1:C:888:LEU:HA	1:C:891:ILE:HD12	1.51	0.92
1:C:2323:HIS:O	1:C:2327:ILE:HG23	1.68	0.92
1:B:2025:LEU:HD11	1:B:2053:ILE:HD11	0.93	0.92
1:C:1974:ILE:CD1	1:C:2000:LEU:HD12	1.99	0.92
1:D:538:LEU:HD22	1:D:587:TYR:CD1	2.04	0.92
1:B:1786:PHE:CE2	1:B:1895:GLN:NE2	2.36	0.91
1:C:2479:ILE:HD12	1:C:2480:LEU:HD23	1.49	0.91
1:B:28:THR:HG21	1:B:152:LEU:HD11	1.52	0.91
1:B:2485:LYS:CG	1:C:2452:GLU:OE2	2.16	0.91
1:B:2513:PHE:HD2	1:C:2513:PHE:CE2	1.88	0.91
1:B:1777:MET:SD	1:B:1891:PHE:HE1	1.86	0.91
1:C:1056:LEU:CD2	1:C:1081:HIS:CD2	2.52	0.91
1:A:2513:PHE:CE2	1:D:2513:PHE:HD2	1.89	0.91
1:D:1448:MET:SD	1:D:1468:VAL:CG2	2.58	0.91
1:D:62:MET:CE	1:D:161:TRP:CE3	2.47	0.91
1:D:458:LYS:HB3	1:D:464:ILE:HD12	1.52	0.91
1:C:1773:HIS:CE1	1:C:1777:MET:CE	2.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:LYS:HB3	1:D:464:ILE:CD1	2.00	0.90
1:A:1954:GLU:N	1:A:1954:GLU:OE2	2.03	0.90
1:B:1250:LEU:HD11	1:B:1264:MET:SD	2.10	0.90
1:B:2536:THR:HG22	1:B:2536:THR:O	1.70	0.90
1:C:95:HIS:CD2	1:D:1922:LEU:HD21	2.06	0.90
1:B:2215:ILE:O	1:B:2219:ILE:CD1	2.19	0.90
1:D:1691:LEU:HD11	1:D:1695:LEU:HD12	0.92	0.90
1:D:1902:ASN:OD1	1:D:1902:ASN:O	1.89	0.90
1:B:986:ARG:NH1	1:B:986:ARG:HB2	1.87	0.90
1:B:1902:ASN:OD1	1:B:1905:CYS:CB	2.19	0.90
1:B:2316:MET:HA	1:B:2316:MET:HE1	1.53	0.90
1:D:1971:THR:HB	1:D:2020:LEU:HD13	1.53	0.89
1:D:2536:THR:O	1:D:2536:THR:HG22	1.71	0.89
1:B:1089:MET:SD	1:B:1603:GLU:HA	2.12	0.89
1:C:1863:MET:HA	1:C:1863:MET:HE3	1.54	0.89
1:B:624:LYS:O	1:B:624:LYS:HD2	1.73	0.89
1:D:1093:LYS:CE	1:D:1599:ILE:HG21	2.02	0.89
1:D:28:THR:HG21	1:D:152:LEU:HD11	1.53	0.89
1:A:812:ILE:HD12	1:A:813:LYS:CE	2.03	0.88
1:D:1784:ARG:O	1:D:1788:VAL:HG13	1.72	0.88
1:B:868:HIS:HE1	1:B:973:GLU:OE1	1.56	0.88
1:D:62:MET:HE2	1:D:161:TRP:CH2	2.04	0.88
1:D:1093:LYS:HE2	1:D:1093:LYS:HA	1.53	0.88
1:D:523:LYS:NZ	1:D:577:GLN:OE1	2.07	0.88
1:A:2485:LYS:HE2	1:B:2452:GLU:OE2	1.74	0.88
1:D:1253:PHE:HA	1:D:1260:GLU:OE1	1.74	0.88
1:A:2513:PHE:CD2	1:B:2513:PHE:CE2	2.61	0.88
1:C:738:ARG:HH21	1:C:926:THR:HG23	1.37	0.88
1:C:893:ASP:OD1	1:C:1054:MET:HE3	1.74	0.88
1:B:989:TYR:CD2	1:B:1035:MET:HE1	2.09	0.87
1:B:1253:PHE:HA	1:B:1260:GLU:OE1	1.74	0.87
1:D:1785:PHE:O	1:D:1788:VAL:HG22	1.75	0.87
1:A:353:CYS:SG	1:A:416:MET:HE1	2.13	0.87
1:C:2479:ILE:HD11	1:C:2480:LEU:CD2	2.03	0.87
1:C:893:ASP:CG	1:C:1054:MET:CE	2.42	0.87
1:C:608:LYS:HD2	1:C:608:LYS:O	1.74	0.87
1:D:856:LYS:O	1:D:860:THR:HG22	1.75	0.87
1:D:2033:TYR:CZ	1:D:2047:ARG:NH2	2.43	0.87
1:D:1659:GLU:OE1	1:D:1749:ILE:HD12	1.73	0.87
1:B:71:TYR:CZ	1:B:94:GLN:HB2	2.10	0.87
1:C:2513:PHE:CD2	1:D:2513:PHE:CE2	2.62	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:MET:HE1	1:B:161:TRP:CZ3	2.10	0.87
1:A:2452:GLU:OE1	1:D:2485:LYS:HD3	1.75	0.87
1:C:265:LEU:HD21	1:C:417:LEU:HD11	1.57	0.86
1:C:2485:LYS:HE2	1:D:2452:GLU:OE2	1.73	0.86
1:D:1660:LYS:HE2	1:D:1660:LYS:CA	2.05	0.86
1:B:62:MET:CE	1:B:161:TRP:CE3	2.58	0.86
1:B:605:LEU:HD12	1:B:609:HIS:HD2	1.40	0.86
1:B:1250:LEU:HD11	1:B:1264:MET:HE1	1.57	0.86
1:B:1892:LEU:HD22	1:B:1903:LEU:HD12	1.58	0.86
1:B:2513:PHE:CD2	1:C:2513:PHE:CZ	2.64	0.86
1:C:254:CYS:O	1:C:255:ASP:OD1	1.92	0.86
1:B:99:MET:HE1	1:C:1922:LEU:CB	2.05	0.85
1:B:2513:PHE:CD2	1:C:2513:PHE:CE2	2.63	0.85
1:D:627:GLU:OE2	1:D:629:ARG:HG3	1.75	0.85
1:A:2452:GLU:OE1	1:D:2485:LYS:CG	2.23	0.85
1:A:2513:PHE:CE2	1:D:2513:PHE:CD2	2.64	0.85
1:C:1934:VAL:O	1:C:1937:VAL:HG12	1.75	0.85
1:D:1977:ASP:O	1:D:1977:ASP:OD2	1.95	0.85
1:D:1063:THR:O	1:D:1071:VAL:HG22	1.77	0.85
1:C:2513:PHE:HD2	1:D:2513:PHE:CE2	1.95	0.85
1:D:2219:ILE:CD1	1:D:2338:GLU:HB2	2.07	0.84
1:B:2117:TYR:O	1:B:2121:THR:HG22	1.77	0.84
1:C:28:THR:HG21	1:C:152:LEU:HD11	1.58	0.84
1:A:2513:PHE:CZ	1:D:2513:PHE:CD2	2.65	0.84
1:D:2117:TYR:O	1:D:2121:THR:HG22	1.77	0.84
1:B:764:MET:HG2	1:B:836:PHE:CZ	2.12	0.84
1:A:2513:PHE:HD2	1:B:2513:PHE:CE2	1.94	0.84
1:A:2513:PHE:CZ	1:D:2513:PHE:HD2	1.95	0.84
1:B:1093:LYS:HA	1:B:1093:LYS:HE2	1.57	0.84
1:C:1747:GLU:HG3	1:C:1751:GLN:OE1	1.78	0.84
1:D:764:MET:HG2	1:D:836:PHE:CZ	2.12	0.84
1:B:1063:THR:O	1:B:1071:VAL:HG22	1.77	0.83
1:B:2513:PHE:HD2	1:C:2513:PHE:CZ	1.94	0.83
1:B:2556:GLU:H	1:B:2556:GLU:CD	1.82	0.83
1:A:1934:VAL:CG1	1:A:1988:LEU:HD13	2.08	0.83
1:D:1531:MET:O	1:D:1531:MET:CE	2.26	0.83
1:B:2316:MET:HA	1:B:2316:MET:CE	2.08	0.83
1:D:1542:MET:SD	1:D:1543:ASP:CA	2.65	0.83
1:C:1250:LEU:CD1	1:C:1264:MET:CE	2.57	0.82
1:C:2388:PHE:HE2	1:D:2223:TYR:CE1	1.98	0.82
1:D:1093:LYS:NZ	1:D:1599:ILE:HD13	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1961:THR:HG22	1:B:1961:THR:O	1.78	0.82
1:C:738:ARG:NH2	1:C:926:THR:HG23	1.94	0.82
1:B:2474:GLY:HA2	1:C:2471:ARG:O	1.79	0.82
1:B:2485:LYS:HG2	1:C:2452:GLU:OE2	1.79	0.82
1:D:788:ARG:HB3	1:D:788:ARG:NH1	1.94	0.82
1:D:2392:LYS:HE2	1:D:2455:CYS:O	1.80	0.82
1:A:1394:GLU:OE1	1:D:545:LYS:HE2	1.80	0.81
1:A:2471:ARG:O	1:D:2474:GLY:HA2	1.79	0.81
1:B:2153:HIS:O	1:B:2157:THR:HG23	1.81	0.81
1:C:250:LYS:HE2	1:C:415:LEU:HD11	1.62	0.81
1:C:2479:ILE:HD12	1:C:2480:LEU:N	1.94	0.81
1:D:1542:MET:SD	1:D:1542:MET:C	2.57	0.81
1:D:2392:LYS:NZ	1:D:2456:ASP:HA	1.95	0.81
1:A:773:LEU:CD1	1:A:777:PHE:HE1	1.93	0.81
1:C:2058:LEU:HD23	1:C:2071:LEU:HD13	1.63	0.81
1:C:28:THR:CG2	1:C:152:LEU:HD11	2.10	0.81
1:B:1751:GLN:O	1:B:1754:ILE:HG22	1.80	0.81
1:D:1250:LEU:HD11	1:D:1264:MET:SD	2.21	0.81
1:C:871:ILE:HD13	1:C:881:LEU:CD2	2.10	0.80
1:C:1974:ILE:CD1	1:C:2000:LEU:CD1	2.59	0.80
1:D:1751:GLN:O	1:D:1754:ILE:HG22	1.80	0.80
1:B:2328:LEU:O	1:B:2332:LEU:CD1	2.30	0.80
1:D:1882:GLU:HG2	1:D:1946:GLU:OE2	1.81	0.80
1:D:1772:PHE:HD1	1:D:1776:MET:CE	1.95	0.80
1:C:376:LYS:HD3	1:C:376:LYS:N	1.97	0.80
1:B:868:HIS:CE1	1:B:973:GLU:OE1	2.35	0.80
1:A:545:LYS:CD	1:B:1394:GLU:OE1	2.22	0.79
1:B:764:MET:CG	1:B:836:PHE:CZ	2.66	0.79
1:A:2009:ASP:OD2	1:A:2011:GLU:OE2	2.00	0.79
1:B:581:MET:HE3	1:B:595:ILE:HG12	1.65	0.79
1:B:71:TYR:OH	1:B:94:GLN:HB2	1.81	0.79
1:C:2324:VAL:O	1:C:2327:ILE:HG12	1.82	0.79
1:D:62:MET:HE2	1:D:161:TRP:CD2	2.17	0.79
1:B:989:TYR:CD2	1:B:1035:MET:CE	2.66	0.79
1:A:140:PRO:HD3	1:B:1292:THR:HG22	1.64	0.79
1:D:804:THR:HG23	1:D:805:GLU:OE2	1.83	0.78
1:A:1430:GLU:O	1:A:1434:SER:OG	2.02	0.78
1:B:28:THR:HG21	1:B:152:LEU:CD1	2.12	0.78
1:C:368:GLU:HA	1:C:368:GLU:OE1	1.83	0.78
1:D:927:MET:C	1:D:927:MET:HE2	2.03	0.78
1:B:605:LEU:HD12	1:B:609:HIS:CD2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2571:PHE:CE2	1:B:2590:VAL:HG11	2.19	0.78
1:D:764:MET:CG	1:D:836:PHE:CZ	2.66	0.78
1:A:2011:GLU:OE1	1:A:2011:GLU:N	2.15	0.78
1:B:523:LYS:HZ1	1:B:577:GLN:NE2	1.81	0.78
1:B:497:MET:O	1:B:497:MET:SD	2.41	0.78
1:B:854:GLU:N	1:B:854:GLU:OE2	2.17	0.78
1:C:2187:LYS:CE	1:C:2191:MET:CE	2.52	0.78
1:D:1430:GLU:O	1:D:1434:SER:OG	2.02	0.78
1:C:1250:LEU:HD21	1:C:1264:MET:HE3	1.64	0.78
1:C:1773:HIS:CE1	1:C:1777:MET:HE1	2.17	0.77
1:D:1691:LEU:HD12	1:D:1695:LEU:HD12	1.61	0.77
1:B:523:LYS:NZ	1:B:577:GLN:NE2	2.32	0.77
1:B:986:ARG:CB	1:B:986:ARG:HH11	1.98	0.77
1:B:2328:LEU:O	1:B:2332:LEU:HD12	1.83	0.77
1:A:854:GLU:N	1:A:854:GLU:OE2	2.17	0.77
1:B:1093:LYS:O	1:B:1093:LYS:HD3	1.84	0.77
1:C:1786:PHE:CE2	1:C:1895:GLN:NE2	2.49	0.77
1:D:28:THR:HG21	1:D:152:LEU:CD1	2.13	0.77
1:D:1941:LEU:O	1:D:1945:THR:HG23	1.85	0.77
1:A:1941:LEU:O	1:A:1945:THR:HG23	1.85	0.77
1:B:99:MET:HE3	1:C:1922:LEU:CG	1.94	0.77
1:B:989:TYR:CE2	1:B:1035:MET:HE2	2.19	0.77
1:B:1941:LEU:O	1:B:1945:THR:HG23	1.85	0.77
1:C:733:LEU:HD22	1:C:780:LEU:HD22	1.65	0.77
1:B:303:LEU:HD23	1:B:368:GLU:HG3	1.66	0.77
1:C:1941:LEU:O	1:C:1945:THR:HG23	1.85	0.77
1:C:893:ASP:OD1	1:C:1054:MET:HE1	1.83	0.77
1:A:319:GLU:OE2	1:A:319:GLU:N	2.16	0.76
1:C:1239:ASN:ND2	1:C:1242:ASN:ND2	2.33	0.76
1:D:1224:ILE:O	1:D:1228:THR:HG23	1.85	0.76
1:D:481:PHE:CE1	1:D:488:ASN:HA	2.19	0.76
1:B:788:ARG:HB3	1:B:788:ARG:NH1	2.00	0.76
1:C:250:LYS:HE2	1:C:415:LEU:CD1	2.15	0.76
1:C:300:TRP:O	1:C:368:GLU:OE2	2.01	0.76
1:C:2388:PHE:CE2	1:D:2223:TYR:HE1	2.00	0.76
1:D:2124:ILE:HG23	1:D:2138:PHE:HE1	1.50	0.76
1:A:2511:LEU:HD21	1:B:2362:VAL:HG23	1.68	0.76
1:B:1430:GLU:O	1:B:1434:SER:OG	2.02	0.76
1:C:265:LEU:CD2	1:C:417:LEU:HD21	2.16	0.76
1:D:1684:ASN:HB3	1:D:1688:LYS:NZ	2.01	0.76
1:B:28:THR:CG2	1:B:152:LEU:HD11	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1349:MET:CE	1:B:1404:ASP:O	2.34	0.76
1:C:265:LEU:CD2	1:C:417:LEU:HD11	2.15	0.76
1:B:354:LEU:HD12	1:B:417:LEU:HB3	1.67	0.75
1:B:2481:ARG:CD	1:C:2400:ASP:OD1	2.28	0.75
1:D:1761:LEU:CD2	1:D:1768:ILE:HG22	2.17	0.75
1:D:1647:LEU:HD21	1:D:1665:VAL:HG13	1.68	0.75
1:C:2555:PHE:O	1:C:2559:ILE:HG23	1.86	0.75
1:B:1116:ARG:HB3	1:B:1120:MET:CE	2.17	0.75
1:D:1089:MET:SD	1:D:1606:LEU:HD12	2.27	0.75
1:B:2124:ILE:HG23	1:B:2138:PHE:HE1	1.50	0.75
1:C:1056:LEU:CD2	1:C:1081:HIS:HD2	1.88	0.75
1:D:458:LYS:CB	1:D:464:ILE:CD1	2.65	0.75
1:B:1772:PHE:HD2	1:B:1776:MET:HE2	1.50	0.74
1:C:1430:GLU:O	1:C:1434:SER:OG	2.02	0.74
1:D:265:LEU:HD13	1:D:417:LEU:HD21	1.69	0.74
1:D:1093:LYS:HE3	1:D:1599:ILE:HG21	1.69	0.74
1:A:526:PHE:CE1	1:A:538:LEU:HD23	2.21	0.74
1:A:652:ILE:O	1:A:656:VAL:HG23	1.86	0.74
1:A:1895:GLN:O	1:A:1900:ASN:ND2	2.21	0.74
1:B:1895:GLN:O	1:B:1900:ASN:ND2	2.21	0.74
1:C:1895:GLN:O	1:C:1900:ASN:ND2	2.21	0.74
1:C:2367:ARG:NH2	1:D:2352:GLU:OE1	2.21	0.74
1:C:2485:LYS:CE	1:D:2452:GLU:OE2	2.35	0.74
1:C:554:ARG:HG2	1:C:590:LEU:HD13	1.66	0.74
1:C:1916:GLY:HA3	1:C:1928:TYR:CD2	2.22	0.74
1:C:1954:GLU:H	1:C:1954:GLU:CD	1.91	0.74
1:C:2485:LYS:CD	1:D:2452:GLU:OE2	2.35	0.74
1:C:2511:LEU:HD21	1:D:2362:VAL:HG23	1.70	0.74
1:D:62:MET:HE3	1:D:161:TRP:CZ3	2.23	0.74
1:B:95:HIS:O	1:B:99:MET:HG3	1.86	0.74
1:B:2485:LYS:CE	1:C:2452:GLU:OE2	2.35	0.73
1:C:1725:GLN:OE1	1:C:1765:ASN:ND2	2.21	0.73
1:B:2556:GLU:OE1	1:B:2556:GLU:N	2.16	0.73
1:C:1320:MET:HA	1:C:1320:MET:HE2	1.69	0.73
1:D:28:THR:CG2	1:D:152:LEU:HD11	2.17	0.73
1:B:1725:GLN:OE1	1:B:1765:ASN:ND2	2.21	0.73
1:D:1895:GLN:O	1:D:1900:ASN:ND2	2.21	0.73
1:A:812:ILE:HD12	1:A:813:LYS:HE2	1.70	0.73
1:A:2485:LYS:CD	1:B:2452:GLU:OE2	2.36	0.73
1:D:10:ILE:HG13	1:D:114:ASP:O	1.88	0.73
1:A:1725:GLN:OE1	1:A:1765:ASN:ND2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2468:HIS:HB3	1:D:2479:ILE:HG21	1.70	0.73
1:B:451:MET:SD	1:B:475:LEU:HD22	2.28	0.73
1:B:592:GLU:HG2	1:B:633:TYR:OH	1.88	0.73
1:D:1725:GLN:OE1	1:D:1765:ASN:ND2	2.21	0.73
1:C:1182:MET:CE	1:C:1193:GLN:OE1	2.36	0.73
1:B:1250:LEU:CG	1:B:1264:MET:HE1	2.19	0.73
1:B:62:MET:HE2	1:B:161:TRP:CD2	2.23	0.73
1:B:1209:LEU:CD2	1:B:1228:THR:CG2	2.67	0.72
1:C:1953:HIS:ND1	1:C:2007:ARG:CZ	2.52	0.72
1:A:2485:LYS:CE	1:B:2452:GLU:OE2	2.37	0.72
1:C:1797:GLN:NE2	1:C:1906:GLU:OE1	2.21	0.72
1:D:1448:MET:SD	1:D:1468:VAL:HG23	2.28	0.72
1:D:652:ILE:O	1:D:656:VAL:HG23	1.89	0.72
1:B:233:GLU:N	1:B:233:GLU:OE2	2.21	0.72
1:D:1093:LYS:HZ1	1:D:1599:ILE:HG21	1.54	0.72
1:B:764:MET:SD	1:B:836:PHE:CZ	2.83	0.72
1:B:605:LEU:CD1	1:B:609:HIS:HD2	2.02	0.72
1:B:782:LEU:HD12	1:B:866:LEU:HA	1.70	0.72
1:C:740:CYS:SG	1:C:751:ILE:HD12	2.29	0.72
1:C:2184:TRP:HZ3	1:C:2187:LYS:HG3	1.55	0.72
1:A:2518:ASP:OD1	1:B:2524:ARG:CD	2.38	0.72
1:D:2219:ILE:HD11	1:D:2338:GLU:HB2	1.70	0.72
1:D:2392:LYS:CE	1:D:2456:ASP:HA	2.19	0.72
1:B:10:ILE:HD12	1:B:111:VAL:HG12	1.72	0.71
1:C:652:ILE:O	1:C:656:VAL:HG23	1.89	0.71
1:D:35:ARG:HH21	1:D:201:LEU:HD23	1.54	0.71
1:C:2162:ASP:OD1	1:C:2164:GLN:N	2.22	0.71
1:D:2219:ILE:HD13	1:D:2338:GLU:HB2	1.72	0.71
1:C:2479:ILE:HD12	1:C:2479:ILE:C	2.11	0.71
1:B:581:MET:CE	1:B:595:ILE:CD1	2.69	0.71
1:D:564:GLN:OE1	1:D:564:GLN:C	2.29	0.71
1:D:764:MET:SD	1:D:836:PHE:CZ	2.83	0.71
1:D:1085:ARG:O	1:D:1089:MET:HG3	1.89	0.71
1:B:652:ILE:O	1:B:656:VAL:HG23	1.89	0.71
1:B:1785:PHE:O	1:B:1788:VAL:CG1	2.38	0.71
1:C:754:GLN:OE1	1:C:754:GLN:HA	1.89	0.71
1:A:1875:ARG:NH2	1:A:1879:LEU:HD11	2.05	0.71
1:B:1055:PHE:O	1:B:1059:LEU:HD23	1.90	0.71
1:C:1182:MET:HE1	1:C:1193:GLN:OE1	1.91	0.71
1:C:1596:GLN:OE1	1:C:1596:GLN:C	2.29	0.71
1:B:761:PHE:CD1	1:B:764:MET:HE2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2216:ASN:ND2	1:B:2345:LEU:CG	2.52	0.71
1:C:893:ASP:CG	1:C:1054:MET:HE3	2.10	0.71
1:B:1250:LEU:CD1	1:B:1264:MET:HE1	2.16	0.71
1:C:1875:ARG:NH2	1:C:1879:LEU:HD11	2.05	0.70
1:C:319:GLU:OE1	1:C:319:GLU:N	2.24	0.70
1:B:71:TYR:OH	1:B:94:GLN:NE2	2.25	0.70
1:B:148:MET:HE3	1:B:190:ALA:HB1	1.73	0.70
1:B:1064:MET:O	1:B:1064:MET:CE	2.39	0.70
1:B:1250:LEU:HD12	1:B:1264:MET:HE2	1.72	0.70
1:B:2162:ASP:OD1	1:B:2164:GLN:N	2.24	0.70
1:C:140:PRO:HD3	1:D:1292:THR:HG22	1.73	0.70
1:B:110:LYS:O	1:B:110:LYS:HD3	1.90	0.70
1:B:764:MET:SD	1:B:836:PHE:CG	2.84	0.70
1:C:871:ILE:HD13	1:C:881:LEU:HD21	1.71	0.70
1:D:764:MET:SD	1:D:836:PHE:CG	2.84	0.70
1:D:2216:ASN:OD1	1:D:2342:SER:HA	1.92	0.70
1:B:1455:ARG:NH2	1:B:1465:GLU:OE2	2.25	0.70
1:C:1776:MET:HA	1:C:1776:MET:CE	2.22	0.70
1:A:607:GLU:HG2	1:A:647:VAL:HG21	1.72	0.70
1:A:2162:ASP:OD1	1:A:2164:GLN:N	2.23	0.70
1:B:564:GLN:C	1:B:564:GLN:OE1	2.29	0.70
1:B:2201:MET:SD	1:B:2300:PHE:CA	2.77	0.70
1:D:1960:VAL:HG13	1:D:1961:THR:HG23	1.73	0.70
1:D:2162:ASP:OD1	1:D:2164:GLN:N	2.24	0.70
1:A:1250:LEU:HD11	1:A:1264:MET:SD	2.31	0.70
1:A:1455:ARG:NH2	1:A:1465:GLU:OE2	2.25	0.70
1:D:1093:LYS:NZ	1:D:1599:ILE:HG21	2.07	0.70
1:B:1336:TYR:CD2	1:B:1345:LEU:HB2	2.27	0.69
1:B:1977:ASP:OD1	1:B:1977:ASP:O	2.10	0.69
1:C:257:TYR:CE2	1:C:258:LYS:HG2	2.27	0.69
1:A:773:LEU:O	1:A:777:PHE:HD1	1.74	0.69
1:B:267:THR:HG23	1:B:413:ILE:O	1.90	0.69
1:C:1793:MET:O	1:C:1797:GLN:HG3	1.92	0.69
1:C:1931:GLU:OE1	1:C:1932:ASP:OD1	2.08	0.69
1:A:2452:GLU:OE1	1:D:2485:LYS:HG2	1.91	0.69
1:B:76:GLN:OE1	1:B:76:GLN:HA	1.92	0.69
1:B:729:TYR:O	1:B:733:LEU:CD2	2.36	0.69
1:C:2518:ASP:OD1	1:D:2524:ARG:CD	2.39	0.69
1:D:1455:ARG:NH2	1:D:1465:GLU:OE2	2.25	0.69
1:C:457:GLU:OE1	1:C:458:LYS:N	2.25	0.69
1:C:394:THR:CG2	1:C:396:THR:HG23	2.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1085:ARG:NH1	1:D:1613:GLU:OE2	2.25	0.69
1:D:1444:PHE:O	1:D:1448:MET:HG2	1.91	0.69
1:A:653:CYS:HA	1:A:739:MET:SD	2.33	0.69
1:A:773:LEU:HD11	1:A:777:PHE:HE1	1.57	0.69
1:A:1784:ARG:O	1:A:1788:VAL:HG23	1.92	0.69
1:B:1085:ARG:NH1	1:B:1613:GLU:OE2	2.25	0.69
1:A:1085:ARG:NH1	1:A:1613:GLU:OE2	2.25	0.69
1:B:2536:THR:O	1:B:2536:THR:CG2	2.41	0.69
1:C:1455:ARG:NH2	1:C:1465:GLU:OE2	2.25	0.69
1:B:1209:LEU:HD23	1:B:1228:THR:CG2	2.17	0.69
1:C:1732:GLY:O	1:C:1735:LYS:HG3	1.93	0.69
1:B:545:LYS:NZ	1:C:1394:GLU:OE1	2.25	0.68
1:B:1902:ASN:OD1	1:B:1905:CYS:HB3	1.92	0.68
1:C:1085:ARG:NH1	1:C:1613:GLU:OE2	2.25	0.68
1:D:761:PHE:CD1	1:D:764:MET:CE	2.77	0.68
1:D:1664:LYS:HE3	1:D:1664:LYS:CA	2.19	0.68
1:D:1902:ASN:ND2	1:D:1905:CYS:HB3	2.09	0.68
1:D:2392:LYS:HE2	1:D:2456:ASP:HA	1.75	0.68
1:D:729:TYR:O	1:D:733:LEU:HD23	1.93	0.68
1:D:1250:LEU:HD11	1:D:1264:MET:CE	2.23	0.68
1:D:2549:ASP:O	1:D:2550:ASN:OD1	2.11	0.68
1:B:523:LYS:NZ	1:B:577:GLN:HE22	1.91	0.68
1:C:1784:ARG:O	1:C:1788:VAL:HG23	1.92	0.68
1:D:1660:LYS:HA	1:D:1660:LYS:CE	2.11	0.68
1:A:1974:ILE:HD12	1:A:2000:LEU:HD12	1.74	0.68
1:C:426:LYS:HG3	1:C:427:GLU:OE1	1.93	0.68
1:D:1761:LEU:HD23	1:D:1768:ILE:CG2	2.24	0.68
1:C:1349:MET:SD	1:C:1406:ILE:HG23	2.33	0.68
1:D:1652:LYS:O	1:D:1652:LYS:CD	2.36	0.68
1:D:1684:ASN:O	1:D:1688:LYS:NZ	2.25	0.68
1:B:989:TYR:CE2	1:B:1035:MET:CE	2.75	0.68
1:B:1790:HIS:HD2	1:B:1790:HIS:O	1.77	0.68
1:B:893:ASP:CG	1:B:1054:MET:CE	2.62	0.68
1:B:2352:GLU:OE1	1:B:2352:GLU:HA	1.94	0.68
1:C:1863:MET:HA	1:C:1863:MET:CE	2.23	0.68
1:D:110:LYS:HD3	1:D:110:LYS:C	2.13	0.68
1:D:1319:ASP:O	1:D:1323:THR:HG23	1.94	0.68
1:B:1793:MET:O	1:B:1797:GLN:HG3	1.94	0.68
1:C:1915:CYS:HB3	1:C:1925:LEU:CD1	2.25	0.68
1:D:1799:GLU:HA	1:D:1799:GLU:OE1	1.94	0.68
1:D:2397:LEU:HD11	1:D:2479:ILE:HD12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:PHE:CD1	1:B:764:MET:CE	2.77	0.67
1:C:1953:HIS:CE1	1:C:2007:ARG:HD2	2.29	0.67
1:C:554:ARG:CG	1:C:590:LEU:CD1	2.71	0.67
1:D:355:VAL:HG22	1:D:356:ALA:H	1.60	0.67
1:B:2049:VAL:O	1:B:2053:ILE:HG22	1.95	0.67
1:C:554:ARG:HG2	1:C:590:LEU:HD12	1.77	0.67
1:C:2389:LEU:HD21	1:D:2339:LEU:CD1	2.24	0.67
1:D:1253:PHE:CA	1:D:1260:GLU:OE1	2.42	0.67
1:B:1880:LEU:HD21	1:B:1888:LEU:HD22	1.76	0.67
1:C:1319:ASP:O	1:C:1323:THR:HG23	1.94	0.67
1:A:623:ARG:NH2	1:A:661:ASN:OD1	2.28	0.67
1:B:623:ARG:NH2	1:B:661:ASN:OD1	2.28	0.67
1:B:1226:ARG:O	1:B:1230:GLN:NE2	2.27	0.67
1:B:1902:ASN:CG	1:B:1905:CYS:HG	1.98	0.67
1:C:537:ARG:NH2	1:C:539:GLU:OE2	2.28	0.67
1:C:623:ARG:NH2	1:C:661:ASN:OD1	2.28	0.67
1:D:1235:PHE:O	1:D:1242:ASN:ND2	2.28	0.67
1:D:1093:LYS:HZ3	1:D:1599:ILE:HD13	1.59	0.67
1:B:990:LEU:HD21	1:B:1035:MET:SD	2.34	0.67
1:B:1064:MET:O	1:B:1064:MET:HE1	1.94	0.67
1:D:1971:THR:CB	1:D:2020:LEU:HD13	2.24	0.67
1:B:581:MET:CE	1:B:595:ILE:HD13	2.25	0.67
1:B:1093:LYS:CE	1:B:1599:ILE:HG21	2.24	0.67
1:B:1319:ASP:O	1:B:1323:THR:HG23	1.94	0.67
1:C:1880:LEU:HD21	1:C:1888:LEU:HD22	1.77	0.67
1:B:1253:PHE:CA	1:B:1260:GLU:OE1	2.42	0.66
1:C:1235:PHE:O	1:C:1242:ASN:ND2	2.28	0.66
1:B:474:GLN:OE1	1:B:474:GLN:HA	1.94	0.66
1:B:1961:THR:O	1:B:1961:THR:CG2	2.43	0.66
1:D:2184:TRP:CE3	1:D:2184:TRP:O	2.48	0.66
1:A:1319:ASP:O	1:A:1323:THR:HG23	1.94	0.66
1:C:805:GLU:OE1	1:C:805:GLU:HA	1.95	0.66
1:B:111:VAL:HG12	1:B:111:VAL:O	1.94	0.66
1:B:986:ARG:NH1	1:B:986:ARG:CB	2.55	0.66
1:B:2189:ARG:HD3	1:B:2195:TYR:CE1	2.31	0.66
1:C:1660:LYS:N	1:C:1660:LYS:HD2	2.10	0.66
1:C:608:LYS:HD2	1:C:608:LYS:C	2.15	0.66
1:C:893:ASP:CG	1:C:1054:MET:HE1	2.13	0.66
1:D:990:LEU:HD13	1:D:1092:PHE:CD2	2.31	0.66
1:C:2381:TYR:CZ	1:C:2385:ILE:HD11	2.31	0.66
1:D:623:ARG:NH2	1:D:661:ASN:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1623:TRP:CB	1:D:1626:LEU:HD11	2.24	0.66
1:A:2381:TYR:CZ	1:A:2385:ILE:HD11	2.31	0.66
1:B:1687:ARG:HG2	1:B:1691:LEU:HD11	1.76	0.66
1:D:1673:LEU:HD13	1:D:1759:HIS:HB3	1.76	0.66
1:D:1880:LEU:HD21	1:D:1888:LEU:HD22	1.76	0.66
1:B:1235:PHE:O	1:B:1242:ASN:ND2	2.28	0.66
1:C:667:ARG:HH12	1:C:754:GLN:CD	1.99	0.66
1:C:2187:LYS:HE3	1:C:2191:MET:HE2	1.72	0.66
1:A:1880:LEU:HD21	1:A:1888:LEU:HD22	1.77	0.66
1:A:320:ASN:ND2	1:A:350:ILE:O	2.29	0.66
1:B:320:ASN:ND2	1:B:350:ILE:O	2.25	0.66
1:B:1772:PHE:CD2	1:B:1776:MET:CE	2.72	0.66
1:B:2468:HIS:HB2	1:B:2479:ILE:HD13	1.78	0.66
1:D:761:PHE:CD1	1:D:764:MET:HE2	2.30	0.65
1:B:2025:LEU:HD12	1:B:2053:ILE:HD11	1.69	0.65
1:B:2216:ASN:HD21	1:B:2345:LEU:HG	1.61	0.65
1:B:2513:PHE:CD2	1:C:2513:PHE:HE2	2.14	0.65
1:A:812:ILE:CD1	1:A:813:LYS:HE3	2.26	0.65
1:A:2389:LEU:HD21	1:B:2339:LEU:CD1	2.26	0.65
1:D:982:ARG:HD3	1:D:986:ARG:HD2	1.77	0.65
1:D:1647:LEU:HD21	1:D:1665:VAL:CG1	2.26	0.65
1:A:2524:ARG:HD3	1:D:2518:ASP:OD1	1.97	0.65
1:B:1093:LYS:HE3	1:B:1599:ILE:HG21	1.77	0.65
1:C:2184:TRP:CE2	1:C:2307:PHE:HZ	2.14	0.65
1:D:1664:LYS:HA	1:D:1664:LYS:CE	2.13	0.65
1:A:656:VAL:CG2	1:A:739:MET:HE1	2.26	0.65
1:A:1235:PHE:O	1:A:1242:ASN:ND2	2.28	0.65
1:C:12:ASP:OD1	1:C:227:PHE:N	2.30	0.65
1:C:740:CYS:SG	1:C:751:ILE:CD1	2.84	0.65
1:C:1320:MET:HA	1:C:1320:MET:CE	2.27	0.65
1:B:99:MET:HE1	1:C:1922:LEU:HB3	1.77	0.65
1:C:28:THR:HG21	1:C:152:LEU:CD1	2.27	0.65
1:B:12:ASP:OD1	1:B:227:PHE:N	2.30	0.65
1:B:2518:ASP:OD1	1:C:2524:ARG:HD3	1.97	0.65
1:D:1684:ASN:C	1:D:1688:LYS:NZ	2.50	0.65
1:A:773:LEU:CD1	1:A:777:PHE:CE1	2.79	0.65
1:C:1110:ILE:HD11	1:C:1182:MET:HE1	1.79	0.65
1:A:812:ILE:HD12	1:A:813:LYS:HE3	1.79	0.65
1:B:1080:LYS:HA	1:B:1080:LYS:HE2	1.79	0.65
1:D:1250:LEU:CD1	1:D:1264:MET:HE2	2.27	0.65
1:A:1206:MET:HA	1:A:1206:MET:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:LYS:O	1:B:624:LYS:CD	2.44	0.64
1:C:1041:THR:O	1:C:1044:MET:CE	2.44	0.64
1:B:764:MET:SD	1:B:765:ALA:N	2.71	0.64
1:C:1250:LEU:CD1	1:C:1264:MET:HE3	2.22	0.64
1:C:2011:GLU:N	1:C:2011:GLU:OE1	2.29	0.64
1:D:1531:MET:O	1:D:1531:MET:HE1	1.97	0.64
1:A:12:ASP:OD1	1:A:227:PHE:N	2.30	0.64
1:A:750:GLU:O	1:A:750:GLU:OE2	2.14	0.64
1:C:1875:ARG:CZ	1:C:1879:LEU:HD11	2.27	0.64
1:B:523:LYS:HZ3	1:B:577:GLN:HE22	1.43	0.64
1:B:1055:PHE:HZ	1:B:1077:LEU:HD13	1.62	0.64
1:D:2597:LYS:HG3	1:D:2597:LYS:O	1.95	0.64
1:D:788:ARG:HB3	1:D:788:ARG:CZ	2.28	0.64
1:D:1902:ASN:HD21	1:D:1905:CYS:CB	1.95	0.64
1:A:1875:ARG:CZ	1:A:1879:LEU:HD11	2.27	0.64
1:B:598:LEU:O	1:B:602:ASN:ND2	2.31	0.64
1:B:768:MET:CE	1:B:768:MET:CA	2.64	0.64
1:C:320:ASN:ND2	1:C:350:ILE:O	2.29	0.64
1:D:354:LEU:HD21	1:D:398:ILE:HD12	1.79	0.64
1:D:1592:ILE:HG22	1:D:1596:GLN:OE1	1.97	0.64
1:B:1592:ILE:HG22	1:B:1596:GLN:OE1	1.97	0.64
1:C:1776:MET:HA	1:C:1776:MET:HE1	1.79	0.64
1:C:2187:LYS:HD2	1:C:2187:LYS:C	2.16	0.64
1:D:764:MET:SD	1:D:765:ALA:N	2.71	0.64
1:B:2348:LEU:HD23	1:B:2352:GLU:HG2	1.79	0.64
1:B:893:ASP:CG	1:B:1054:MET:HE1	2.18	0.63
1:C:1974:ILE:HD12	1:C:2000:LEU:CD1	2.27	0.63
1:D:354:LEU:HD21	1:D:398:ILE:CD1	2.27	0.63
1:B:1250:LEU:CG	1:B:1264:MET:CE	2.76	0.63
1:B:2184:TRP:CE3	1:B:2184:TRP:O	2.51	0.63
1:C:457:GLU:C	1:C:457:GLU:CD	2.57	0.63
1:D:426:LYS:HG3	1:D:427:GLU:OE1	1.99	0.63
1:D:2536:THR:O	1:D:2536:THR:CG2	2.42	0.63
1:B:764:MET:CG	1:B:836:PHE:CE2	2.82	0.63
1:C:394:THR:CG2	1:C:396:THR:CG2	2.75	0.63
1:D:598:LEU:O	1:D:602:ASN:ND2	2.31	0.63
1:A:2513:PHE:HZ	1:D:2513:PHE:CD2	2.16	0.63
1:B:2219:ILE:HD11	1:B:2282:LEU:HD22	1.80	0.63
1:C:2184:TRP:CE2	1:C:2307:PHE:CZ	2.87	0.63
1:D:519:PHE:CE1	1:D:560:LEU:HD11	2.33	0.63
1:D:990:LEU:HD13	1:D:1092:PHE:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2348:LEU:O	1:C:2348:LEU:HD23	1.99	0.63
1:B:581:MET:HE3	1:B:595:ILE:CG1	2.29	0.63
1:B:1325:LEU:CD2	1:B:1332:VAL:CG1	2.77	0.63
1:A:598:LEU:O	1:A:602:ASN:ND2	2.31	0.63
1:D:2280:PRO:HA	1:D:2283:ASN:OD1	1.99	0.63
1:B:2556:GLU:CD	1:B:2556:GLU:N	2.51	0.62
1:D:761:PHE:O	1:D:764:MET:CE	2.44	0.62
1:A:305:ARG:NH1	1:A:365:SER:OG	2.32	0.62
1:B:261:LEU:CD1	1:B:311:THR:HG21	2.29	0.62
1:B:1785:PHE:O	1:B:1788:VAL:HG13	1.99	0.62
1:A:2513:PHE:HE2	1:D:2513:PHE:CD2	2.14	0.62
1:B:1729:ASP:C	1:B:1729:ASP:OD1	2.37	0.62
1:C:1206:MET:HE3	1:C:1206:MET:HA	1.80	0.62
1:C:1953:HIS:CE1	1:C:2007:ARG:CD	2.82	0.62
1:D:160:SER:O	1:D:162:LEU:HD12	1.99	0.62
1:C:1916:GLY:HA3	1:C:1928:TYR:CE2	2.34	0.62
1:C:2513:PHE:CE2	1:D:2513:PHE:HE2	2.17	0.62
1:D:62:MET:HE2	1:D:161:TRP:CZ2	2.34	0.62
1:A:2513:PHE:CE2	1:B:2513:PHE:HE2	2.16	0.62
1:C:1673:LEU:O	1:C:1721:ILE:CD1	2.47	0.62
1:D:802:LEU:CD2	1:D:804:THR:HG22	2.29	0.62
1:B:5:SER:HB2	1:C:374:LEU:CD2	2.29	0.62
1:B:153:ASP:OD2	1:B:155:THR:HG22	1.99	0.62
1:B:305:ARG:NH1	1:B:365:SER:OG	2.32	0.62
1:C:598:LEU:O	1:C:602:ASN:ND2	2.33	0.62
1:D:1243:GLN:OE1	1:D:1271:ASN:ND2	2.33	0.62
1:A:1243:GLN:OE1	1:A:1271:ASN:ND2	2.33	0.62
1:B:1785:PHE:O	1:B:1788:VAL:HG12	1.99	0.62
1:D:305:ARG:NH1	1:D:365:SER:OG	2.32	0.62
1:D:1209:LEU:HD12	1:D:1212:ILE:HD12	1.82	0.62
1:B:1651:THR:OG1	1:B:1665:VAL:HG11	2.00	0.62
1:B:1734:THR:HG23	1:B:1772:PHE:CE1	2.35	0.62
1:C:305:ARG:NH1	1:C:365:SER:OG	2.32	0.62
1:C:537:ARG:HD3	1:C:540:GLU:OE1	2.00	0.62
1:D:10:ILE:HD12	1:D:111:VAL:HG12	1.82	0.62
1:D:250:LYS:HE2	1:D:415:LEU:HD11	1.81	0.62
1:D:261:LEU:CD1	1:D:311:THR:HG21	2.29	0.62
1:D:764:MET:CG	1:D:836:PHE:CE2	2.82	0.62
1:B:768:MET:HE3	1:B:768:MET:CA	2.14	0.62
1:C:1747:GLU:O	1:C:1751:GLN:HG3	1.99	0.62
1:A:374:LEU:CD2	1:D:5:SER:HB2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2328:LEU:O	1:B:2332:LEU:HD13	1.99	0.62
1:B:99:MET:HE2	1:C:1922:LEU:HD12	0.62	0.61
1:B:581:MET:HE3	1:B:595:ILE:CD1	2.29	0.61
1:B:1243:GLN:OE1	1:B:1271:ASN:ND2	2.33	0.61
1:C:2479:ILE:CD1	1:C:2480:LEU:CD2	2.61	0.61
1:D:927:MET:C	1:D:927:MET:CE	2.68	0.61
1:B:160:SER:O	1:B:162:LEU:HD12	1.99	0.61
1:B:982:ARG:HD3	1:B:986:ARG:HH12	1.65	0.61
1:C:802:LEU:CD2	1:C:804:THR:HG22	2.29	0.61
1:D:1623:TRP:HB2	1:D:1626:LEU:CD1	2.30	0.61
1:D:2014:GLU:OE2	1:D:2014:GLU:HA	2.00	0.61
1:B:538:LEU:HD22	1:B:587:TYR:CG	2.35	0.61
1:B:761:PHE:O	1:B:764:MET:CE	2.44	0.61
1:C:1363:MET:HA	1:C:1366:ILE:HD12	1.82	0.61
1:D:1761:LEU:HD23	1:D:1768:ILE:HG22	1.79	0.61
1:B:581:MET:HE2	1:B:595:ILE:CD1	2.30	0.61
1:B:977:PHE:O	1:B:981:VAL:HG23	2.01	0.61
1:B:1797:GLN:OE1	1:B:1906:GLU:OE1	2.18	0.61
1:C:977:PHE:O	1:C:981:VAL:HG23	2.01	0.61
1:A:773:LEU:HD11	1:A:777:PHE:CE1	2.35	0.61
1:D:1206:MET:HA	1:D:1206:MET:HE3	1.83	0.61
1:D:977:PHE:O	1:D:981:VAL:HG23	2.01	0.61
1:D:1592:ILE:HG23	1:D:1596:GLN:HE22	1.66	0.61
1:D:1685:GLN:O	1:D:1688:LYS:HG3	2.00	0.61
1:D:2292:ASN:ND2	1:D:2292:ASN:O	2.33	0.61
1:A:977:PHE:O	1:A:981:VAL:HG23	2.01	0.61
1:B:250:LYS:HE2	1:B:415:LEU:HD11	1.81	0.61
1:C:265:LEU:HD23	1:C:417:LEU:HD21	1.82	0.61
1:C:368:GLU:OE1	1:C:368:GLU:CA	2.48	0.61
1:B:99:MET:CE	1:C:1922:LEU:CD1	0.61	0.60
1:D:802:LEU:HB3	1:D:805:GLU:HG2	1.82	0.60
1:A:2513:PHE:CE2	1:B:2513:PHE:CE2	2.88	0.60
1:C:1968:ASP:OD1	1:C:2019:SER:OG	2.09	0.60
1:A:2452:GLU:CG	1:D:2485:LYS:HE3	2.30	0.60
1:B:89:LEU:HD11	1:C:1927:LEU:HD21	1.83	0.60
1:C:2349:ILE:HG12	1:C:2359:ILE:CD1	2.31	0.60
1:D:1684:ASN:C	1:D:1688:LYS:HZ2	2.04	0.60
1:D:250:LYS:HB2	1:D:265:LEU:HD23	1.81	0.60
1:D:1250:LEU:CD1	1:D:1264:MET:CE	2.79	0.60
1:B:624:LYS:HD2	1:B:624:LYS:C	2.22	0.60
1:D:927:MET:O	1:D:927:MET:CE	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:HIS:HD2	1:D:138:ARG:CZ	2.12	0.60
1:A:2368:SER:OG	1:B:2354:THR:CG2	2.49	0.60
1:D:62:MET:HE2	1:D:161:TRP:CE2	2.36	0.60
1:A:786:VAL:HG21	1:A:866:LEU:HD11	1.84	0.60
1:B:581:MET:HE2	1:B:595:ILE:HD13	1.82	0.60
1:B:1592:ILE:HG23	1:B:1596:GLN:HE22	1.66	0.60
1:B:2352:GLU:OE1	1:B:2352:GLU:CA	2.50	0.60
1:C:2513:PHE:CE2	1:D:2513:PHE:CE2	2.89	0.60
1:D:1652:LYS:HD2	1:D:1652:LYS:C	2.20	0.60
1:B:1621:LEU:HD23	1:B:1672:MET:HE2	1.84	0.60
1:B:2513:PHE:CD2	1:C:2513:PHE:HZ	2.16	0.60
1:A:884:LEU:HD12	1:A:884:LEU:O	2.01	0.60
1:D:2201:MET:SD	1:D:2300:PHE:HA	2.42	0.60
1:B:889:LEU:HD12	1:B:975:LEU:HD21	1.81	0.60
1:B:1064:MET:CE	1:B:1064:MET:C	2.70	0.60
1:B:1611:GLN:OE1	1:B:1611:GLN:N	2.35	0.60
1:C:786:VAL:HG21	1:C:866:LEU:HD11	1.84	0.60
1:B:2571:PHE:CE2	1:B:2590:VAL:HG21	2.36	0.59
1:B:1764:GLY:O	1:B:1883:ASN:ND2	2.35	0.59
1:C:257:TYR:CE2	1:C:258:LYS:CG	2.85	0.59
1:B:1651:THR:HG22	1:B:1736:LEU:HD11	1.83	0.59
1:A:812:ILE:CD1	1:A:813:LYS:CE	2.79	0.59
1:C:99:MET:HA	1:C:102:LYS:HE3	1.84	0.59
1:C:2549:ASP:OD1	1:C:2550:ASN:ND2	2.36	0.59
1:B:2280:PRO:HA	1:B:2283:ASN:OD1	2.02	0.59
1:A:2549:ASP:OD1	1:A:2550:ASN:ND2	2.36	0.59
1:B:1688:LYS:HA	1:B:1691:LEU:HD12	1.84	0.59
1:D:2292:ASN:HD22	1:D:2292:ASN:C	2.06	0.59
1:A:374:LEU:HD21	1:D:5:SER:CB	2.33	0.59
1:B:2549:ASP:OD1	1:B:2550:ASN:ND2	2.36	0.59
1:C:153:ASP:OD1	1:C:155:THR:HG22	2.03	0.59
1:D:1902:ASN:HD21	1:D:1905:CYS:HB3	1.64	0.59
1:A:1910:PHE:CE2	1:A:1914:MET:HE2	2.38	0.59
1:C:250:LYS:CD	1:C:415:LEU:HD12	2.33	0.59
1:D:1623:TRP:CB	1:D:1626:LEU:CD1	2.81	0.59
1:B:5:SER:CB	1:C:374:LEU:HD21	2.33	0.59
1:C:1957:THR:O	1:C:1961:THR:HG23	2.03	0.59
1:C:2327:ILE:HG13	1:C:2328:LEU:N	2.16	0.59
1:B:1032:ALA:HA	1:B:1035:MET:HE3	1.85	0.58
1:C:265:LEU:HD21	1:C:417:LEU:HD21	1.84	0.58
1:A:1764:GLY:O	1:A:1883:ASN:ND2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1097:LEU:CD1	1:B:1595:LEU:HD22	2.33	0.58
1:B:1737:VAL:CG2	1:B:1753:SER:O	2.51	0.58
1:B:2011:GLU:OE1	1:B:2011:GLU:N	2.36	0.58
1:B:2571:PHE:HE2	1:B:2590:VAL:HG11	1.67	0.58
1:C:1974:ILE:HD11	1:C:2000:LEU:CD1	2.33	0.58
1:A:1371:LEU:HD12	1:A:1371:LEU:O	2.04	0.58
1:B:624:LYS:CD	1:B:624:LYS:C	2.71	0.58
1:D:1097:LEU:CD1	1:D:1595:LEU:HD22	2.33	0.58
1:A:1968:ASP:OD1	1:A:2019:SER:OG	2.09	0.58
1:B:1055:PHE:CZ	1:B:1077:LEU:HD13	2.38	0.58
1:C:2368:SER:OG	1:D:2354:THR:CG2	2.52	0.58
1:B:1093:LYS:NZ	1:B:1599:ILE:HD13	2.18	0.58
1:B:2598:ASN:OD1	1:B:2599:LEU:N	2.37	0.58
1:C:2468:HIS:HB3	1:C:2479:ILE:HG21	1.84	0.58
1:D:1737:VAL:CG2	1:D:1753:SER:O	2.51	0.58
1:A:1086:GLN:OE1	1:A:1086:GLN:O	2.22	0.58
1:A:2598:ASN:OD1	1:A:2599:LEU:N	2.37	0.58
1:B:10:ILE:HD12	1:B:111:VAL:CG1	2.34	0.58
1:B:402:ASN:O	1:B:402:ASN:ND2	2.30	0.58
1:C:1773:HIS:CE1	1:C:1777:MET:HE2	2.38	0.58
1:D:1660:LYS:HD2	1:D:1660:LYS:N	2.19	0.58
1:D:2598:ASN:OD1	1:D:2599:LEU:N	2.37	0.58
1:B:889:LEU:HD23	1:B:1054:MET:HG3	1.86	0.58
1:B:1648:ILE:HD11	1:B:1669:LEU:HD11	1.86	0.58
1:B:2133:MET:HE2	1:B:2608:MET:HG3	1.86	0.58
1:A:2021:ARG:HB2	1:A:2024:GLU:OE1	2.04	0.57
1:C:2281:THR:HA	1:C:2284:ILE:CG2	2.34	0.57
1:B:764:MET:SD	1:B:764:MET:C	2.83	0.57
1:B:1325:LEU:CD2	1:B:1332:VAL:HG11	2.34	0.57
1:B:2050:GLY:O	1:B:2053:ILE:HG23	2.05	0.57
1:B:2510:ASN:HB3	1:C:2513:PHE:CD1	2.39	0.57
1:D:153:ASP:OD1	1:D:155:THR:HG22	2.05	0.57
1:C:727:SER:HA	1:C:730:ARG:HD3	1.85	0.57
1:C:1751:GLN:HG2	1:C:1869:ILE:HD13	1.86	0.57
1:D:2033:TYR:CE1	1:D:2047:ARG:NH2	2.66	0.57
1:B:1371:LEU:HD12	1:B:1371:LEU:O	2.03	0.57
1:C:1250:LEU:CD2	1:C:1264:MET:HE3	2.32	0.57
1:B:2468:HIS:CB	1:B:2479:ILE:HD13	2.35	0.57
1:C:1742:THR:HG21	1:C:1781:LYS:HE2	1.87	0.57
1:C:1974:ILE:HD12	1:C:2000:LEU:HD11	1.86	0.57
1:D:1927:LEU:H	1:D:1927:LEU:HD12	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:THR:OG1	1:B:413:ILE:HG22	2.04	0.57
1:B:2481:ARG:HD2	1:C:2400:ASP:OD1	2.04	0.57
1:C:2598:ASN:OD1	1:C:2599:LEU:N	2.37	0.57
1:B:505:ARG:O	1:B:509:MET:HG2	2.05	0.57
1:C:768:MET:CE	1:C:768:MET:CA	2.67	0.57
1:D:1954:GLU:HA	1:D:1954:GLU:OE2	2.05	0.57
1:C:2058:LEU:HD23	1:C:2071:LEU:CD1	2.34	0.57
1:D:611:THR:OG1	1:D:612:LYS:N	2.38	0.57
1:D:764:MET:SD	1:D:764:MET:C	2.83	0.57
1:B:111:VAL:O	1:B:111:VAL:CG1	2.53	0.57
1:B:611:THR:OG1	1:B:612:LYS:N	2.38	0.57
1:C:2154:ARG:HG3	1:C:2154:ARG:HH11	1.70	0.57
1:D:1685:GLN:HA	1:D:1688:LYS:HD2	1.85	0.57
1:B:398:ILE:HD13	1:B:419:THR:HG22	1.87	0.56
1:B:1050:GLU:CD	1:B:1053:ARG:NH2	2.58	0.56
1:B:1105:GLU:OE2	1:B:1109:VAL:HG11	2.05	0.56
1:B:1669:LEU:HD23	1:B:1672:MET:HE3	1.86	0.56
1:C:1793:MET:CE	1:C:1903:LEU:HD22	2.35	0.56
1:D:1542:MET:SD	1:D:1543:ASP:HA	2.45	0.56
1:B:840:TYR:CE2	1:B:860:THR:HG22	2.40	0.56
1:C:554:ARG:CG	1:C:590:LEU:HD13	2.33	0.56
1:C:969:LEU:O	1:C:973:GLU:HG3	2.05	0.56
1:D:927:MET:SD	1:D:927:MET:C	2.83	0.56
1:A:611:THR:OG1	1:A:612:LYS:N	2.38	0.56
1:B:1325:LEU:CD2	1:B:1332:VAL:HG12	2.36	0.56
1:B:1336:TYR:HD2	1:B:1345:LEU:HB2	1.66	0.56
1:B:1527:ARG:O	1:B:1531:MET:HG2	2.05	0.56
1:B:2226:MET:SD	1:B:2226:MET:C	2.84	0.56
1:C:457:GLU:OE1	1:C:457:GLU:C	2.43	0.56
1:C:608:LYS:C	1:C:608:LYS:CD	2.74	0.56
1:C:1773:HIS:HE1	1:C:1777:MET:HE1	1.66	0.56
1:D:481:PHE:HE1	1:D:488:ASN:HA	1.67	0.56
1:B:1325:LEU:HD22	1:B:1333:VAL:CG2	2.35	0.56
1:B:1325:LEU:HD22	1:B:1333:VAL:HG23	1.88	0.56
1:D:495:ASP:C	1:D:495:ASP:OD1	2.42	0.56
1:D:1619:ASP:OD2	1:D:1687:ARG:NH2	2.38	0.56
1:A:1619:ASP:OD2	1:A:1687:ARG:NH2	2.38	0.56
1:B:1325:LEU:HD21	1:B:1332:VAL:CG1	2.35	0.56
1:D:2481:ARG:O	1:D:2483:PRO:HD3	2.06	0.56
1:C:19:GLU:O	1:C:19:GLU:CD	2.44	0.56
1:C:1619:ASP:OD2	1:C:1687:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1684:ASN:HB3	1:D:1688:LYS:HZ3	1.70	0.56
1:A:969:LEU:O	1:A:973:GLU:HG3	2.06	0.56
1:A:2513:PHE:CD1	1:D:2510:ASN:HB3	2.40	0.56
1:B:19:GLU:OE1	1:B:23:ASN:HB3	2.05	0.56
1:B:1064:MET:HE1	1:B:1064:MET:C	2.26	0.56
1:B:1349:MET:HE1	1:B:1404:ASP:O	2.06	0.56
1:B:1619:ASP:OD2	1:B:1687:ARG:NH2	2.38	0.56
1:B:2050:GLY:HA2	1:B:2053:ILE:CG2	2.36	0.56
1:B:2468:HIS:HB3	1:B:2479:ILE:HG21	1.88	0.56
1:B:2485:LYS:HE2	1:C:2452:GLU:OE2	2.06	0.56
1:D:19:GLU:O	1:D:19:GLU:HG3	2.05	0.56
1:D:1085:ARG:O	1:D:1089:MET:CG	2.52	0.56
1:A:1120:MET:SD	1:A:1172:VAL:HG22	2.46	0.56
1:A:1288:HIS:HD2	1:D:138:ARG:NH2	2.00	0.56
1:B:2189:ARG:HD3	1:B:2195:TYR:CZ	2.39	0.56
1:C:639:VAL:HG21	1:C:738:ARG:CD	2.36	0.56
1:C:884:LEU:HD12	1:C:884:LEU:O	2.06	0.56
1:C:2187:LYS:CD	1:C:2191:MET:HE3	2.35	0.56
1:C:2281:THR:O	1:C:2284:ILE:CG2	2.54	0.56
1:C:2281:THR:O	1:C:2284:ILE:HG23	2.05	0.56
1:D:802:LEU:HD22	1:D:805:GLU:HG2	1.88	0.56
1:A:805:GLU:HA	1:A:805:GLU:OE1	2.06	0.56
1:B:1176:LEU:HD21	1:B:1206:MET:HE1	1.86	0.56
1:C:1596:GLN:OE1	1:C:1596:GLN:O	2.24	0.56
1:D:872:TYR:OH	1:D:935:VAL:HG22	2.05	0.56
1:D:884:LEU:HD12	1:D:884:LEU:O	2.06	0.56
1:D:1734:THR:HG23	1:D:1772:PHE:CE2	2.40	0.56
1:A:2513:PHE:HE1	1:D:2510:ASN:O	1.89	0.56
1:B:884:LEU:O	1:B:884:LEU:HD12	2.06	0.56
1:C:854:GLU:OE1	1:C:854:GLU:N	2.37	0.56
1:C:1371:LEU:HD12	1:C:1371:LEU:O	2.06	0.56
1:D:2226:MET:C	1:D:2226:MET:SD	2.84	0.56
1:B:99:MET:CE	1:C:1922:LEU:HD13	0.81	0.55
1:B:872:TYR:OH	1:B:935:VAL:HG22	2.05	0.55
1:C:398:ILE:HD13	1:C:419:THR:HG22	1.87	0.55
1:C:1918:THR:O	1:C:1922:LEU:HG	2.06	0.55
1:C:2485:LYS:HD3	1:D:2452:GLU:OE2	2.06	0.55
1:D:2124:ILE:HG23	1:D:2138:PHE:CE1	2.38	0.55
1:C:2280:PRO:O	1:C:2284:ILE:HG22	2.06	0.55
1:D:10:ILE:CD1	1:D:111:VAL:HG12	2.36	0.55
1:D:1081:HIS:HD2	1:D:1082:PHE:CE2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1908:LEU:HD22	1:D:1959:ILE:HG12	1.88	0.55
1:D:1975:LEU:CD2	1:D:2024:GLU:HB3	2.37	0.55
1:A:398:ILE:HD13	1:A:419:THR:HG22	1.87	0.55
1:A:750:GLU:OE2	1:A:754:GLN:HG3	2.07	0.55
1:C:605:LEU:HD12	1:C:609:HIS:CD2	2.41	0.55
1:B:209:GLU:HG3	1:B:210:VAL:N	2.21	0.55
1:B:231:LEU:O	1:B:236:LYS:NZ	2.38	0.55
1:B:788:ARG:HB3	1:B:788:ARG:HH11	1.72	0.55
1:B:893:ASP:CG	1:B:1054:MET:HE3	2.25	0.55
1:B:2510:ASN:O	1:C:2513:PHE:HE1	1.89	0.55
1:C:111:VAL:O	1:C:111:VAL:HG12	2.07	0.55
1:C:233:GLU:HA	1:C:233:GLU:OE1	2.06	0.55
1:D:398:ILE:HD13	1:D:419:THR:HG22	1.87	0.55
1:B:1116:ARG:HB3	1:B:1120:MET:HE2	1.86	0.55
1:D:76:GLN:OE1	1:D:76:GLN:HA	2.07	0.55
1:A:622:VAL:O	1:A:626:ARG:N	2.38	0.55
1:C:1362:LEU:HG	1:C:1366:ILE:HD11	1.89	0.55
1:C:2389:LEU:HD21	1:D:2339:LEU:HD11	1.89	0.55
1:A:105:ASP:OD2	1:A:105:ASP:C	2.44	0.55
1:A:1265:GLN:HG3	1:A:1305:THR:HG21	1.89	0.55
1:B:1687:ARG:O	1:B:1691:LEU:CG	2.43	0.55
1:D:1952:CYS:O	1:D:1956:GLN:HG3	2.07	0.55
1:A:111:VAL:O	1:A:111:VAL:HG12	2.07	0.55
1:B:2481:ARG:NE	1:C:2400:ASP:OD1	2.40	0.55
1:C:1256:PRO:HA	1:C:1289:LEU:HD21	1.89	0.55
1:C:2009:ASP:OD2	1:C:2011:GLU:OE2	2.25	0.55
1:B:1729:ASP:OD1	1:B:1729:ASP:O	2.25	0.54
1:A:605:LEU:HD12	1:A:609:HIS:CD2	2.41	0.54
1:A:1793:MET:O	1:A:1797:GLN:HG3	2.08	0.54
1:A:2164:GLN:HA	1:A:2164:GLN:OE1	2.07	0.54
1:B:481:PHE:CE2	1:B:488:ASN:HA	2.42	0.54
1:B:1050:GLU:CD	1:B:1053:ARG:CZ	2.69	0.54
1:B:2311:TYR:O	1:B:2314:MET:HE3	2.08	0.54
1:C:650:GLU:HG2	1:C:651:LEU:HD23	1.90	0.54
1:C:1362:LEU:O	1:C:1366:ILE:CG1	2.47	0.54
1:D:564:GLN:HB3	1:D:574:ILE:HD12	1.90	0.54
1:D:982:ARG:CD	1:D:986:ARG:HD2	2.36	0.54
1:A:1886:ARG:NH2	1:A:1951:PRO:O	2.41	0.54
1:A:2485:LYS:HG2	1:B:2452:GLU:OE2	2.07	0.54
1:C:1621:LEU:HD12	1:C:1643:PHE:HE2	1.73	0.54
1:D:1253:PHE:HB2	1:D:1264:MET:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLN:HB3	1:A:574:ILE:HD12	1.90	0.54
1:B:622:VAL:O	1:B:626:ARG:N	2.38	0.54
1:B:1773:HIS:HE1	1:B:1891:PHE:CD1	2.25	0.54
1:C:622:VAL:O	1:C:626:ARG:N	2.38	0.54
1:D:622:VAL:O	1:D:626:ARG:N	2.38	0.54
1:B:1116:ARG:C	1:B:1120:MET:CE	2.76	0.54
1:C:1182:MET:HE2	1:C:1193:GLN:OE1	2.08	0.54
1:D:1761:LEU:HD21	1:D:1768:ILE:HG22	1.90	0.54
1:D:1772:PHE:HD1	1:D:1776:MET:HE2	1.70	0.54
1:B:1974:ILE:HD11	1:B:1997:SER:CA	2.38	0.54
1:C:608:LYS:HG3	1:C:609:HIS:CD2	2.43	0.54
1:C:733:LEU:HD13	1:C:776:SER:OG	2.08	0.54
1:C:1793:MET:HE3	1:C:1903:LEU:HD22	1.90	0.54
1:B:99:MET:HE2	1:C:1922:LEU:CD1	1.32	0.53
1:B:889:LEU:HD11	1:B:975:LEU:CD2	2.32	0.53
1:B:1093:LYS:HE2	1:B:1599:ILE:HD13	1.89	0.53
1:B:1886:ARG:NH2	1:B:1951:PRO:O	2.41	0.53
1:B:2376:ALA:HB2	1:B:2508:VAL:HG11	1.90	0.53
1:C:28:THR:HG22	1:C:152:LEU:HD11	1.90	0.53
1:C:611:THR:OG1	1:C:612:LYS:N	2.38	0.53
1:C:867:ALA:O	1:C:871:ILE:HG13	2.08	0.53
1:C:1265:GLN:HG3	1:C:1305:THR:HG21	1.89	0.53
1:D:1319:ASP:HB2	1:D:1320:MET:HE2	1.91	0.53
1:B:2216:ASN:HD22	1:B:2345:LEU:HG	1.70	0.53
1:C:1953:HIS:CE1	1:C:2007:ARG:NH1	2.51	0.53
1:A:2368:SER:OG	1:B:2354:THR:HG21	2.08	0.53
1:B:868:HIS:HD2	1:B:868:HIS:O	1.91	0.53
1:B:1685:GLN:OE1	1:B:1688:LYS:HD2	2.07	0.53
1:C:257:TYR:CZ	1:C:258:LYS:HG2	2.44	0.53
1:A:140:PRO:HG3	1:B:1292:THR:HA	1.90	0.53
1:B:2124:ILE:HG23	1:B:2138:PHE:CE1	2.38	0.53
1:B:2571:PHE:HE2	1:B:2590:VAL:HG21	1.72	0.53
1:C:1886:ARG:NH2	1:C:1951:PRO:O	2.41	0.53
1:D:990:LEU:CD1	1:D:1092:PHE:CD2	2.91	0.53
1:A:92:LYS:HB3	1:B:1924:LEU:HD21	1.89	0.53
1:A:1061:HIS:ND1	1:A:1061:HIS:O	2.42	0.53
1:B:986:ARG:HH11	1:B:986:ARG:HB3	1.73	0.53
1:D:2376:ALA:HB2	1:D:2508:VAL:HG11	1.90	0.53
1:A:2164:GLN:OE1	1:A:2164:GLN:CA	2.55	0.53
1:C:2281:THR:HA	1:C:2284:ILE:HG22	1.89	0.53
1:D:1684:ASN:HB3	1:D:1688:LYS:HZ1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1886:ARG:NH2	1:D:1951:PRO:O	2.41	0.53
1:D:2389:LEU:HB3	1:D:2390:PHE:CD2	2.44	0.53
1:B:1737:VAL:HG21	1:B:1753:SER:O	2.09	0.53
1:C:2058:LEU:CD2	1:C:2071:LEU:HD13	2.37	0.53
1:D:111:VAL:HG12	1:D:111:VAL:O	2.09	0.53
1:D:231:LEU:O	1:D:236:LYS:NZ	2.38	0.53
1:D:990:LEU:HD21	1:D:1032:ALA:HB2	1.91	0.53
1:B:2279:GLY:C	1:B:2283:ASN:OD1	2.46	0.53
1:C:564:GLN:HB3	1:C:574:ILE:HD12	1.89	0.53
1:C:825:ASP:OD1	1:C:826:LYS:N	2.42	0.53
1:C:1055:PHE:CE1	1:C:1059:LEU:HD11	2.44	0.53
1:C:2376:ALA:HB2	1:C:2508:VAL:HG11	1.90	0.53
1:D:402:ASN:O	1:D:402:ASN:ND2	2.30	0.53
1:A:656:VAL:HG21	1:A:739:MET:HE1	1.91	0.53
1:B:164:ILE:HG23	1:B:164:ILE:O	2.09	0.53
1:B:1790:HIS:O	1:B:1790:HIS:CD2	2.59	0.53
1:C:730:ARG:HH21	1:C:772:ASP:HB2	1.73	0.53
1:C:2485:LYS:HG2	1:D:2452:GLU:OE2	2.09	0.53
1:D:164:ILE:HG23	1:D:164:ILE:O	2.09	0.53
1:B:1250:LEU:HG	1:B:1264:MET:HE1	1.90	0.53
1:D:782:LEU:HD23	1:D:782:LEU:C	2.30	0.53
1:D:2279:GLY:C	1:D:2283:ASN:OD1	2.46	0.53
1:B:261:LEU:HD11	1:B:311:THR:HG21	1.90	0.52
1:B:840:TYR:HE2	1:B:860:THR:HG22	1.74	0.52
1:B:1055:PHE:CE1	1:B:1059:LEU:HD21	2.43	0.52
1:D:261:LEU:HD11	1:D:311:THR:HG21	1.91	0.52
1:A:164:ILE:HG23	1:A:164:ILE:O	2.09	0.52
1:A:261:LEU:CD2	1:A:311:THR:HG21	2.39	0.52
1:B:806:ILE:O	1:B:995:LYS:NZ	2.39	0.52
1:B:825:ASP:OD1	1:B:826:LYS:N	2.42	0.52
1:B:1116:ARG:C	1:B:1120:MET:HE3	2.29	0.52
1:B:1551:MET:N	1:B:1551:MET:SD	2.82	0.52
1:B:619:VAL:CG2	1:B:655:CYS:SG	2.89	0.52
1:B:1543:ASP:OD1	1:B:1544:LEU:N	2.42	0.52
1:C:1954:GLU:N	1:C:1954:GLU:CD	2.56	0.52
1:D:1793:MET:O	1:D:1797:GLN:HG3	2.07	0.52
1:A:2485:LYS:HD3	1:B:2452:GLU:OE2	2.07	0.52
1:B:2518:ASP:OD1	1:C:2524:ARG:CD	2.58	0.52
1:D:1975:LEU:HD21	1:D:2024:GLU:HB3	1.90	0.52
1:A:825:ASP:OD1	1:A:826:LYS:N	2.42	0.52
1:A:2376:ALA:HB2	1:A:2508:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2215:ILE:O	1:B:2219:ILE:HD13	2.09	0.52
1:B:2555:PHE:O	1:B:2559:ILE:HG23	2.09	0.52
1:C:164:ILE:O	1:C:164:ILE:HG23	2.09	0.52
1:C:782:LEU:C	1:C:782:LEU:HD23	2.30	0.52
1:A:231:LEU:O	1:A:236:LYS:NZ	2.38	0.52
1:B:1952:CYS:O	1:B:1956:GLN:HG3	2.08	0.52
1:D:538:LEU:HD22	1:D:587:TYR:CG	2.42	0.52
1:D:813:LYS:HZ2	1:D:813:LYS:HB3	1.73	0.52
1:A:997:GLU:HG2	1:A:1028:ILE:HD11	1.92	0.52
1:A:1055:PHE:CZ	1:A:1059:LEU:HD11	2.44	0.52
1:C:997:GLU:HG2	1:C:1028:ILE:HD11	1.92	0.52
1:D:2389:LEU:HB3	1:D:2390:PHE:CE2	2.45	0.52
1:A:782:LEU:HD23	1:A:782:LEU:C	2.30	0.52
1:C:667:ARG:NH1	1:C:754:GLN:CD	2.63	0.52
1:D:1649:GLN:OE1	1:D:1649:GLN:HA	2.09	0.52
1:D:1737:VAL:HG21	1:D:1753:SER:O	2.09	0.52
1:B:1093:LYS:CE	1:B:1599:ILE:HD13	2.39	0.52
1:B:1105:GLU:OE2	1:B:1109:VAL:CG1	2.57	0.52
1:B:2396:ILE:C	1:B:2397:LEU:HD12	2.30	0.52
1:B:931:ARG:NH2	1:B:966:GLU:OE2	2.43	0.52
1:B:1772:PHE:CD2	1:B:1776:MET:HE2	2.39	0.52
1:C:666:ILE:HG12	1:C:696:TRP:HB3	1.91	0.52
1:C:733:LEU:CD2	1:C:780:LEU:HD22	2.36	0.52
1:D:825:ASP:OD1	1:D:826:LYS:N	2.42	0.52
1:B:354:LEU:HD11	1:B:398:ILE:HD12	1.93	0.51
1:B:791:GLN:HB3	1:B:873:PHE:CD1	2.45	0.51
1:C:647:VAL:O	1:C:651:LEU:HG	2.10	0.51
1:C:806:ILE:O	1:C:995:LYS:NZ	2.39	0.51
1:C:1214:TYR:CD2	1:C:1221:MET:HE2	2.45	0.51
1:D:2033:TYR:CE1	1:D:2047:ARG:NE	2.74	0.51
1:A:2389:LEU:HD21	1:B:2339:LEU:HD11	1.92	0.51
1:B:1380:ASN:OD1	1:B:1381:VAL:N	2.44	0.51
1:C:1380:ASN:OD1	1:C:1381:VAL:N	2.44	0.51
1:D:523:LYS:HE3	1:D:580:MET:SD	2.50	0.51
1:D:1543:ASP:OD1	1:D:1544:LEU:N	2.42	0.51
1:B:10:ILE:HG13	1:B:114:ASP:O	2.10	0.51
1:B:764:MET:HG3	1:B:836:PHE:CE2	2.46	0.51
1:B:1951:PRO:HG3	1:B:2006:SER:OG	2.09	0.51
1:D:806:ILE:O	1:D:995:LYS:NZ	2.39	0.51
1:D:997:GLU:HG2	1:D:1028:ILE:HD11	1.92	0.51
1:A:1543:ASP:OD1	1:A:1544:LEU:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2524:ARG:CD	1:D:2518:ASP:OD1	2.58	0.51
1:B:997:GLU:HG2	1:B:1028:ILE:HD11	1.92	0.51
1:C:931:ARG:NH2	1:C:966:GLU:OE2	2.43	0.51
1:C:1543:ASP:OD1	1:C:1544:LEU:N	2.42	0.51
1:D:1055:PHE:CZ	1:D:1059:LEU:HD11	2.45	0.51
1:D:2292:ASN:ND2	1:D:2292:ASN:C	2.64	0.51
1:D:2571:PHE:HE1	1:D:2590:VAL:HG21	1.75	0.51
1:D:497:MET:SD	1:D:497:MET:C	2.89	0.51
1:D:1197:LEU:N	1:D:1197:LEU:HD23	2.25	0.51
1:B:523:LYS:HE3	1:B:580:MET:SD	2.50	0.51
1:B:1250:LEU:HG	1:B:1264:MET:CE	2.41	0.51
1:D:2057:ALA:O	1:D:2061:SER:OG	2.27	0.51
1:D:2146:PHE:CE2	1:D:2186:ARG:HD2	2.46	0.51
1:B:17:TYR:CE2	1:B:19:GLU:HG2	2.46	0.51
1:B:238:GLY:N	1:B:285:VAL:O	2.42	0.51
1:B:402:ASN:O	1:B:404:PRO:HD3	2.10	0.51
1:B:582:GLN:HE22	1:B:614:GLU:HB3	1.76	0.51
1:B:1064:MET:O	1:B:1064:MET:HE2	2.10	0.51
1:C:667:ARG:HH12	1:C:754:GLN:NE2	2.08	0.51
1:D:581:MET:HB3	1:D:595:ILE:HD11	1.93	0.51
1:D:1951:PRO:HG3	1:D:2006:SER:OG	2.11	0.51
1:B:564:GLN:HB3	1:B:574:ILE:HD12	1.91	0.51
1:B:976:GLN:OE1	1:B:976:GLN:HA	2.11	0.51
1:B:1614:LEU:O	1:B:1618:VAL:HG23	2.11	0.51
1:B:1790:HIS:CD2	1:B:1790:HIS:C	2.84	0.51
1:B:1875:ARG:NH2	1:B:1879:LEU:HD11	2.26	0.51
1:B:2474:GLY:CA	1:C:2471:ARG:O	2.55	0.51
1:D:355:VAL:HG22	1:D:356:ALA:N	2.25	0.51
1:D:1531:MET:O	1:D:1531:MET:HE3	2.09	0.51
1:C:250:LYS:HE2	1:C:415:LEU:HD12	1.93	0.51
1:C:250:LYS:CE	1:C:415:LEU:CD1	2.88	0.51
1:C:1945:THR:HG22	1:C:1999:LEU:HB2	1.93	0.51
1:D:976:GLN:HA	1:D:976:GLN:OE1	2.11	0.51
1:D:1380:ASN:OD1	1:D:1381:VAL:N	2.44	0.51
1:B:1651:THR:HG21	1:B:1736:LEU:HD21	1.93	0.51
1:C:1915:CYS:HB3	1:C:1925:LEU:HD11	1.93	0.51
1:D:1210:LEU:HD21	1:D:1228:THR:OG1	2.11	0.51
1:D:2522:ASP:C	1:D:2522:ASP:OD1	2.49	0.51
1:A:1120:MET:CE	1:A:1172:VAL:HG22	2.42	0.50
1:B:408:GLU:N	1:B:408:GLU:OE2	2.43	0.50
1:B:927:MET:O	1:B:927:MET:SD	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LEU:O	1:C:236:LYS:NZ	2.38	0.50
1:C:1655:MET:HE1	1:C:1744:THR:HA	1.92	0.50
1:D:764:MET:HG3	1:D:836:PHE:CE2	2.46	0.50
1:D:882:LEU:O	1:D:885:THR:HG22	2.12	0.50
1:D:1875:ARG:NH2	1:D:1879:LEU:HD11	2.26	0.50
1:D:1977:ASP:OD2	1:D:1977:ASP:C	2.48	0.50
1:B:538:LEU:CD2	1:B:589:ILE:HD11	2.42	0.50
1:B:2297:VAL:HG21	1:B:2327:ILE:HD11	1.92	0.50
1:A:1059:LEU:HD21	1:A:1077:LEU:HB2	1.93	0.50
1:B:497:MET:SD	1:B:497:MET:C	2.90	0.50
1:B:2188:LEU:HD12	1:B:2188:LEU:O	2.11	0.50
1:B:2387:GLY:O	1:B:2391:LEU:N	2.44	0.50
1:C:1250:LEU:CG	1:C:1264:MET:HE3	2.41	0.50
1:C:2368:SER:OG	1:D:2354:THR:HG21	2.10	0.50
1:A:931:ARG:NH2	1:A:966:GLU:OE2	2.43	0.50
1:B:1945:THR:HG22	1:B:1999:LEU:HB2	1.93	0.50
1:D:2571:PHE:HE1	1:D:2590:VAL:HG11	1.77	0.50
1:B:407:ILE:HG13	1:B:408:GLU:OE2	2.11	0.50
1:B:1761:LEU:CD2	1:B:1768:ILE:HG22	2.41	0.50
1:C:2188:LEU:O	1:C:2188:LEU:HD12	2.11	0.50
1:D:2297:VAL:HG21	1:D:2327:ILE:HD11	1.92	0.50
1:A:763:CYS:SG	1:A:777:PHE:CE2	3.05	0.50
1:B:1225:LEU:HA	1:B:1228:THR:OG1	2.12	0.50
1:B:1325:LEU:HD21	1:B:1332:VAL:HG12	1.93	0.50
1:B:2522:ASP:C	1:B:2522:ASP:OD1	2.49	0.50
1:C:882:LEU:O	1:C:885:THR:HG22	2.12	0.50
1:D:1448:MET:SD	1:D:1468:VAL:HG21	2.51	0.50
1:A:526:PHE:CD1	1:A:538:LEU:HD23	2.46	0.50
1:A:1910:PHE:CE2	1:A:1914:MET:CE	2.95	0.50
1:A:2524:ARG:NE	1:D:2518:ASP:OD1	2.45	0.50
1:B:1622:HIS:CE1	1:B:1672:MET:HG3	2.47	0.50
1:C:29:LEU:HD22	1:C:204:ASN:OD1	2.12	0.50
1:C:2043:GLU:OE1	1:C:2043:GLU:HA	2.11	0.50
1:D:402:ASN:O	1:D:404:PRO:HD3	2.11	0.50
1:A:972:LEU:HD22	1:A:1077:LEU:HD12	1.94	0.50
1:B:169:LYS:HA	1:B:169:LYS:HE2	1.94	0.50
1:B:592:GLU:CG	1:B:633:TYR:OH	2.59	0.50
1:B:1773:HIS:O	1:B:1777:MET:HG2	2.12	0.50
1:D:458:LYS:HB2	1:D:464:ILE:HD11	1.94	0.50
1:D:484:SER:HB3	1:D:486:VAL:HG23	1.94	0.50
1:D:1592:ILE:O	1:D:1596:GLN:OE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:THR:O	1:A:1095:VAL:HG23	2.12	0.50
1:A:2188:LEU:HD12	1:A:2188:LEU:O	2.11	0.50
1:B:1091:THR:O	1:B:1095:VAL:HG23	2.12	0.50
1:B:1325:LEU:HD23	1:B:1332:VAL:HG11	1.94	0.50
1:C:1033:GLU:OE2	1:C:1609:LEU:HD11	2.11	0.50
1:C:2332:LEU:O	1:C:2336:ALA:N	2.45	0.50
1:D:2043:GLU:HA	1:D:2043:GLU:OE2	2.12	0.50
1:D:2332:LEU:O	1:D:2336:ALA:N	2.45	0.50
1:A:2297:VAL:HG21	1:A:2327:ILE:HD11	1.92	0.49
1:A:2471:ARG:O	1:D:2474:GLY:CA	2.55	0.49
1:B:2219:ILE:HD11	1:B:2282:LEU:CD2	2.41	0.49
1:C:1091:THR:O	1:C:1095:VAL:HG23	2.12	0.49
1:D:289:HIS:NE2	1:D:294:ARG:HD3	2.27	0.49
1:D:1093:LYS:CE	1:D:1599:ILE:HD13	2.41	0.49
1:D:1794:LYS:NZ	1:D:1906:GLU:OE2	2.44	0.49
1:A:36:CYS:SG	1:A:152:LEU:HD21	2.52	0.49
1:A:1910:PHE:CZ	1:A:1914:MET:HE1	2.47	0.49
1:A:2387:GLY:O	1:A:2391:LEU:N	2.44	0.49
1:B:481:PHE:CZ	1:B:488:ASN:HA	2.48	0.49
1:C:238:GLY:N	1:C:285:VAL:O	2.42	0.49
1:A:806:ILE:O	1:A:995:LYS:NZ	2.39	0.49
1:A:1380:ASN:OD1	1:A:1381:VAL:N	2.44	0.49
1:B:812:ILE:HG13	1:B:813:LYS:N	2.28	0.49
1:B:2518:ASP:OD1	1:C:2524:ARG:NE	2.44	0.49
1:C:406:ASP:N	1:C:406:ASP:OD1	2.46	0.49
1:D:1082:PHE:CD1	1:D:1617:LEU:HB2	2.47	0.49
1:D:1091:THR:O	1:D:1095:VAL:HG23	2.12	0.49
1:D:1945:THR:HG22	1:D:1999:LEU:HB2	1.93	0.49
1:A:1055:PHE:CE2	1:A:1059:LEU:HD11	2.47	0.49
1:A:2332:LEU:O	1:A:2336:ALA:N	2.45	0.49
1:B:868:HIS:CD2	1:B:868:HIS:C	2.85	0.49
1:B:1592:ILE:O	1:B:1596:GLN:OE1	2.30	0.49
1:B:2513:PHE:CE2	1:C:2513:PHE:HE2	2.30	0.49
1:C:1180:ASN:OD1	1:C:1234:LYS:NZ	2.44	0.49
1:D:2555:PHE:O	1:D:2559:ILE:HG23	2.12	0.49
1:B:2201:MET:HG2	1:B:2299:SER:HB2	1.95	0.49
1:D:34:ASP:OD1	1:D:34:ASP:N	2.33	0.49
1:B:1116:ARG:O	1:B:1120:MET:HE2	2.11	0.49
1:B:2216:ASN:OD1	1:B:2342:SER:HA	2.13	0.49
1:D:406:ASP:OD1	1:D:406:ASP:N	2.46	0.49
1:D:2188:LEU:HD12	1:D:2188:LEU:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:LYS:HA	1:B:1080:LYS:CE	2.39	0.49
1:B:1080:LYS:HE2	1:B:1080:LYS:CA	2.38	0.49
1:C:2397:LEU:HD11	1:C:2479:ILE:HD13	1.92	0.49
1:D:733:LEU:CD1	1:D:780:LEU:HD22	2.43	0.49
1:D:1082:PHE:CD2	1:D:1082:PHE:N	2.81	0.49
1:A:1945:THR:HG22	1:A:1999:LEU:HB2	1.93	0.49
1:B:99:MET:HE3	1:C:1922:LEU:CD1	0.78	0.49
1:B:255:ASP:OD1	1:B:280:ASN:ND2	2.46	0.49
1:B:406:ASP:OD1	1:B:406:ASP:N	2.46	0.49
1:B:1685:GLN:O	1:B:1688:LYS:HG2	2.13	0.49
1:B:1773:HIS:CE1	1:B:1891:PHE:CD1	3.01	0.49
1:C:7:PHE:CE2	1:D:374:LEU:HD12	2.48	0.49
1:C:362:ASP:N	1:C:362:ASP:OD1	2.45	0.49
1:C:639:VAL:CG2	1:C:738:ARG:CD	2.91	0.49
1:C:2507:ILE:O	1:C:2511:LEU:N	2.45	0.49
1:D:1622:HIS:CE1	1:D:1672:MET:HG3	2.47	0.49
1:D:1623:TRP:HB3	1:D:1626:LEU:HG	1.95	0.49
1:D:2468:HIS:CB	1:D:2479:ILE:HG21	2.41	0.49
1:D:2507:ILE:O	1:D:2511:LEU:N	2.45	0.49
1:A:1180:ASN:OD1	1:A:1234:LYS:NZ	2.44	0.49
1:B:387:VAL:HG21	1:B:431:ILE:HD11	1.95	0.49
1:B:982:ARG:CD	1:B:986:ARG:HH12	2.26	0.49
1:B:989:TYR:CD2	1:B:1035:MET:HE2	2.41	0.49
1:B:2507:ILE:O	1:B:2511:LEU:N	2.45	0.49
1:D:1055:PHE:CE2	1:D:1059:LEU:HD11	2.48	0.49
1:D:1059:LEU:HD21	1:D:1077:LEU:HB3	1.94	0.49
1:A:726:LEU:O	1:A:730:ARG:HG3	2.12	0.49
1:A:2511:LEU:HD21	1:B:2362:VAL:CG2	2.39	0.49
1:A:2513:PHE:CE1	1:D:2510:ASN:O	2.66	0.49
1:B:1209:LEU:HD21	1:B:1228:THR:HG21	1.89	0.49
1:B:1601:ALA:HA	1:B:1604:GLU:OE2	2.12	0.49
1:B:2291:THR:O	1:B:2294:ILE:HG22	2.13	0.49
1:B:2364:ARG:NH1	1:B:2522:ASP:OD2	2.46	0.49
1:D:726:LEU:O	1:D:730:ARG:HG3	2.12	0.49
1:A:255:ASP:OD1	1:A:280:ASN:ND2	2.46	0.48
1:A:882:LEU:O	1:A:885:THR:HG22	2.12	0.48
1:A:1089:MET:SD	1:A:1606:LEU:HD12	2.53	0.48
1:C:36:CYS:SG	1:C:152:LEU:HD21	2.53	0.48
1:C:639:VAL:HG21	1:C:738:ARG:HD2	1.94	0.48
1:C:639:VAL:CG2	1:C:738:ARG:HD2	2.43	0.48
1:C:802:LEU:HD23	1:C:803:TRP:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1438:TRP:CE3	1:C:1497:ILE:HG21	2.48	0.48
1:C:2387:GLY:O	1:C:2391:LEU:N	2.44	0.48
1:D:241:VAL:HG22	1:D:285:VAL:HG23	1.94	0.48
1:D:538:LEU:HD23	1:D:589:ILE:HD11	1.94	0.48
1:A:2054:TYR:CE1	1:A:2071:LEU:HD22	2.48	0.48
1:A:2212:ALA:O	1:A:2216:ASN:ND2	2.46	0.48
1:A:2474:GLY:HA2	1:B:2471:ARG:O	2.13	0.48
1:A:2513:PHE:HE2	1:D:2513:PHE:CE2	2.31	0.48
1:B:28:THR:CG2	1:B:152:LEU:CD1	2.85	0.48
1:B:99:MET:SD	1:C:1922:LEU:HD11	2.31	0.48
1:B:538:LEU:HD23	1:B:541:LEU:HD12	1.95	0.48
1:B:882:LEU:O	1:B:885:THR:HG22	2.12	0.48
1:C:223:LEU:HD23	1:C:294:ARG:HH22	1.78	0.48
1:C:1732:GLY:O	1:C:1735:LYS:CG	2.61	0.48
1:C:2396:ILE:CG2	1:C:2396:ILE:O	2.61	0.48
1:D:62:MET:HE3	1:D:161:TRP:CE3	2.40	0.48
1:D:1063:THR:O	1:D:1071:VAL:CG2	2.57	0.48
1:D:2571:PHE:CE1	1:D:2590:VAL:HG11	2.48	0.48
1:A:860:THR:O	1:A:864:VAL:HG23	2.13	0.48
1:B:1438:TRP:CE3	1:B:1497:ILE:HG21	2.48	0.48
1:B:1792:ARG:HG2	1:B:1873:ILE:CD1	2.44	0.48
1:C:802:LEU:HD22	1:C:805:GLU:HG2	1.94	0.48
1:C:1250:LEU:CD1	1:C:1264:MET:SD	2.89	0.48
1:C:1974:ILE:HD13	1:C:2000:LEU:HD12	1.89	0.48
1:A:1438:TRP:CE3	1:A:1497:ILE:HG21	2.48	0.48
1:A:2007:ARG:NH2	1:A:2011:GLU:OE2	2.47	0.48
1:B:1600:THR:O	1:B:1604:GLU:OE2	2.32	0.48
1:D:1093:LYS:NZ	1:D:1599:ILE:CD1	2.73	0.48
1:D:1438:TRP:CE3	1:D:1497:ILE:HG21	2.48	0.48
1:D:1773:HIS:O	1:D:1777:MET:HG3	2.14	0.48
1:D:1957:THR:HA	1:D:1960:VAL:CG1	2.43	0.48
1:A:406:ASP:OD1	1:A:406:ASP:N	2.46	0.48
1:B:29:LEU:HD21	1:B:37:VAL:HG11	1.95	0.48
1:B:538:LEU:HD23	1:B:589:ILE:HD11	1.94	0.48
1:D:641:ASN:C	1:D:642:HIS:ND1	2.67	0.48
1:D:802:LEU:HD23	1:D:803:TRP:N	2.28	0.48
1:D:1999:LEU:O	1:D:2003:LEU:HD23	2.12	0.48
1:B:986:ARG:HB2	1:B:986:ARG:CZ	2.43	0.48
1:D:255:ASP:OD1	1:D:280:ASN:ND2	2.46	0.48
1:D:1055:PHE:HZ	1:D:1077:LEU:HD13	1.78	0.48
1:D:1063:THR:C	1:D:1071:VAL:HG22	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1189:MET:CE	1:D:1192:LYS:HD2	2.44	0.48
1:A:238:GLY:N	1:A:285:VAL:O	2.42	0.48
1:A:1773:HIS:HB2	1:A:1888:LEU:HD21	1.96	0.48
1:B:788:ARG:HH11	1:B:788:ARG:CB	2.26	0.48
1:B:927:MET:O	1:B:927:MET:HE2	2.14	0.48
1:B:1206:MET:HA	1:B:1206:MET:HE3	1.95	0.48
1:D:522:LEU:HD21	1:D:556:CYS:CB	2.44	0.48
1:D:788:ARG:NH1	1:D:788:ARG:CB	2.72	0.48
1:D:1331:ASP:OD1	1:D:1331:ASP:N	2.47	0.48
1:D:1761:LEU:CD2	1:D:1768:ILE:CG2	2.87	0.48
1:D:1785:PHE:HE1	1:D:1789:LEU:HD11	1.79	0.48
1:D:2209:PHE:HD2	1:D:2351:ARG:HH21	1.60	0.48
1:B:1331:ASP:OD1	1:B:1331:ASP:N	2.47	0.48
1:B:2597:LYS:HG3	1:B:2597:LYS:O	2.14	0.48
1:C:759:LEU:HD23	1:C:759:LEU:C	2.33	0.48
1:C:1773:HIS:HB2	1:C:1888:LEU:HD21	1.96	0.48
1:C:2162:ASP:OD1	1:C:2162:ASP:C	2.51	0.48
1:C:2212:ALA:O	1:C:2216:ASN:ND2	2.46	0.48
1:C:2474:GLY:HA2	1:D:2471:ARG:O	2.14	0.48
1:D:2162:ASP:OD1	1:D:2162:ASP:C	2.52	0.48
1:A:1256:PRO:HA	1:A:1289:LEU:HD21	1.95	0.48
1:A:1981:LEU:HD23	1:A:1989:VAL:HG23	1.96	0.48
1:B:1912:ASP:C	1:B:1912:ASP:OD1	2.51	0.48
1:C:1785:PHE:HE1	1:C:1789:LEU:HD11	1.79	0.48
1:C:2215:ILE:HG22	1:C:2219:ILE:HD11	1.96	0.48
1:D:1773:HIS:HB2	1:D:1888:LEU:HD21	1.96	0.48
1:D:1910:PHE:CZ	1:D:1914:MET:HE1	2.49	0.48
1:D:2014:GLU:OE2	1:D:2014:GLU:CA	2.61	0.48
1:D:2311:TYR:O	1:D:2314:MET:HE3	2.14	0.48
1:A:7:PHE:CE2	1:B:374:LEU:HD12	2.49	0.48
1:A:709:ARG:NH1	1:A:768:MET:SD	2.87	0.48
1:B:31:LEU:N	1:B:447:ASP:OD2	2.43	0.48
1:B:1981:LEU:HD23	1:B:1989:VAL:HG23	1.96	0.48
1:B:2332:LEU:O	1:B:2336:ALA:N	2.45	0.48
1:C:1089:MET:SD	1:C:1606:LEU:HD12	2.54	0.48
1:C:2187:LYS:C	1:C:2187:LYS:CD	2.81	0.48
1:D:522:LEU:HD21	1:D:556:CYS:HB2	1.95	0.48
1:D:1882:GLU:CG	1:D:1946:GLU:OE2	2.58	0.48
1:A:168:TRP:CH2	1:B:425:ASP:HB2	2.48	0.47
1:A:1288:HIS:NE2	1:D:138:ARG:CZ	2.63	0.47
1:B:2162:ASP:OD1	1:B:2162:ASP:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLU:O	1:C:19:GLU:OE1	2.31	0.47
1:C:607:GLU:C	1:C:607:GLU:OE1	2.52	0.47
1:C:887:THR:O	1:C:891:ILE:HG13	2.14	0.47
1:C:1915:CYS:O	1:C:1925:LEU:HD12	2.14	0.47
1:C:2184:TRP:CZ2	1:C:2307:PHE:HZ	2.32	0.47
1:D:1080:LYS:NZ	1:D:1087:GLU:CD	2.67	0.47
1:D:1093:LYS:O	1:D:1093:LYS:HD3	2.14	0.47
1:D:2390:PHE:CD2	1:D:2390:PHE:N	2.82	0.47
1:A:374:LEU:CD2	1:D:5:SER:CB	2.92	0.47
1:B:1256:PRO:HA	1:B:1289:LEU:HD21	1.96	0.47
1:B:2118:GLU:HA	1:B:2121:THR:CG2	2.45	0.47
1:B:2510:ASN:O	1:C:2513:PHE:CE1	2.65	0.47
1:C:1218:ASP:CB	1:C:1221:MET:HG2	2.44	0.47
1:D:110:LYS:HE2	1:D:110:LYS:HA	1.96	0.47
1:D:1787:LYS:O	1:D:1791:ASP:OD1	2.32	0.47
1:D:2364:ARG:NH1	1:D:2522:ASP:OD2	2.46	0.47
1:B:1063:THR:C	1:B:1071:VAL:HG22	2.34	0.47
1:B:2022:PRO:O	1:B:2026:VAL:HG13	2.14	0.47
1:C:31:LEU:N	1:C:447:ASP:OD2	2.43	0.47
1:D:788:ARG:HB3	1:D:788:ARG:HH11	1.75	0.47
1:D:1660:LYS:N	1:D:1660:LYS:CD	2.76	0.47
1:D:2022:PRO:O	1:D:2026:VAL:HG13	2.14	0.47
1:A:656:VAL:HB	1:A:739:MET:CE	2.44	0.47
1:B:772:ASP:OD1	1:B:773:LEU:N	2.47	0.47
1:B:1116:ARG:O	1:B:1120:MET:CE	2.62	0.47
1:C:245:HIS:O	1:C:249:GLU:N	2.47	0.47
1:D:1981:LEU:HD23	1:D:1989:VAL:HG23	1.96	0.47
1:A:656:VAL:HG21	1:A:739:MET:CE	2.44	0.47
1:A:1785:PHE:HE1	1:A:1789:LEU:HD11	1.79	0.47
1:B:585:ILE:HG23	1:B:592:GLU:OE2	2.14	0.47
1:B:1082:PHE:CE2	1:B:1617:LEU:HD13	2.50	0.47
1:B:1863:MET:HE1	1:B:1867:VAL:HB	1.95	0.47
1:C:1655:MET:HE2	1:C:1740:LEU:HD22	1.96	0.47
1:C:2485:LYS:CG	1:D:2452:GLU:OE2	2.63	0.47
1:A:245:HIS:O	1:A:249:GLU:N	2.47	0.47
1:A:2507:ILE:O	1:A:2511:LEU:N	2.45	0.47
1:B:62:MET:HE2	1:B:161:TRP:CH2	2.49	0.47
1:B:1667:ARG:NH1	1:B:1752:GLU:OE2	2.48	0.47
1:C:608:LYS:O	1:C:608:LYS:CD	2.55	0.47
1:D:458:LYS:CB	1:D:464:ILE:HD11	2.41	0.47
1:D:1056:LEU:HD12	1:D:1694:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1448:MET:SD	1:D:1468:VAL:HG22	2.52	0.47
1:A:1235:PHE:O	1:A:1235:PHE:CD1	2.68	0.47
1:A:2022:PRO:O	1:A:2026:VAL:HG13	2.14	0.47
1:A:2485:LYS:CG	1:B:2452:GLU:OE2	2.62	0.47
1:B:893:ASP:OD2	1:B:1054:MET:HE1	2.14	0.47
1:B:1206:MET:CE	1:B:1228:THR:HG22	2.44	0.47
1:B:1616:VAL:HG22	1:B:1691:LEU:HD21	1.97	0.47
1:B:1687:ARG:CG	1:B:1691:LEU:HD11	2.41	0.47
1:B:2188:LEU:HD11	1:B:2195:TYR:HA	1.97	0.47
1:C:29:LEU:HD13	1:C:204:ASN:OD1	2.14	0.47
1:C:545:LYS:CD	1:D:1394:GLU:OE1	2.33	0.47
1:C:772:ASP:OD1	1:C:773:LEU:N	2.47	0.47
1:C:1120:MET:SD	1:C:1127:TRP:NE1	2.88	0.47
1:C:1863:MET:CE	1:C:1867:VAL:HG21	2.45	0.47
1:C:2011:GLU:HA	1:C:2014:GLU:OE2	2.14	0.47
1:C:2022:PRO:O	1:C:2026:VAL:HG13	2.14	0.47
1:D:245:HIS:O	1:D:249:GLU:N	2.47	0.47
1:D:772:ASP:OD1	1:D:773:LEU:N	2.47	0.47
1:D:964:VAL:O	1:D:968:LYS:HG3	2.15	0.47
1:D:1974:ILE:CG2	1:D:1975:LEU:N	2.78	0.47
1:D:2118:GLU:HA	1:D:2121:THR:CG2	2.44	0.47
1:D:2133:MET:HG2	1:D:2606:ARG:HH21	1.80	0.47
1:A:2400:ASP:HB2	1:D:2481:ARG:CG	2.45	0.47
1:D:1256:PRO:HA	1:D:1289:LEU:HD21	1.96	0.47
1:D:1338:ASP:OD1	1:D:1339:LYS:N	2.47	0.47
1:D:1747:GLU:OE1	1:D:1792:ARG:NH1	2.48	0.47
1:A:461:GLU:HA	1:A:461:GLU:OE2	2.13	0.47
1:A:1063:THR:HG21	1:A:1643:PHE:HE1	1.79	0.47
1:A:1963:GLU:OE1	1:A:1963:GLU:N	2.46	0.47
1:B:2054:TYR:CE1	1:B:2071:LEU:HD22	2.50	0.47
1:A:2188:LEU:HD11	1:A:2195:TYR:HA	1.97	0.47
1:A:2400:ASP:HB2	1:D:2481:ARG:HG2	1.96	0.47
1:B:5:SER:CB	1:C:374:LEU:CD2	2.92	0.47
1:B:1785:PHE:HE1	1:B:1789:LEU:HD11	1.79	0.47
1:C:1235:PHE:O	1:C:1235:PHE:CD1	2.68	0.47
1:C:1366:ILE:O	1:C:1370:ASP:OD1	2.33	0.47
1:C:1912:ASP:OD1	1:C:1917:SER:HA	2.15	0.47
1:C:1981:LEU:HD23	1:C:1989:VAL:HG23	1.96	0.47
1:D:250:LYS:HE2	1:D:415:LEU:CD1	2.44	0.47
1:D:2188:LEU:HD11	1:D:2195:TYR:HA	1.97	0.47
1:D:2332:LEU:HD22	1:D:2336:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:VAL:HB	1:A:739:MET:HE3	1.98	0.46
1:A:772:ASP:OD1	1:A:773:LEU:N	2.47	0.46
1:A:877:SER:OG	1:A:880:GLU:HG3	2.14	0.46
1:A:1331:ASP:OD1	1:A:1331:ASP:N	2.47	0.46
1:A:2162:ASP:OD1	1:A:2162:ASP:C	2.52	0.46
1:C:1331:ASP:OD1	1:C:1331:ASP:N	2.47	0.46
1:D:1673:LEU:HD23	1:D:1673:LEU:O	2.15	0.46
1:B:137:LYS:HA	1:B:148:MET:SD	2.56	0.46
1:B:245:HIS:O	1:B:249:GLU:N	2.47	0.46
1:B:250:LYS:HE2	1:B:415:LEU:CD1	2.44	0.46
1:B:1616:VAL:HG13	1:B:1691:LEU:HD23	1.98	0.46
1:C:253:THR:HG23	1:C:280:ASN:HB3	1.97	0.46
1:C:1673:LEU:O	1:C:1721:ILE:HD11	2.14	0.46
1:D:2387:GLY:O	1:D:2391:LEU:N	2.44	0.46
1:A:2381:TYR:CE2	1:B:2342:SER:HB2	2.50	0.46
1:B:561:ARG:O	1:B:564:GLN:NE2	2.48	0.46
1:C:71:TYR:OH	1:C:75:LYS:NZ	2.48	0.46
1:C:1762:ASP:OD2	1:C:1762:ASP:C	2.54	0.46
1:D:94:GLN:HE21	1:D:98:GLN:HE22	1.63	0.46
1:D:1235:PHE:O	1:D:1235:PHE:CD1	2.68	0.46
1:D:2054:TYR:CE1	1:D:2071:LEU:HD22	2.50	0.46
1:A:2215:ILE:HG22	1:A:2219:ILE:HD11	1.96	0.46
1:B:110:LYS:HA	1:B:110:LYS:HE2	1.97	0.46
1:B:1550:SER:C	1:B:1551:MET:SD	2.94	0.46
1:C:1054:MET:SD	1:C:1057:ARG:NH2	2.88	0.46
1:C:1902:ASN:C	1:C:1902:ASN:OD1	2.54	0.46
1:C:1963:GLU:OE1	1:C:1963:GLU:N	2.46	0.46
1:D:10:ILE:HD12	1:D:114:ASP:HB2	1.95	0.46
1:D:1652:LYS:HZ2	1:D:1739:ASP:HB3	1.81	0.46
1:A:1094:GLN:O	1:A:1096:GLN:OE1	2.33	0.46
1:C:1055:PHE:CD1	1:C:1059:LEU:HD11	2.51	0.46
1:C:1673:LEU:HD11	1:C:1760:LEU:HD13	1.98	0.46
1:C:2055:ILE:O	1:C:2059:GLN:HG3	2.16	0.46
1:D:1621:LEU:HD11	1:D:1644:LEU:CD1	2.45	0.46
1:D:2216:ASN:ND2	1:D:2345:LEU:HG	2.30	0.46
1:A:607:GLU:HG2	1:A:647:VAL:CG2	2.43	0.46
1:B:1784:ARG:O	1:B:1788:VAL:HG12	2.16	0.46
1:C:1890:ASN:OD1	1:C:1893:ARG:NH1	2.49	0.46
1:C:2511:LEU:HD21	1:D:2362:VAL:CG2	2.41	0.46
1:D:523:LYS:CE	1:D:577:GLN:OE1	2.63	0.46
1:A:1176:LEU:HD12	1:A:1224:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:PHE:C	1:B:861:PHE:CD2	2.89	0.46
1:B:2050:GLY:O	1:B:2053:ILE:CG2	2.64	0.46
1:C:99:MET:SD	1:C:102:LYS:NZ	2.80	0.46
1:C:168:TRP:CH2	1:D:425:ASP:HB2	2.50	0.46
1:C:2375:LEU:HD22	1:D:2355:LEU:HD11	1.97	0.46
1:D:1056:LEU:HD12	1:D:1694:TYR:CD1	2.51	0.46
1:D:1448:MET:CE	1:D:1472:VAL:HG11	2.45	0.46
1:A:31:LEU:N	1:A:447:ASP:OD2	2.43	0.46
1:B:1176:LEU:HD12	1:B:1224:ILE:HG23	1.97	0.46
1:B:2513:PHE:CE2	1:B:2517:ILE:HD11	2.51	0.46
1:C:261:LEU:CD2	1:C:311:THR:HG21	2.46	0.46
1:C:1086:GLN:OE1	1:C:1086:GLN:O	2.34	0.46
1:C:1176:LEU:HD12	1:C:1224:ILE:HG23	1.97	0.46
1:B:1338:ASP:OD1	1:B:1339:LYS:N	2.47	0.46
1:B:1786:PHE:CE2	1:B:1892:LEU:HD23	2.51	0.46
1:C:200:GLU:HG3	1:C:208:LYS:NZ	2.30	0.46
1:C:1055:PHE:CZ	1:C:1059:LEU:HD11	2.51	0.46
1:C:2188:LEU:HD11	1:C:2195:TYR:HA	1.97	0.46
1:D:1684:ASN:CB	1:D:1688:LYS:HZ3	2.29	0.46
1:B:790:PRO:O	1:B:792:GLU:OE2	2.33	0.46
1:B:2055:ILE:O	1:B:2059:GLN:HG3	2.16	0.46
1:C:99:MET:HA	1:C:102:LYS:CE	2.45	0.46
1:C:1250:LEU:CG	1:C:1264:MET:CE	2.94	0.46
1:C:1910:PHE:CZ	1:C:1914:MET:HE1	2.51	0.46
1:C:2054:TYR:CE1	1:C:2071:LEU:HD22	2.50	0.46
1:C:2389:LEU:HD21	1:D:2339:LEU:HD13	1.98	0.46
1:D:788:ARG:HH12	1:D:790:PRO:HD3	1.81	0.46
1:D:2513:PHE:CE2	1:D:2517:ILE:HD11	2.51	0.46
1:A:374:LEU:HD21	1:D:5:SER:HB3	1.98	0.45
1:A:2215:ILE:O	1:A:2219:ILE:HG13	2.17	0.45
1:B:788:ARG:HB3	1:B:788:ARG:CZ	2.45	0.45
1:B:791:GLN:HB3	1:B:873:PHE:CE1	2.51	0.45
1:C:2582:ASP:O	1:C:2582:ASP:OD2	2.33	0.45
1:D:238:GLY:N	1:D:285:VAL:O	2.42	0.45
1:D:538:LEU:CD2	1:D:589:ILE:HD11	2.46	0.45
1:D:761:PHE:CE1	1:D:764:MET:HE1	2.51	0.45
1:B:10:ILE:CD1	1:B:111:VAL:HG12	2.44	0.45
1:B:1428:MET:HB2	1:B:1431:ILE:HD12	1.98	0.45
1:C:574:ILE:CG2	1:C:581:MET:HE3	2.46	0.45
1:A:802:LEU:CD2	1:A:804:THR:HG22	2.47	0.45
1:A:1890:ASN:OD1	1:A:1893:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1427:GLU:O	1:B:1428:MET:HE1	2.16	0.45
1:B:1742:THR:HG21	1:B:1781:LYS:HE2	1.99	0.45
1:C:2007:ARG:CG	1:C:2009:ASP:OD1	2.52	0.45
1:D:788:ARG:CB	1:D:788:ARG:HH11	2.28	0.45
1:D:1063:THR:HG21	1:D:1643:PHE:HE1	1.81	0.45
1:D:2209:PHE:HD2	1:D:2351:ARG:NH2	2.13	0.45
1:B:71:TYR:CZ	1:B:75:LYS:HE3	2.52	0.45
1:C:1094:GLN:O	1:C:1096:GLN:NE2	2.50	0.45
1:A:878:PHE:O	1:A:882:LEU:HD12	2.17	0.45
1:A:2375:LEU:HD22	1:B:2355:LEU:HD11	1.99	0.45
1:A:2513:PHE:CE2	1:A:2517:ILE:HD11	2.51	0.45
1:B:927:MET:O	1:B:927:MET:CE	2.65	0.45
1:C:554:ARG:CB	1:C:590:LEU:HD13	2.46	0.45
1:D:802:LEU:HD21	1:D:804:THR:HG22	1.98	0.45
1:D:1604:GLU:CD	1:D:1604:GLU:O	2.55	0.45
1:B:29:LEU:CD2	1:B:37:VAL:CG1	2.95	0.45
1:B:34:ASP:OD1	1:B:34:ASP:N	2.33	0.45
1:B:522:LEU:HD22	1:B:584:GLN:HE22	1.82	0.45
1:B:854:GLU:O	1:B:858:LYS:HG3	2.17	0.45
1:B:1235:PHE:O	1:B:1235:PHE:CD1	2.68	0.45
1:B:2069:HIS:HA	1:B:2072:LYS:NZ	2.32	0.45
1:C:95:HIS:CD2	1:D:1922:LEU:CD2	2.91	0.45
1:C:2184:TRP:HA	1:C:2184:TRP:CE3	2.52	0.45
1:C:2513:PHE:CE2	1:C:2517:ILE:HD11	2.51	0.45
1:D:743:ARG:NH1	1:D:788:ARG:N	2.65	0.45
1:D:1912:ASP:OD2	1:D:1917:SER:HA	2.15	0.45
1:D:2279:GLY:O	1:D:2283:ASN:CG	2.53	0.45
1:A:370:ASP:C	1:A:370:ASP:OD1	2.55	0.45
1:A:666:ILE:N	1:A:732:GLN:HE22	2.14	0.45
1:B:481:PHE:HD2	1:B:486:VAL:O	1.99	0.45
1:B:759:LEU:HD23	1:B:759:LEU:C	2.37	0.45
1:B:861:PHE:CD2	1:B:861:PHE:O	2.69	0.45
1:B:1253:PHE:O	1:B:1260:GLU:OE1	2.35	0.45
1:C:1804:VAL:CG1	1:C:1928:TYR:CE1	2.99	0.45
1:C:1974:ILE:CD1	1:C:2000:LEU:HD11	2.40	0.45
1:D:1176:LEU:HD12	1:D:1224:ILE:HG23	1.97	0.45
1:D:1253:PHE:O	1:D:1260:GLU:OE1	2.35	0.45
1:A:416:MET:HG3	1:A:417:LEU:N	2.32	0.45
1:A:1612:ALA:O	1:A:1616:VAL:HG23	2.17	0.45
1:A:1902:ASN:C	1:A:1902:ASN:OD1	2.54	0.45
1:A:2057:ALA:O	1:A:2061:SER:OG	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1912:ASP:OD1	1:B:1917:SER:HA	2.17	0.45
1:C:370:ASP:OD1	1:C:370:ASP:C	2.55	0.45
1:C:2184:TRP:CZ2	1:C:2307:PHE:CZ	3.05	0.45
1:D:256:GLU:CG	1:D:256:GLU:O	2.64	0.45
1:D:629:ARG:HG3	1:D:629:ARG:HH11	1.81	0.45
1:D:768:MET:CE	1:D:768:MET:CA	2.68	0.45
1:A:261:LEU:HD22	1:A:311:THR:HG21	1.98	0.45
1:A:759:LEU:HD23	1:A:759:LEU:C	2.37	0.45
1:A:1790:HIS:HE1	1:A:1794:LYS:HE2	1.82	0.45
1:B:62:MET:CE	1:B:161:TRP:CH2	2.97	0.45
1:B:733:LEU:HD12	1:B:780:LEU:HD22	1.98	0.45
1:B:987:ILE:HD11	1:B:1091:THR:HB	1.99	0.45
1:B:1063:THR:HG21	1:B:1643:PHE:HE1	1.81	0.45
1:B:1349:MET:HE2	1:B:1404:ASP:O	2.14	0.45
1:B:1612:ALA:O	1:B:1616:VAL:HG23	2.17	0.45
1:C:2215:ILE:O	1:C:2219:ILE:HG13	2.17	0.45
1:D:982:ARG:HD3	1:D:986:ARG:CD	2.44	0.45
1:A:71:TYR:OH	1:A:75:LYS:NZ	2.50	0.45
1:B:291:ASP:HB3	1:B:294:ARG:HB2	1.99	0.45
1:B:990:LEU:CD2	1:B:1035:MET:SD	3.03	0.45
1:B:1059:LEU:HD12	1:B:1074:ALA:O	2.17	0.45
1:B:2133:MET:HG2	1:B:2606:ARG:HH21	1.81	0.45
1:C:95:HIS:O	1:C:99:MET:HG2	2.17	0.45
1:C:308:HIS:O	1:C:312:GLY:N	2.48	0.45
1:C:2184:TRP:HA	1:C:2184:TRP:HE3	1.82	0.45
1:D:519:PHE:HE1	1:D:560:LEU:HD11	1.81	0.45
1:D:878:PHE:O	1:D:882:LEU:HD12	2.17	0.45
1:D:1950:GLY:N	1:D:1951:PRO:HA	2.32	0.45
1:A:1502:LEU:HD13	1:A:1529:LEU:HB3	2.00	0.44
1:A:1882:GLU:HG2	1:A:1946:GLU:OE1	2.17	0.44
1:B:878:PHE:O	1:B:882:LEU:HD12	2.17	0.44
1:B:1960:VAL:HG22	1:B:1967:ILE:HD12	2.00	0.44
1:B:2580:LYS:HA	1:B:2583:TYR:CD2	2.52	0.44
1:C:140:PRO:HG3	1:D:1292:THR:HA	1.99	0.44
1:C:773:LEU:HD11	1:C:777:PHE:HE1	1.81	0.44
1:C:2402:LEU:C	1:C:2402:LEU:HD12	2.37	0.44
1:D:1684:ASN:CB	1:D:1688:LYS:NZ	2.78	0.44
1:D:1685:GLN:HA	1:D:1688:LYS:CD	2.48	0.44
1:B:5:SER:HB3	1:C:374:LEU:HD21	1.99	0.44
1:B:1411:MET:SD	1:B:1411:MET:C	2.96	0.44
1:B:2050:GLY:HA2	1:B:2053:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1950:GLY:N	1:C:1951:PRO:HA	2.32	0.44
1:D:35:ARG:HH11	1:D:35:ARG:HG3	1.81	0.44
1:D:105:ASP:C	1:D:105:ASP:OD1	2.56	0.44
1:D:1197:LEU:HD13	1:D:1231:PHE:HZ	1.82	0.44
1:D:1612:ALA:O	1:D:1616:VAL:HG23	2.17	0.44
1:C:574:ILE:CG2	1:C:581:MET:CE	2.95	0.44
1:C:878:PHE:O	1:C:882:LEU:HD12	2.17	0.44
1:C:1502:LEU:HD13	1:C:1529:LEU:HB3	2.00	0.44
1:C:1804:VAL:HG13	1:C:1928:TYR:CE1	2.53	0.44
1:C:2327:ILE:CG1	1:C:2328:LEU:N	2.80	0.44
1:C:2479:ILE:HD12	1:C:2480:LEU:CA	2.48	0.44
1:D:495:ASP:OD1	1:D:495:ASP:O	2.36	0.44
1:D:1663:ILE:HD13	1:D:1748:LYS:HG2	1.99	0.44
1:D:1890:ASN:OD1	1:D:1893:ARG:NH1	2.49	0.44
1:A:95:HIS:O	1:A:99:MET:HG2	2.17	0.44
1:B:2288:LEU:HA	1:B:2288:LEU:HD23	1.78	0.44
1:C:29:LEU:CD2	1:C:204:ASN:OD1	2.66	0.44
1:C:265:LEU:HD21	1:C:417:LEU:CD1	2.38	0.44
1:C:802:LEU:HD21	1:C:804:THR:HG22	1.98	0.44
1:C:1041:THR:O	1:C:1044:MET:HE1	2.17	0.44
1:C:1960:VAL:HG22	1:C:1967:ILE:HD12	2.00	0.44
1:C:2513:PHE:HE2	1:D:2513:PHE:HE2	1.64	0.44
1:D:990:LEU:HD23	1:D:990:LEU:HA	1.86	0.44
1:D:1182:MET:N	1:D:1182:MET:SD	2.91	0.44
1:D:1448:MET:HE3	1:D:1472:VAL:HG11	1.99	0.44
1:D:1902:ASN:OD1	1:D:1902:ASN:C	2.54	0.44
1:D:2219:ILE:HD12	1:D:2338:GLU:O	2.18	0.44
1:D:2280:PRO:CA	1:D:2283:ASN:OD1	2.64	0.44
1:A:405:ILE:O	1:A:405:ILE:HG22	2.18	0.44
1:A:1960:VAL:HG22	1:A:1967:ILE:HD12	2.00	0.44
1:B:72:TRP:O	1:B:76:GLN:HG2	2.17	0.44
1:B:1182:MET:N	1:B:1182:MET:SD	2.91	0.44
1:B:1684:ASN:O	1:B:1688:LYS:HG2	2.17	0.44
1:C:105:ASP:OD1	1:C:105:ASP:C	2.56	0.44
1:C:405:ILE:HG22	1:C:405:ILE:O	2.18	0.44
1:C:2184:TRP:CZ3	1:C:2187:LYS:HG3	2.44	0.44
1:D:460:ASN:OD1	1:D:460:ASN:C	2.55	0.44
1:D:600:HIS:CE1	1:D:601:ASN:HB2	2.52	0.44
1:D:2153:HIS:O	1:D:2157:THR:OG1	2.35	0.44
1:B:1218:ASP:O	1:B:1219:ALA:HB3	2.18	0.44
1:B:2219:ILE:HD12	1:B:2219:ILE:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1895:GLN:OE1	1:C:1895:GLN:N	2.51	0.44
1:D:1910:PHE:CE2	1:D:1914:MET:CE	3.00	0.44
1:B:1502:LEU:HD13	1:B:1529:LEU:HB3	2.00	0.44
1:B:1950:GLY:N	1:B:1951:PRO:HA	2.32	0.44
1:C:537:ARG:HD3	1:C:540:GLU:CD	2.38	0.44
1:D:1097:LEU:HD12	1:D:1595:LEU:HD22	2.00	0.44
1:D:1902:ASN:ND2	1:D:1905:CYS:CB	2.58	0.44
1:B:1290:LEU:HD23	1:B:1290:LEU:HA	1.85	0.44
1:C:92:LYS:HB3	1:D:1924:LEU:HD21	1.98	0.44
1:C:250:LYS:CE	1:C:415:LEU:HD12	2.48	0.44
1:C:639:VAL:HG21	1:C:738:ARG:HD3	2.00	0.44
1:D:773:LEU:HD11	1:D:777:PHE:HE1	1.81	0.44
1:D:1400:VAL:HG11	1:D:1440:LEU:CD2	2.48	0.44
1:D:1684:ASN:C	1:D:1688:LYS:HZ3	2.19	0.44
1:D:1685:GLN:HA	1:D:1688:LYS:CG	2.48	0.44
1:A:666:ILE:H	1:A:732:GLN:HE22	1.65	0.44
1:A:987:ILE:HD11	1:A:1091:THR:HB	1.99	0.44
1:B:1229:HIS:ND1	1:B:1263:THR:HG21	2.33	0.44
1:B:2513:PHE:CZ	1:B:2517:ILE:HD11	2.53	0.44
1:C:740:CYS:SG	1:C:751:ILE:HD13	2.58	0.44
1:C:1338:ASP:OD1	1:C:1339:LYS:N	2.47	0.44
1:C:2513:PHE:CZ	1:C:2517:ILE:HD11	2.53	0.44
1:D:405:ILE:O	1:D:405:ILE:HG22	2.18	0.44
1:D:629:ARG:O	1:D:633:TYR:CD1	2.70	0.44
1:D:759:LEU:HD23	1:D:759:LEU:C	2.37	0.44
1:A:1218:ASP:O	1:A:1219:ALA:HB3	2.18	0.43
1:B:713:GLN:OE1	1:B:713:GLN:HA	2.18	0.43
1:B:1542:MET:C	1:B:1542:MET:SD	2.96	0.43
1:C:98:GLN:O	1:C:102:LYS:HG3	2.17	0.43
1:C:396:THR:OG1	1:C:419:THR:HB	2.18	0.43
1:D:987:ILE:HD11	1:D:1091:THR:HB	1.99	0.43
1:D:1502:LEU:HD13	1:D:1529:LEU:HB3	2.00	0.43
1:A:2513:PHE:CZ	1:A:2517:ILE:HD11	2.53	0.43
1:B:105:ASP:C	1:B:105:ASP:OD1	2.56	0.43
1:B:1116:ARG:C	1:B:1120:MET:HE2	2.39	0.43
1:C:869:ASN:O	1:C:873:PHE:CD2	2.71	0.43
1:C:1229:HIS:ND1	1:C:1263:THR:HG21	2.33	0.43
1:C:1400:VAL:HG11	1:C:1440:LEU:CD2	2.48	0.43
1:D:854:GLU:O	1:D:858:LYS:HG3	2.17	0.43
1:A:1960:VAL:HG22	1:A:1967:ILE:CD1	2.49	0.43
1:B:1063:THR:O	1:B:1071:VAL:CG2	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:LYS:N	1:C:376:LYS:CD	2.68	0.43
1:C:564:GLN:C	1:C:564:GLN:OE1	2.57	0.43
1:C:1214:TYR:HB2	1:C:1221:MET:CE	2.48	0.43
1:C:1218:ASP:O	1:C:1219:ALA:HB3	2.18	0.43
1:C:1612:ALA:O	1:C:1616:VAL:HG23	2.17	0.43
1:C:1960:VAL:HG22	1:C:1967:ILE:CD1	2.49	0.43
1:C:2281:THR:CA	1:C:2284:ILE:HG22	2.48	0.43
1:D:241:VAL:HG12	1:D:433:SER:HA	2.00	0.43
1:D:761:PHE:CD1	1:D:764:MET:HE1	2.50	0.43
1:D:1218:ASP:O	1:D:1219:ALA:HB3	2.18	0.43
1:D:2396:ILE:C	1:D:2397:LEU:HD12	2.39	0.43
1:B:648:THR:HA	1:B:651:LEU:HD12	1.99	0.43
1:B:2201:MET:CG	1:B:2299:SER:HB2	2.48	0.43
1:C:987:ILE:HD11	1:C:1091:THR:HB	1.99	0.43
1:C:1610:VAL:O	1:C:1614:LEU:HD23	2.19	0.43
1:D:370:ASP:C	1:D:370:ASP:OD1	2.57	0.43
1:D:743:ARG:NH1	1:D:788:ARG:O	2.51	0.43
1:D:1542:MET:CG	1:D:1543:ASP:N	2.80	0.43
1:D:1971:THR:CG2	1:D:2020:LEU:HD13	2.48	0.43
1:A:1400:VAL:HG11	1:A:1440:LEU:CD2	2.48	0.43
1:A:1950:GLY:N	1:A:1951:PRO:HA	2.32	0.43
1:A:2375:LEU:HD21	1:B:2359:ILE:HD11	2.00	0.43
1:B:405:ILE:O	1:B:405:ILE:HG22	2.18	0.43
1:B:1400:VAL:HG11	1:B:1440:LEU:CD2	2.48	0.43
1:B:1875:ARG:CZ	1:B:1879:LEU:HD11	2.49	0.43
1:B:1881:CYS:SG	1:B:1892:LEU:HD12	2.58	0.43
1:B:2057:ALA:O	1:B:2061:SER:OG	2.27	0.43
1:B:2215:ILE:HG23	1:B:2219:ILE:HD11	2.00	0.43
1:C:375:GLN:C	1:C:376:LYS:HD3	2.37	0.43
1:D:743:ARG:HH11	1:D:788:ARG:N	2.16	0.43
1:D:2513:PHE:CZ	1:D:2517:ILE:HD11	2.53	0.43
1:A:146:ASN:N	1:A:146:ASN:OD1	2.50	0.43
1:A:1229:HIS:ND1	1:A:1263:THR:HG21	2.33	0.43
1:B:71:TYR:CD2	1:B:93:LEU:HB3	2.54	0.43
1:C:2479:ILE:CD1	1:C:2479:ILE:C	2.82	0.43
1:D:9:HIS:HB2	1:D:12:ASP:OD2	2.18	0.43
1:D:311:THR:HG22	1:D:313:ASN:OD1	2.18	0.43
1:D:458:LYS:HB2	1:D:464:ILE:CD1	2.44	0.43
1:D:481:PHE:CE1	1:D:488:ASN:CA	2.96	0.43
1:D:664:ILE:HG13	1:D:665:LEU:HD12	2.00	0.43
1:D:1531:MET:O	1:D:1531:MET:SD	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1623:TRP:HB3	1:D:1626:LEU:CG	2.48	0.43
1:A:1188:GLN:HB2	1:A:1189:MET:CE	2.48	0.43
1:B:241:VAL:HG12	1:B:433:SER:HA	1.99	0.43
1:B:982:ARG:HD3	1:B:986:ARG:NH1	2.33	0.43
1:B:2397:LEU:HD21	1:B:2464:THR:HG23	1.99	0.43
1:C:29:LEU:CD1	1:C:204:ASN:OD1	2.66	0.43
1:D:1236:CYS:SG	1:D:1246:LEU:HD12	2.59	0.43
1:D:1626:LEU:HD12	1:D:1695:LEU:HD22	2.00	0.43
1:A:231:LEU:HD23	1:A:231:LEU:H	1.84	0.43
1:A:2208:SER:N	1:A:2292:ASN:OD1	2.52	0.43
1:B:29:LEU:CD2	1:B:37:VAL:HG11	2.48	0.43
1:B:288:VAL:HG23	1:B:303:LEU:C	2.39	0.43
1:B:773:LEU:O	1:B:777:PHE:HD1	2.02	0.43
1:B:1206:MET:HA	1:B:1206:MET:CE	2.49	0.43
1:C:64:ARG:HG3	1:C:104:ASN:OD1	2.18	0.43
1:C:146:ASN:OD1	1:C:146:ASN:N	2.50	0.43
1:C:871:ILE:HG12	1:C:876:TYR:CD1	2.54	0.43
1:C:1320:MET:CE	1:C:1320:MET:CA	2.97	0.43
1:A:773:LEU:CG	1:A:777:PHE:HE1	2.30	0.43
1:A:2314:MET:HE1	1:A:2315:VAL:HG23	2.01	0.43
1:B:311:THR:HG22	1:B:313:ASN:OD1	2.19	0.43
1:B:564:GLN:OE1	1:B:565:GLU:N	2.52	0.43
1:B:1616:VAL:HG11	1:B:1690:LEU:HB3	2.01	0.43
1:B:1660:LYS:N	1:B:1660:LYS:HD2	2.33	0.43
1:C:231:LEU:HG	1:C:234:VAL:HG23	2.01	0.43
1:C:2348:LEU:HD23	1:C:2348:LEU:C	2.40	0.43
1:D:241:VAL:CG2	1:D:285:VAL:CG2	2.97	0.43
1:D:493:VAL:HG11	1:D:555:LEU:HD21	2.01	0.43
1:D:498:VAL:CG2	1:D:565:GLU:OE1	2.67	0.43
1:A:664:ILE:HG13	1:A:665:LEU:HD12	2.01	0.43
1:B:370:ASP:C	1:B:370:ASP:OD1	2.57	0.43
1:B:2511:LEU:HD21	1:C:2362:VAL:HG23	2.01	0.43
1:C:941:LEU:HD13	1:C:1096:GLN:OE1	2.18	0.43
1:C:1214:TYR:CB	1:C:1221:MET:HE1	2.48	0.43
1:C:1236:CYS:SG	1:C:1246:LEU:HD12	2.59	0.43
1:C:1910:PHE:CE1	1:C:1914:MET:HE2	2.54	0.43
1:D:773:LEU:O	1:D:777:PHE:HD1	2.02	0.43
1:D:1229:HIS:ND1	1:D:1263:THR:HG21	2.33	0.43
1:D:1448:MET:CE	1:D:1468:VAL:HG23	2.49	0.43
1:D:2604:ARG:HG2	1:D:2604:ARG:HH11	1.83	0.43
1:B:1890:ASN:OD1	1:B:1893:ARG:NH1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD23	1:C:651:LEU:N	2.34	0.42
1:C:1793:MET:HG2	1:C:1870:MET:SD	2.59	0.42
1:D:2392:LYS:HE2	1:D:2456:ASP:CA	2.46	0.42
1:A:869:ASN:O	1:A:873:PHE:CD2	2.71	0.42
1:A:1061:HIS:CE1	1:A:1065:HIS:NE2	2.87	0.42
1:A:1338:ASP:OD1	1:A:1339:LYS:N	2.47	0.42
1:B:1077:LEU:HA	1:B:1077:LEU:HD23	1.80	0.42
1:B:1685:GLN:O	1:B:1688:LYS:CG	2.67	0.42
1:B:2213:VAL:HG12	1:B:2217:ILE:HD11	2.02	0.42
1:C:2154:ARG:HH11	1:C:2154:ARG:CG	2.31	0.42
1:C:2375:LEU:HD21	1:D:2359:ILE:HD11	2.01	0.42
1:D:31:LEU:N	1:D:447:ASP:OD2	2.43	0.42
1:A:493:VAL:HG11	1:A:555:LEU:HD21	2.01	0.42
1:B:1787:LYS:HG3	1:B:1901:TYR:OH	2.18	0.42
1:D:729:TYR:CZ	1:D:733:LEU:HD21	2.54	0.42
1:A:5:SER:HB2	1:B:374:LEU:CD2	2.49	0.42
1:A:656:VAL:CG2	1:A:739:MET:CE	2.97	0.42
1:A:812:ILE:HD11	1:A:813:LYS:HE3	2.01	0.42
1:B:1427:GLU:O	1:B:1428:MET:CE	2.66	0.42
1:B:2479:ILE:HG13	1:B:2480:LEU:HD23	2.02	0.42
1:B:2580:LYS:HA	1:B:2583:TYR:CE2	2.54	0.42
1:C:1094:GLN:O	1:C:1096:GLN:OE1	2.37	0.42
1:D:1875:ARG:CZ	1:D:1879:LEU:HD11	2.49	0.42
1:A:1616:VAL:HG11	1:A:1690:LEU:HB3	2.01	0.42
1:A:2355:LEU:HD11	1:D:2375:LEU:HD22	2.02	0.42
1:B:802:LEU:HD23	1:B:803:TRP:N	2.34	0.42
1:B:1960:VAL:HG22	1:B:1967:ILE:CD1	2.48	0.42
1:B:2279:GLY:O	1:B:2283:ASN:CG	2.54	0.42
1:C:294:ARG:HG3	1:C:294:ARG:NH1	2.35	0.42
1:C:493:VAL:HG11	1:C:555:LEU:HD21	2.01	0.42
1:C:773:LEU:O	1:C:777:PHE:HD1	2.02	0.42
1:C:1366:ILE:O	1:C:1370:ASP:CG	2.58	0.42
1:C:2208:SER:N	1:C:2292:ASN:OD1	2.52	0.42
1:D:9:HIS:O	1:D:12:ASP:OD2	2.37	0.42
1:D:231:LEU:H	1:D:231:LEU:HD23	1.84	0.42
1:D:354:LEU:HD12	1:D:417:LEU:HB2	2.01	0.42
1:D:538:LEU:HD23	1:D:541:LEU:HD12	2.01	0.42
1:B:96:ALA:HA	1:B:99:MET:HE2	2.00	0.42
1:B:110:LYS:HD3	1:B:110:LYS:C	2.40	0.42
1:B:155:THR:HG23	1:B:156:GLY:N	2.35	0.42
1:B:263:VAL:HG12	1:B:355:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:VAL:HG23	1:B:303:LEU:O	2.20	0.42
1:B:861:PHE:O	1:B:861:PHE:HD2	2.03	0.42
1:B:1790:HIS:ND1	1:B:1901:TYR:HD2	2.17	0.42
1:B:1863:MET:CE	1:B:1867:VAL:HB	2.50	0.42
1:C:233:GLU:OE1	1:C:233:GLU:CA	2.67	0.42
1:C:294:ARG:HG3	1:C:294:ARG:HH11	1.84	0.42
1:C:812:ILE:HG12	1:C:813:LYS:NZ	2.35	0.42
1:D:155:THR:HG23	1:D:156:GLY:N	2.35	0.42
1:D:2381:TYR:CZ	1:D:2385:ILE:HD11	2.54	0.42
1:B:95:HIS:NE2	1:B:99:MET:SD	2.93	0.42
1:B:729:TYR:CZ	1:B:733:LEU:HD21	2.54	0.42
1:B:2117:TYR:O	1:B:2121:THR:CG2	2.60	0.42
1:C:738:ARG:HH21	1:C:926:THR:CG2	2.21	0.42
1:C:1428:MET:HB2	1:C:1431:ILE:HD12	2.01	0.42
1:C:1742:THR:HG21	1:C:1781:LYS:CE	2.48	0.42
1:D:263:VAL:HG12	1:D:355:VAL:HA	2.02	0.42
1:D:1077:LEU:HD23	1:D:1077:LEU:HA	1.82	0.42
1:D:1777:MET:HG2	1:D:1891:PHE:CZ	2.54	0.42
1:D:1788:VAL:CG2	1:D:1789:LEU:N	2.82	0.42
1:A:1059:LEU:HD21	1:A:1077:LEU:CB	2.50	0.42
1:B:1035:MET:H	1:B:1035:MET:HG2	1.68	0.42
1:B:2280:PRO:CA	1:B:2283:ASN:OD1	2.68	0.42
1:C:893:ASP:OD2	1:C:1054:MET:HE1	2.19	0.42
1:C:1718:TRP:HZ3	1:C:1762:ASP:OD2	2.03	0.42
1:C:1863:MET:HE2	1:C:1867:VAL:HG21	2.01	0.42
1:C:1974:ILE:HD11	1:C:2000:LEU:HD12	1.89	0.42
1:C:2381:TYR:CE2	1:D:2342:SER:HB2	2.54	0.42
1:D:500:LYS:O	1:D:500:LYS:CG	2.68	0.42
1:D:2571:PHE:CE1	1:D:2590:VAL:HG21	2.53	0.42
1:A:2214:PHE:CD1	1:A:2269:ILE:CD1	3.03	0.42
1:C:2518:ASP:OD1	1:D:2524:ARG:NE	2.53	0.42
1:D:272:SER:HB2	1:D:275:SER:OG	2.19	0.42
1:D:2563:HIS:O	4:D:3003:ATP:N6	2.53	0.42
1:A:2518:ASP:OD1	1:B:2524:ARG:NE	2.53	0.42
1:B:860:THR:O	1:B:864:VAL:HG23	2.20	0.42
1:B:2261:ILE:O	1:B:2261:ILE:HG22	2.20	0.42
1:C:155:THR:HG23	1:C:156:GLY:N	2.35	0.42
1:C:231:LEU:HD23	1:C:231:LEU:H	1.84	0.42
1:C:311:THR:HG22	1:C:313:ASN:OD1	2.19	0.42
1:C:1411:MET:C	1:C:1411:MET:SD	2.98	0.42
1:C:2349:ILE:HG12	1:C:2359:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LYS:HG3	1:D:138:ARG:HD2	2.01	0.42
1:D:354:LEU:HD12	1:D:417:LEU:CB	2.49	0.42
1:D:1089:MET:CE	1:D:1603:GLU:HA	2.50	0.42
1:D:1206:MET:HA	1:D:1206:MET:CE	2.49	0.42
1:D:1616:VAL:HG11	1:D:1690:LEU:HB3	2.01	0.42
1:D:1790:HIS:C	1:D:1790:HIS:ND1	2.74	0.42
1:D:2020:LEU:HD12	1:D:2020:LEU:HA	1.85	0.42
1:A:203:ASP:OD1	1:A:204:ASN:N	2.53	0.41
1:A:645:ILE:HB	1:A:648:THR:HG22	2.02	0.41
1:A:719:ASN:OD1	1:A:721:HIS:N	2.53	0.41
1:A:1033:GLU:OE2	1:A:1682:ARG:NH2	2.52	0.41
1:A:1236:CYS:SG	1:A:1246:LEU:HD12	2.60	0.41
1:B:2375:LEU:HD22	1:C:2355:LEU:HD11	2.01	0.41
1:B:2563:HIS:O	4:B:3003:ATP:N6	2.53	0.41
1:C:5:SER:HB2	1:D:374:LEU:CD2	2.50	0.41
1:C:109:LYS:NZ	1:C:109:LYS:HB2	2.35	0.41
1:C:234:VAL:CG1	1:C:380:PHE:HB3	2.50	0.41
1:C:554:ARG:HD3	1:C:590:LEU:HD11	2.02	0.41
1:C:664:ILE:HG13	1:C:665:LEU:HD12	2.01	0.41
1:C:2388:PHE:CE2	1:D:2223:TYR:CE1	2.88	0.41
1:D:860:THR:O	1:D:864:VAL:HG23	2.20	0.41
1:A:140:PRO:CD	1:B:1292:THR:HG22	2.41	0.41
1:A:719:ASN:OD1	1:A:720:ALA:N	2.53	0.41
1:A:2389:LEU:HD21	1:B:2339:LEU:HD13	2.00	0.41
1:B:99:MET:CE	1:C:1922:LEU:HD12	0.94	0.41
1:B:364:ALA:O	1:B:391:HIS:NE2	2.54	0.41
1:B:1250:LEU:HD21	1:B:1264:MET:HE1	2.01	0.41
1:B:1793:MET:HG2	1:B:1870:MET:SD	2.60	0.41
1:C:173:ASN:OD1	1:C:174:GLY:N	2.54	0.41
1:D:788:ARG:NH1	1:D:790:PRO:CD	2.83	0.41
1:D:802:LEU:HD13	1:D:805:GLU:HG2	2.01	0.41
1:D:2347:ASP:O	1:D:2347:ASP:OD1	2.38	0.41
1:A:2563:HIS:O	4:A:3003:ATP:N6	2.53	0.41
1:B:493:VAL:HG11	1:B:555:LEU:HD21	2.01	0.41
1:C:203:ASP:OD1	1:C:204:ASN:N	2.53	0.41
1:C:364:ALA:O	1:C:391:HIS:NE2	2.54	0.41
1:D:749:ASP:O	1:D:753:GLN:HG3	2.21	0.41
1:D:773:LEU:CD1	1:D:777:PHE:HE1	2.33	0.41
1:D:1290:LEU:HD23	1:D:1290:LEU:HA	1.85	0.41
1:D:1349:MET:SD	1:D:1406:ILE:HG23	2.60	0.41
1:A:1349:MET:SD	1:A:1406:ILE:HG23	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:HD23	1:B:231:LEU:H	1.84	0.41
1:B:538:LEU:HB3	1:B:587:TYR:CZ	2.56	0.41
1:B:664:ILE:HG13	1:B:665:LEU:HD12	2.01	0.41
1:B:1080:LYS:HZ3	1:B:1087:GLU:CD	2.24	0.41
1:B:1250:LEU:CD2	1:B:1264:MET:HE1	2.50	0.41
1:B:1734:THR:HG23	1:B:1772:PHE:CD1	2.55	0.41
1:C:773:LEU:CD1	1:C:777:PHE:HE1	2.33	0.41
1:C:1099:ILE:HG22	1:C:1099:ILE:O	2.21	0.41
1:D:2261:ILE:O	1:D:2261:ILE:HG22	2.20	0.41
1:A:1099:ILE:HG22	1:A:1099:ILE:O	2.21	0.41
1:A:2261:ILE:O	1:A:2261:ILE:HG22	2.20	0.41
1:B:203:ASP:OD1	1:B:204:ASN:N	2.53	0.41
1:B:1321:ILE:O	1:B:1325:LEU:HB2	2.20	0.41
1:B:1621:LEU:HD12	1:B:1643:PHE:HE2	1.85	0.41
1:B:1761:LEU:HD23	1:B:1768:ILE:CG2	2.50	0.41
1:B:1974:ILE:HD11	1:B:1997:SER:HA	2.01	0.41
1:B:2347:ASP:O	1:B:2347:ASP:OD1	2.38	0.41
1:C:747:ALA:O	1:C:751:ILE:HG13	2.20	0.41
1:C:1366:ILE:HG13	1:C:1366:ILE:H	1.64	0.41
1:C:1616:VAL:HG11	1:C:1690:LEU:HB3	2.01	0.41
1:D:1080:LYS:HZ3	1:D:1087:GLU:CD	2.23	0.41
1:D:2189:ARG:HG2	1:D:2189:ARG:NH1	2.35	0.41
1:A:92:LYS:CB	1:B:1924:LEU:HD21	2.50	0.41
1:A:1527:ARG:O	1:A:1531:MET:HG2	2.20	0.41
1:A:1650:HIS:CD2	1:A:1654:LEU:HD23	2.56	0.41
1:C:368:GLU:CD	1:C:369:LEU:H	2.23	0.41
1:C:813:LYS:HA	1:C:813:LYS:HD3	1.95	0.41
1:D:1349:MET:SD	1:D:1349:MET:C	2.99	0.41
1:D:1650:HIS:CD2	1:D:1654:LEU:HD23	2.56	0.41
1:A:719:ASN:OD1	1:A:719:ASN:C	2.59	0.41
1:A:2007:ARG:NH1	1:A:2012:ASN:OD1	2.54	0.41
1:A:2311:TYR:O	1:A:2314:MET:HE3	2.21	0.41
1:A:2362:VAL:HG23	1:D:2511:LEU:HD21	2.01	0.41
1:B:557:TYR:CD2	1:B:589:ILE:HG22	2.56	0.41
1:C:1762:ASP:OD2	1:C:1763:GLY:N	2.53	0.41
1:D:982:ARG:C	1:D:982:ARG:HD2	2.41	0.41
1:D:1059:LEU:HD21	1:D:1077:LEU:CB	2.51	0.41
1:D:1623:TRP:HB3	1:D:1626:LEU:HD11	2.00	0.41
1:D:1773:HIS:CE1	1:D:1777:MET:SD	3.13	0.41
1:D:1792:ARG:HE	1:D:1792:ARG:HB2	1.70	0.41
1:D:2550:ASN:OD1	1:D:2550:ASN:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:LEU:HD12	1:A:888:LEU:HG	2.02	0.41
1:A:1915:CYS:HB3	1:A:1925:LEU:HD13	2.02	0.41
1:B:557:TYR:HD2	1:B:589:ILE:HG22	1.85	0.41
1:B:727:SER:HA	1:B:730:ARG:NH2	2.36	0.41
1:B:1099:ILE:O	1:B:1099:ILE:HG22	2.21	0.41
1:C:95:HIS:HD2	1:D:1922:LEU:HD21	1.73	0.41
1:D:71:TYR:OH	1:D:75:LYS:NZ	2.50	0.41
1:D:203:ASP:OD1	1:D:204:ASN:N	2.53	0.41
1:D:645:ILE:HB	1:D:648:THR:HG22	2.02	0.41
1:D:757:VAL:HG12	1:D:785:HIS:CD2	2.56	0.41
1:A:173:ASN:OD1	1:A:174:GLY:N	2.54	0.41
1:A:1790:HIS:NE2	1:A:1906:GLU:OE2	2.53	0.41
1:A:1797:GLN:NE2	1:A:1906:GLU:OE1	2.54	0.41
1:A:2214:PHE:HD1	1:A:2269:ILE:CD1	2.34	0.41
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.84	0.41
1:B:1032:ALA:O	1:B:1035:MET:HG2	2.20	0.41
1:B:1097:LEU:HD12	1:B:1595:LEU:HD22	1.99	0.41
1:B:1650:HIS:CD2	1:B:1654:LEU:HD23	2.56	0.41
1:B:1684:ASN:O	1:B:1688:LYS:HE3	2.20	0.41
1:B:1902:ASN:ND2	1:B:1905:CYS:HG	2.08	0.41
1:B:1915:CYS:HB3	1:B:1925:LEU:HD13	2.02	0.41
1:B:2025:LEU:CD1	1:B:2053:ILE:CD1	2.51	0.41
1:C:1056:LEU:HD11	1:C:1082:PHE:CZ	2.55	0.41
1:C:1863:MET:HE3	1:C:1863:MET:CA	2.39	0.41
1:C:1937:VAL:HG13	1:C:1938:ILE:N	2.36	0.41
1:C:2563:HIS:O	4:C:3003:ATP:N6	2.53	0.41
1:D:28:THR:CG2	1:D:152:LEU:CD1	2.87	0.41
1:D:1321:ILE:HG22	1:D:1325:LEU:HD12	2.03	0.41
1:D:1761:LEU:HD23	1:D:1761:LEU:HA	1.97	0.41
1:D:1915:CYS:HB3	1:D:1925:LEU:HD13	2.02	0.41
1:A:364:ALA:O	1:A:391:HIS:NE2	2.54	0.41
1:A:1349:MET:SD	1:A:1349:MET:C	2.99	0.41
1:B:19:GLU:OE1	1:B:19:GLU:HA	2.21	0.41
1:B:645:ILE:HB	1:B:648:THR:CG2	2.51	0.41
1:B:1349:MET:HE1	1:B:1404:ASP:C	2.41	0.41
1:B:2522:ASP:OD1	1:B:2522:ASP:O	2.39	0.41
1:C:261:LEU:HD22	1:C:311:THR:HG21	2.03	0.41
1:C:537:ARG:HH11	1:C:537:ARG:HG2	1.85	0.41
1:C:1059:LEU:HD21	1:C:1077:LEU:HB3	2.02	0.41
1:C:2184:TRP:NE1	1:C:2307:PHE:CE1	2.89	0.41
1:D:265:LEU:CD1	1:D:417:LEU:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LEU:HD11	1:D:398:ILE:HD12	2.03	0.41
1:D:2483:PRO:HG3	1:D:2493:ARG:NH1	2.36	0.41
1:A:2533:ILE:O	1:A:2537:THR:OG1	2.35	0.40
1:B:1185:VAL:O	1:B:1189:MET:HB2	2.21	0.40
1:B:2485:LYS:HG2	1:C:2452:GLU:CD	2.41	0.40
1:C:1596:GLN:NE2	1:C:1600:THR:OG1	2.54	0.40
1:C:1790:HIS:NE2	1:C:1906:GLU:OE2	2.53	0.40
1:C:2261:ILE:O	1:C:2261:ILE:HG22	2.20	0.40
1:D:35:ARG:HG3	1:D:35:ARG:NH1	2.36	0.40
1:D:63:ASN:O	1:D:161:TRP:HZ2	2.04	0.40
1:D:308:HIS:O	1:D:312:GLY:N	2.48	0.40
1:D:785:HIS:O	1:D:788:ARG:HG3	2.20	0.40
1:D:990:LEU:HD21	1:D:1032:ALA:CB	2.50	0.40
1:D:1772:PHE:CD1	1:D:1776:MET:CE	2.87	0.40
1:D:1785:PHE:CE1	1:D:1789:LEU:HD11	2.56	0.40
1:D:1788:VAL:HG23	1:D:1789:LEU:N	2.36	0.40
1:D:1797:GLN:NE2	1:D:1906:GLU:OE1	2.54	0.40
1:D:1882:GLU:HA	1:D:1946:GLU:OE2	2.22	0.40
1:B:1093:LYS:HD3	1:B:1093:LYS:C	2.37	0.40
1:B:1116:ARG:HB3	1:B:1120:MET:HE1	2.01	0.40
1:B:2054:TYR:HE2	1:B:2121:THR:HG21	1.87	0.40
1:B:2189:ARG:CD	1:B:2195:TYR:CZ	3.03	0.40
1:D:1652:LYS:NZ	1:D:1739:ASP:HB3	2.35	0.40
1:D:2522:ASP:OD1	1:D:2522:ASP:O	2.39	0.40
1:A:1065:HIS:HD1	1:A:1070:LEU:HD23	1.86	0.40
1:B:383:ARG:NH1	1:B:384:ASN:OD1	2.55	0.40
1:B:1892:LEU:HD23	1:B:1892:LEU:HA	1.84	0.40
1:D:366:LEU:HD13	1:D:392:LEU:HD23	2.04	0.40
1:D:648:THR:HA	1:D:651:LEU:HD12	2.03	0.40
1:D:1319:ASP:HB2	1:D:1320:MET:CE	2.51	0.40
1:D:1924:LEU:HB3	1:D:1927:LEU:HD13	2.03	0.40
1:A:366:LEU:HD13	1:A:392:LEU:HD23	2.04	0.40
1:A:802:LEU:HD22	1:A:805:GLU:HG2	2.04	0.40
1:B:749:ASP:O	1:B:753:GLN:HG3	2.20	0.40
1:B:1792:ARG:HD2	1:B:1869:ILE:HG21	2.03	0.40
1:B:2029:ILE:HG12	1:B:2053:ILE:HG23	2.02	0.40
1:C:366:LEU:HD13	1:C:392:LEU:HD23	2.04	0.40
1:C:383:ARG:NH1	1:C:384:ASN:OD1	2.55	0.40
1:C:888:LEU:HA	1:C:891:ILE:CD1	2.36	0.40
1:C:1206:MET:HA	1:C:1206:MET:CE	2.49	0.40
1:D:364:ALA:O	1:D:391:HIS:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ARG:NH1	1:D:384:ASN:OD1	2.55	0.40
1:D:619:VAL:O	1:D:622:VAL:HG12	2.21	0.40
1:D:822:SER:HA	1:D:825:ASP:OD2	2.22	0.40
1:D:1253:PHE:HB2	1:D:1264:MET:CE	2.50	0.40
1:D:2054:TYR:HE2	1:D:2121:THR:HG21	1.87	0.40
1:D:2560:LYS:HB2	1:D:2560:LYS:HE2	1.90	0.40
1:A:308:HIS:O	1:A:312:GLY:N	2.48	0.40
1:A:1428:MET:HB2	1:A:1431:ILE:HD12	2.04	0.40
1:B:366:LEU:HD13	1:B:392:LEU:HD23	2.04	0.40
1:B:802:LEU:HD22	1:B:804:THR:HG22	2.04	0.40
1:B:1761:LEU:HD23	1:B:1761:LEU:HA	1.96	0.40
1:C:376:LYS:O	1:C:379:SER:HB2	2.21	0.40
1:C:719:ASN:ND2	1:C:722:ASP:OD1	2.55	0.40
1:C:1182:MET:SD	1:C:1182:MET:C	3.00	0.40
1:C:1250:LEU:CD1	1:C:1264:MET:HE1	2.47	0.40
1:D:761:PHE:CE1	1:D:764:MET:CE	3.05	0.40
1:D:963:VAL:O	1:D:967:THR:HG22	2.22	0.40
1:D:1623:TRP:HB2	1:D:1626:LEU:HD12	2.02	0.40
1:D:1916:GLY:HA3	1:D:1928:TYR:CD1	2.57	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	2238/2671 (84%)	2209 (99%)	29 (1%)	0	100	100
1	B	2238/2671 (84%)	2210 (99%)	28 (1%)	0	100	100
1	C	2238/2671 (84%)	2210 (99%)	28 (1%)	0	100	100
1	D	2238/2671 (84%)	2209 (99%)	29 (1%)	0	100	100
All	All	8952/10684 (84%)	8838 (99%)	114 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	2021/2385 (85%)	1990 (98%)	31 (2%)	60	77
1	B	2021/2385 (85%)	1969 (97%)	52 (3%)	41	66
1	C	2021/2385 (85%)	1990 (98%)	31 (2%)	60	77
1	D	2021/2385 (85%)	1970 (98%)	51 (2%)	42	67
All	All	8084/9540 (85%)	7919 (98%)	165 (2%)	50	72

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LYS
1	A	172	SER
1	A	186	ASN
1	A	255	ASP
1	A	301	ASN
1	A	567	TYR
1	A	707	SER
1	A	816	ASP
1	A	869	ASN
1	A	882	LEU
1	A	988	SER
1	A	1064	MET
1	A	1067	TYR
1	A	1083	SER
1	A	1086	GLN
1	A	1182	MET
1	A	1235	PHE
1	A	1622	HIS
1	A	1673	LEU
1	A	1743	SER
1	A	1759	HIS
1	A	1771	SER

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Mol	Chain	Res	Type
1	A	1891	PHE
1	A	2162	ASP
1	A	2190	SER
1	A	2206	SER
1	A	2361	SER
1	A	2461	CYS
1	A	2488	SER
1	A	2604	ARG
1	A	2608	MET
1	B	19	GLU
1	B	46	ASP
1	B	94	GLN
1	B	146	ASN
1	B	172	SER
1	B	186	ASN
1	B	239	ASP
1	B	255	ASP
1	B	301	ASN
1	B	402	ASN
1	B	450	SER
1	B	564	GLN
1	B	567	TYR
1	B	600	HIS
1	B	601	ASN
1	B	707	SER
1	B	764	MET
1	B	782	LEU
1	B	816	ASP
1	B	861	PHE
1	B	869	ASN
1	B	872	TYR
1	B	882	LEU
1	B	927	MET
1	B	988	SER
1	B	1064	MET
1	B	1067	TYR
1	B	1083	SER
1	B	1235	PHE
1	B	1264	MET
1	B	1290	LEU
1	B	1325	LEU
1	B	1673	LEU

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Mol	Chain	Res	Type
1	B	1743	SER
1	B	1759	HIS
1	B	1771	SER
1	B	1772	PHE
1	B	1891	PHE
1	B	1946	GLU
1	B	2019	SER
1	B	2129	GLN
1	B	2162	ASP
1	B	2184	TRP
1	B	2190	SER
1	B	2206	SER
1	B	2226	MET
1	B	2316	MET
1	B	2347	ASP
1	B	2352	GLU
1	B	2361	SER
1	B	2461	CYS
1	B	2488	SER
1	C	169	LYS
1	C	172	SER
1	C	186	ASN
1	C	257	TYR
1	C	289	HIS
1	C	301	ASN
1	C	567	TYR
1	C	707	SER
1	C	816	ASP
1	C	882	LEU
1	C	988	SER
1	C	1044	MET
1	C	1064	MET
1	C	1067	TYR
1	C	1083	SER
1	C	1235	PHE
1	C	1622	HIS
1	C	1743	SER
1	C	1759	HIS
1	C	1771	SER
1	C	1891	PHE
1	C	1958	CYS
1	C	2160	GLU

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Mol	Chain	Res	Type
1	C	2162	ASP
1	C	2190	SER
1	C	2206	SER
1	C	2361	SER
1	C	2461	CYS
1	C	2488	SER
1	C	2604	ARG
1	C	2608	MET
1	D	146	ASN
1	D	169	LYS
1	D	172	SER
1	D	186	ASN
1	D	239	ASP
1	D	255	ASP
1	D	301	ASN
1	D	402	ASN
1	D	450	SER
1	D	497	MET
1	D	564	GLN
1	D	567	TYR
1	D	601	ASN
1	D	642	HIS
1	D	707	SER
1	D	764	MET
1	D	816	ASP
1	D	869	ASN
1	D	872	TYR
1	D	882	LEU
1	D	927	MET
1	D	988	SER
1	D	1064	MET
1	D	1067	TYR
1	D	1082	PHE
1	D	1083	SER
1	D	1089	MET
1	D	1234	LYS
1	D	1235	PHE
1	D	1290	LEU
1	D	1542	MET
1	D	1688	LYS
1	D	1743	SER
1	D	1771	SER

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Mol	Chain	Res	Type
1	D	1772	PHE
1	D	1891	PHE
1	D	2019	SER
1	D	2162	ASP
1	D	2184	TRP
1	D	2190	SER
1	D	2201	MET
1	D	2206	SER
1	D	2226	MET
1	D	2288	LEU
1	D	2292	ASN
1	D	2337	HIS
1	D	2347	ASP
1	D	2361	SER
1	D	2390	PHE
1	D	2461	CYS
1	D	2488	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	HIS
1	A	732	GLN
1	A	1061	HIS
1	A	1090	HIS
1	A	1765	ASN
1	A	2550	ASN
1	B	94	GLN
1	B	577	GLN
1	B	609	HIS
1	B	868	HIS
1	B	1090	HIS
1	B	1622	HIS
1	B	1765	ASN
1	B	1773	HIS
1	B	1790	HIS
1	B	1797	GLN
1	B	2550	ASN
1	C	95	HIS
1	C	609	HIS
1	C	1242	ASN
1	C	1765	ASN

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Mol	Chain	Res	Type
1	C	1773	HIS
1	C	2550	ASN
1	D	290	HIS
1	D	1090	HIS
1	D	1622	HIS
1	D	1765	ASN
1	D	1902	ASN

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	$\# Z > 2$
3	I3P	B	3002	-	24,24,24	2.18	3 (12%)	39,39,39	0.86	0
3	I3P	D	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	0
4	ATP	C	3003	-	28,33,33	0.65	0	34,52,52	0.91	1 (2%)
4	ATP	D	3003	-	28,33,33	0.64	0	34,52,52	0.91	1 (2%)
4	ATP	B	3003	-	28,33,33	0.64	0	34,52,52	0.91	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	I3P	C	3002	-	24,24,24	2.18	3 (12%)	39,39,39	0.86	0
3	I3P	A	3002	-	24,24,24	2.18	3 (12%)	39,39,39	0.86	0
4	ATP	A	3003	-	28,33,33	0.65	0	34,52,52	0.91	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I3P	B	3002	-	-	1/15/39/39	0/1/1/1
3	I3P	D	3002	-	-	1/15/39/39	0/1/1/1
4	ATP	C	3003	-	-	8/18/38/38	0/3/3/3
4	ATP	D	3003	-	-	8/18/38/38	0/3/3/3
4	ATP	B	3003	-	-	8/18/38/38	0/3/3/3
3	I3P	C	3002	-	-	1/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	1/15/39/39	0/1/1/1
4	ATP	A	3003	-	-	8/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3002	I3P	P4-O4	6.08	1.70	1.59
3	D	3002	I3P	P4-O4	6.08	1.70	1.59
3	A	3002	I3P	P4-O4	6.05	1.70	1.59
3	C	3002	I3P	P4-O4	6.05	1.70	1.59
3	D	3002	I3P	P5-O5	5.92	1.69	1.59
3	A	3002	I3P	P5-O5	5.90	1.69	1.59
3	C	3002	I3P	P5-O5	5.90	1.69	1.59
3	B	3002	I3P	P5-O5	5.86	1.69	1.59
3	D	3002	I3P	P1-O1	5.68	1.69	1.59
3	A	3002	I3P	P1-O1	5.68	1.69	1.59
3	C	3002	I3P	P1-O1	5.67	1.69	1.59
3	B	3002	I3P	P1-O1	5.66	1.69	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3003	ATP	C5-C6-N6	2.35	123.89	120.31
4	C	3003	ATP	C5-C6-N6	2.32	123.85	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3003	ATP	C5-C6-N6	2.31	123.83	120.31
4	B	3003	ATP	C5-C6-N6	2.26	123.76	120.31

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3003	ATP	PB-O3B-PG-O3G
4	A	3003	ATP	C5'-O5'-PA-O1A
4	A	3003	ATP	C5'-O5'-PA-O2A
4	A	3003	ATP	C5'-O5'-PA-O3A
4	B	3003	ATP	PB-O3B-PG-O3G
4	B	3003	ATP	C5'-O5'-PA-O1A
4	B	3003	ATP	C5'-O5'-PA-O2A
4	B	3003	ATP	C5'-O5'-PA-O3A
4	C	3003	ATP	PB-O3B-PG-O3G
4	C	3003	ATP	C5'-O5'-PA-O1A
4	C	3003	ATP	C5'-O5'-PA-O2A
4	C	3003	ATP	C5'-O5'-PA-O3A
4	D	3003	ATP	PB-O3B-PG-O3G
4	D	3003	ATP	C5'-O5'-PA-O1A
4	D	3003	ATP	C5'-O5'-PA-O2A
4	D	3003	ATP	C5'-O5'-PA-O3A
4	A	3003	ATP	C3'-C4'-C5'-O5'
4	B	3003	ATP	C3'-C4'-C5'-O5'
4	C	3003	ATP	C3'-C4'-C5'-O5'
4	D	3003	ATP	C3'-C4'-C5'-O5'
4	A	3003	ATP	O4'-C4'-C5'-O5'
4	B	3003	ATP	O4'-C4'-C5'-O5'
4	C	3003	ATP	O4'-C4'-C5'-O5'
4	D	3003	ATP	O4'-C4'-C5'-O5'
3	A	3002	I3P	C5-O5-P5-O52
3	B	3002	I3P	C5-O5-P5-O52
3	C	3002	I3P	C5-O5-P5-O52
3	D	3002	I3P	C5-O5-P5-O52
4	A	3003	ATP	PB-O3B-PG-O1G
4	B	3003	ATP	PB-O3B-PG-O1G
4	C	3003	ATP	PB-O3B-PG-O1G
4	D	3003	ATP	PB-O3B-PG-O1G
4	A	3003	ATP	PB-O3B-PG-O2G
4	B	3003	ATP	PB-O3B-PG-O2G
4	C	3003	ATP	PB-O3B-PG-O2G

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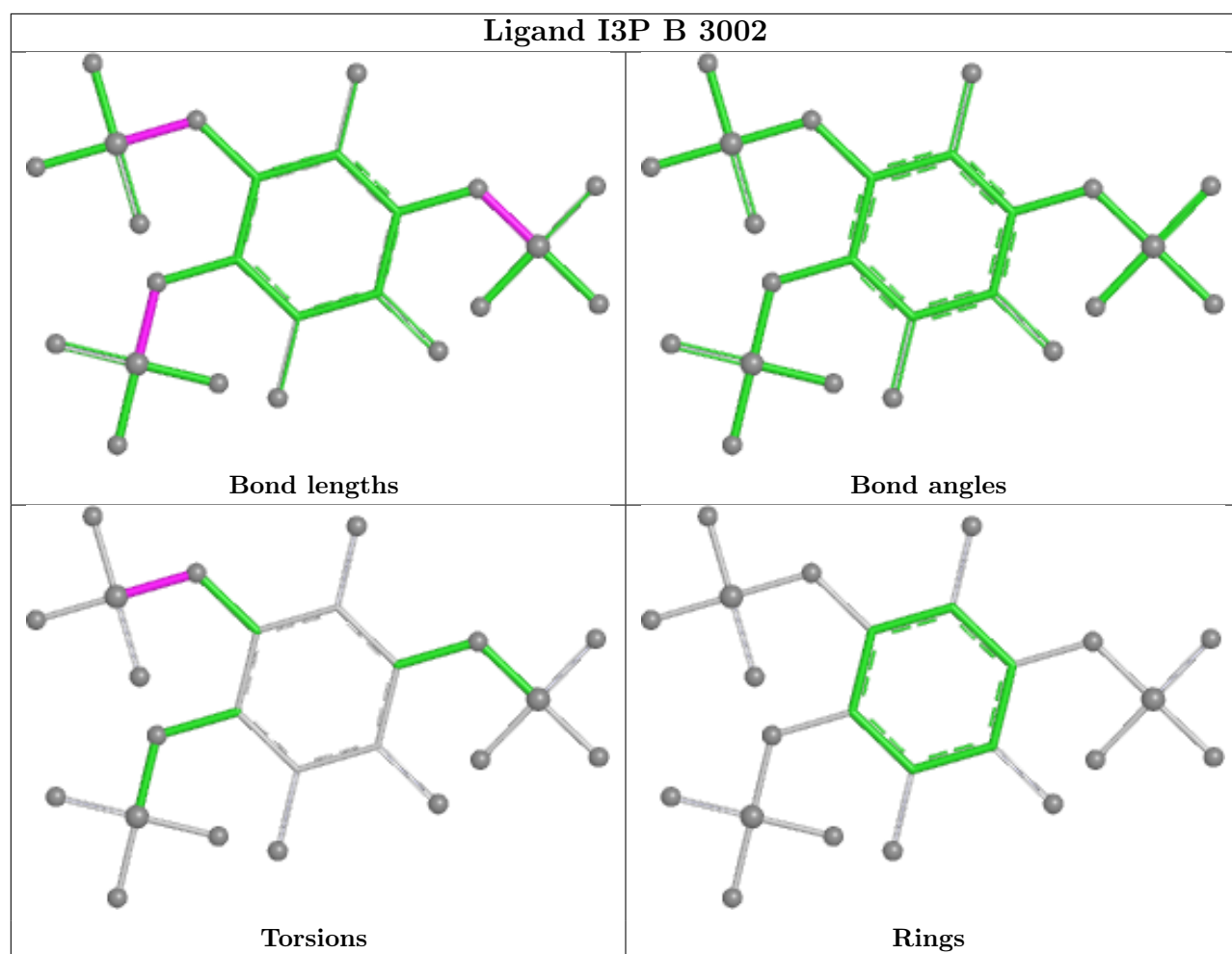
Mol	Chain	Res	Type	Atoms
4	D	3003	ATP	PB-O3B-PG-O2G

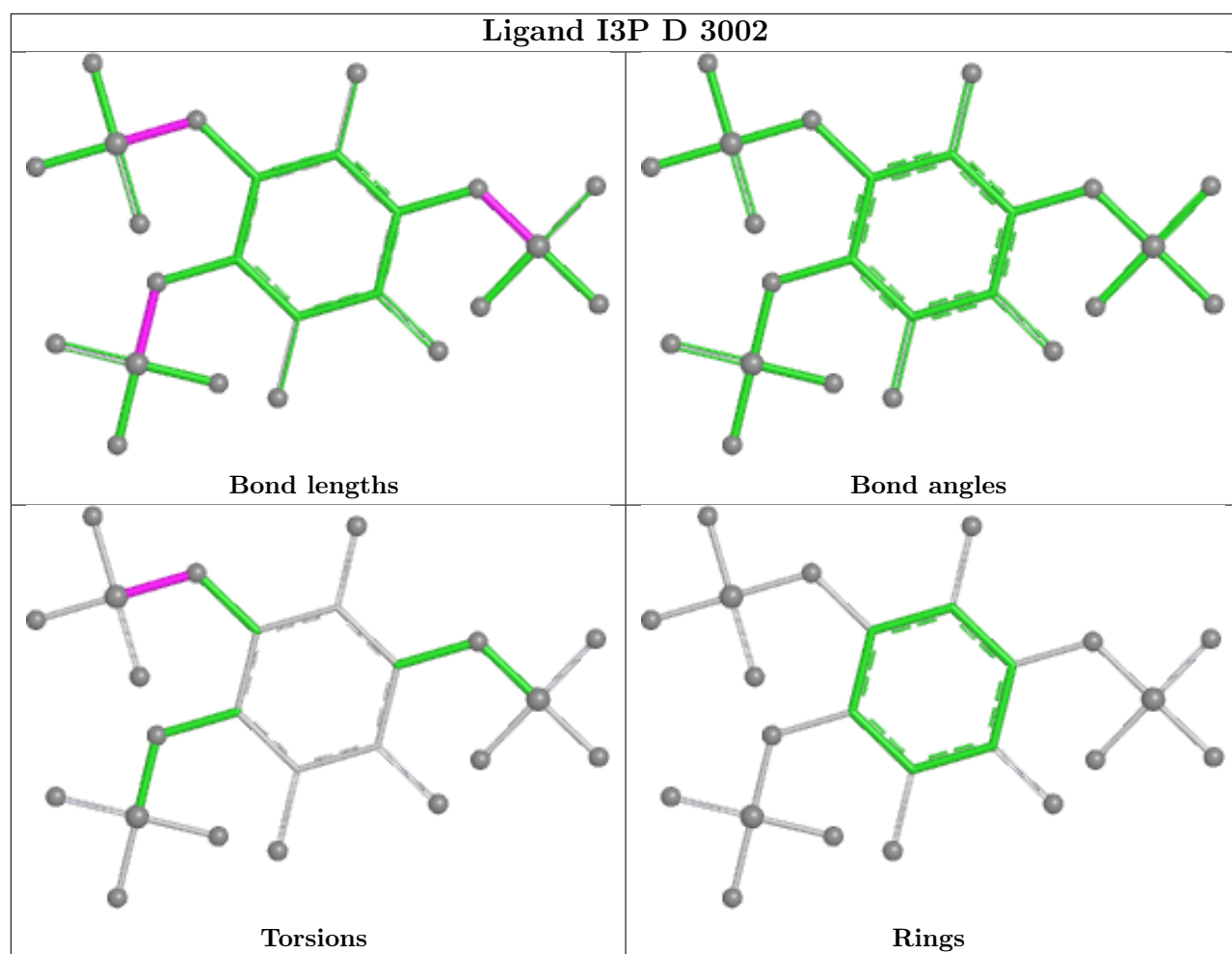
There are no ring outliers.

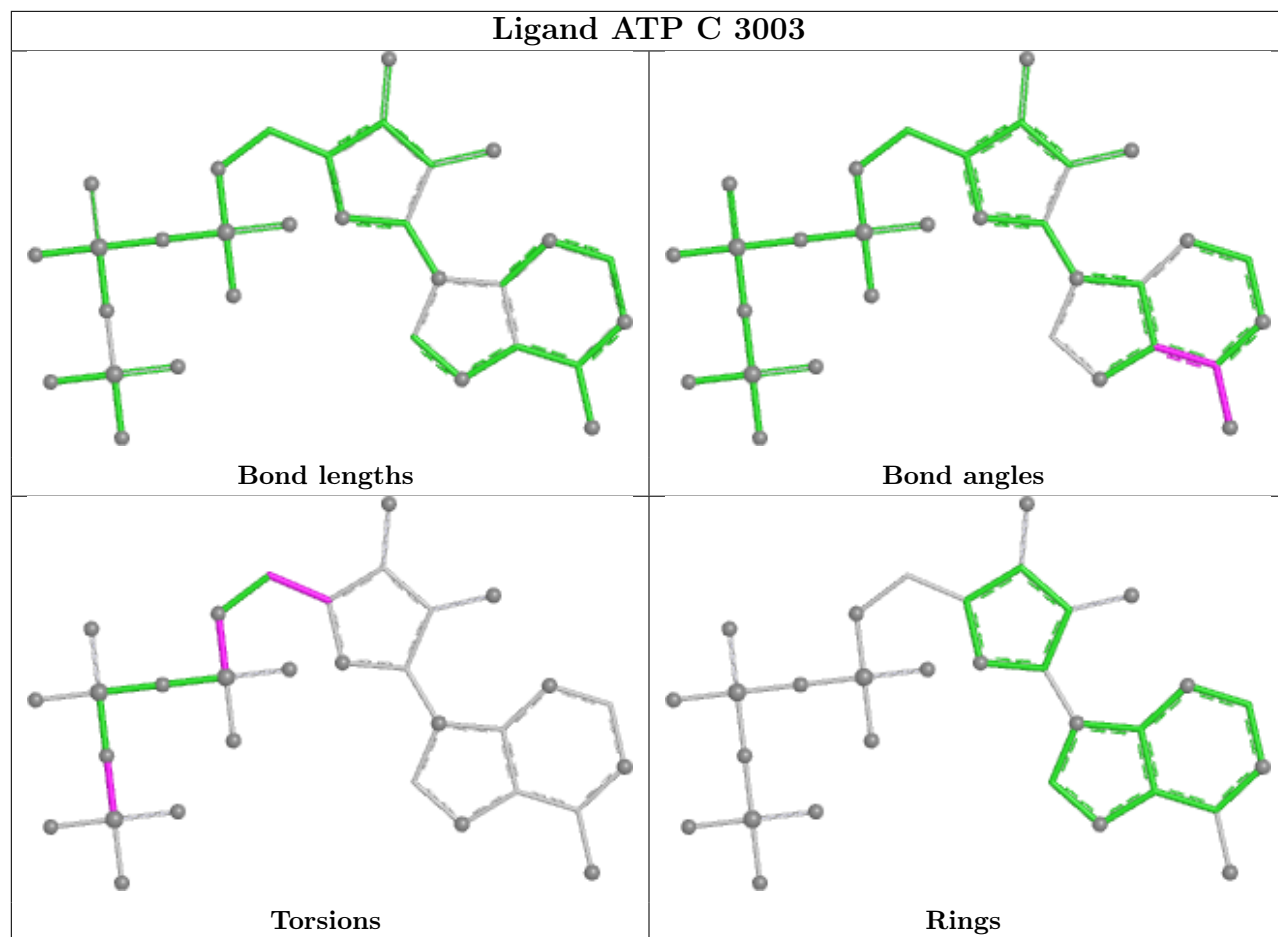
4 monomers are involved in 4 short contacts:

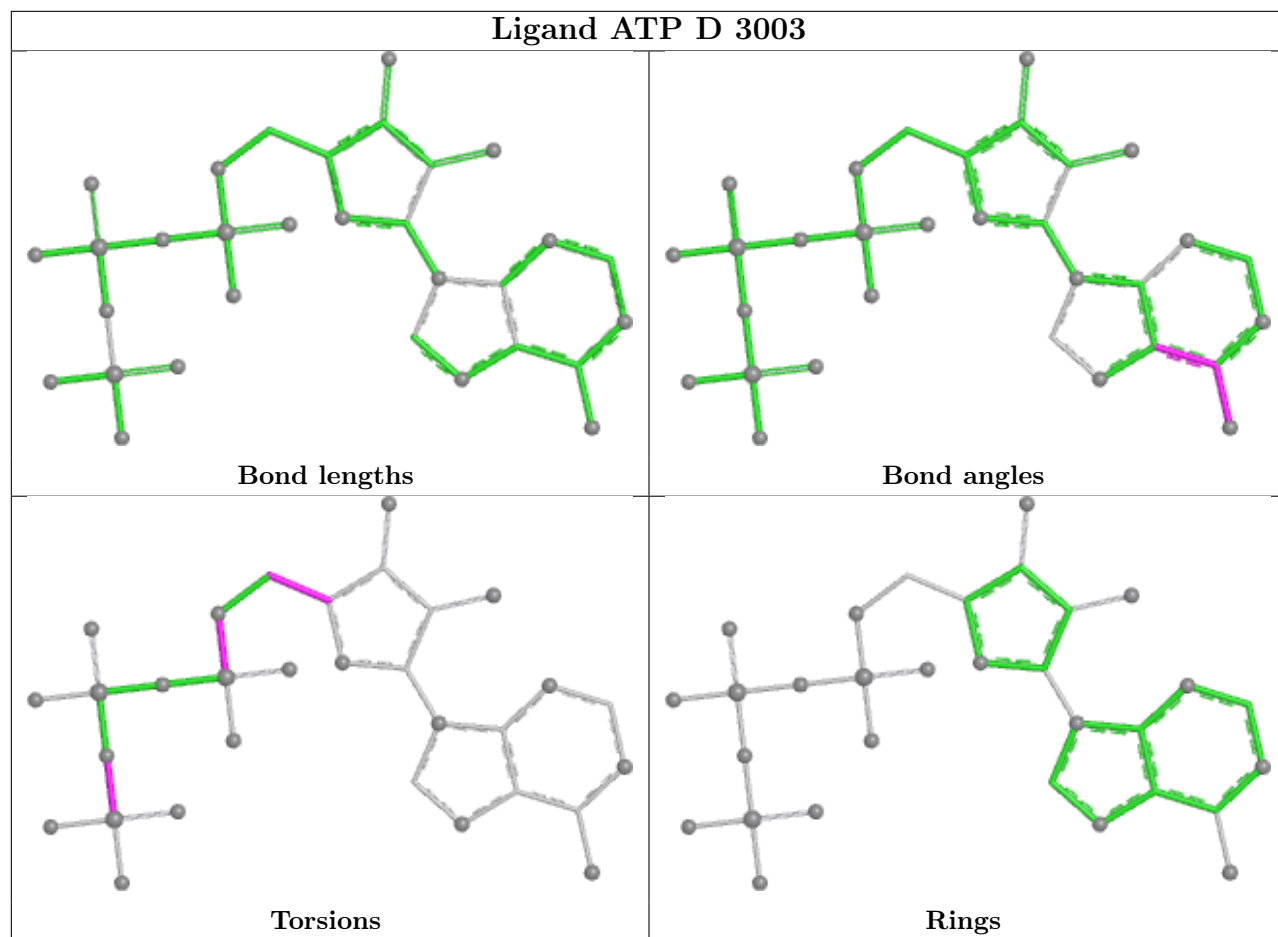
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3003	ATP	1	0
4	D	3003	ATP	1	0
4	B	3003	ATP	1	0
4	A	3003	ATP	1	0

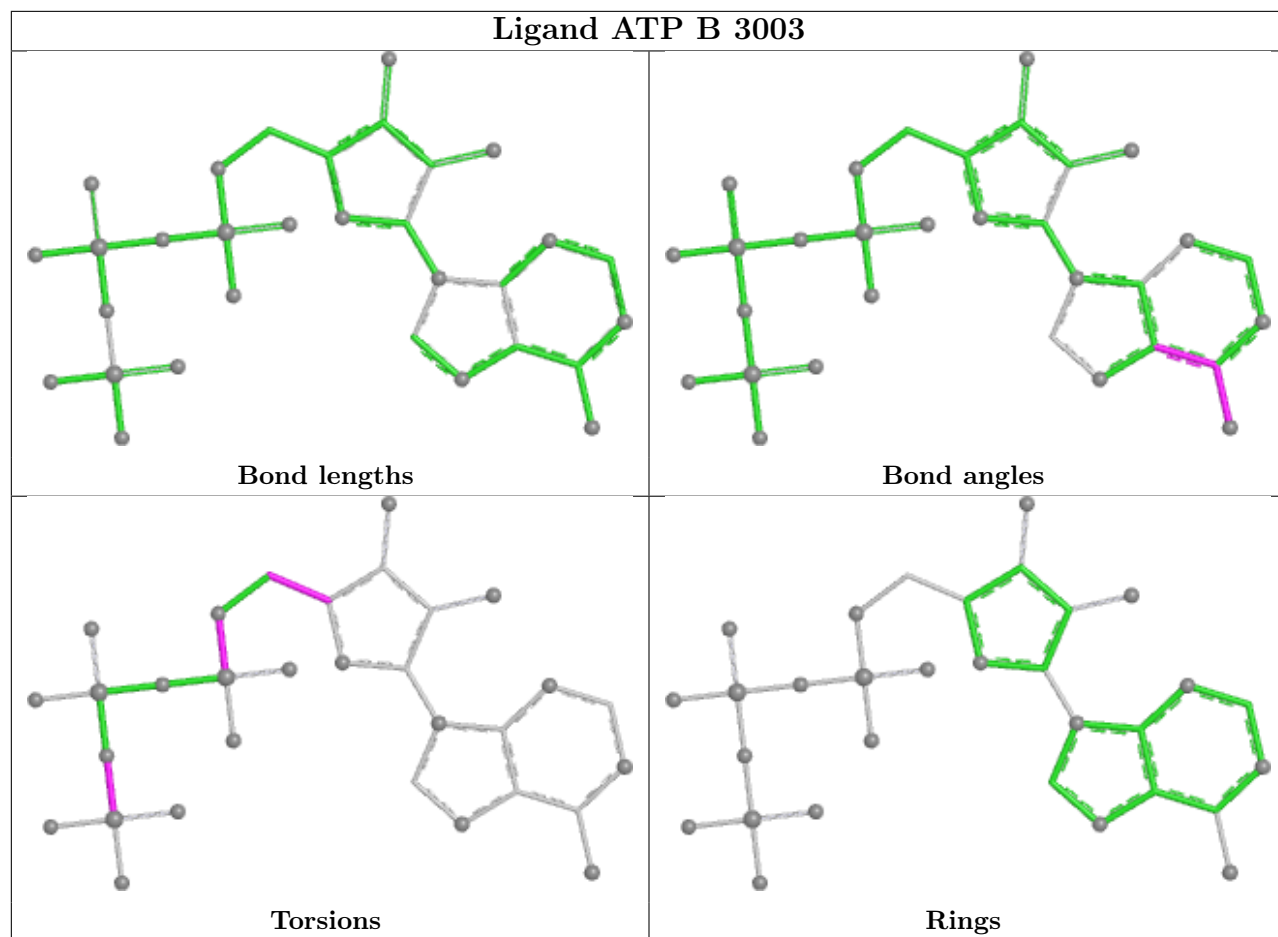
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

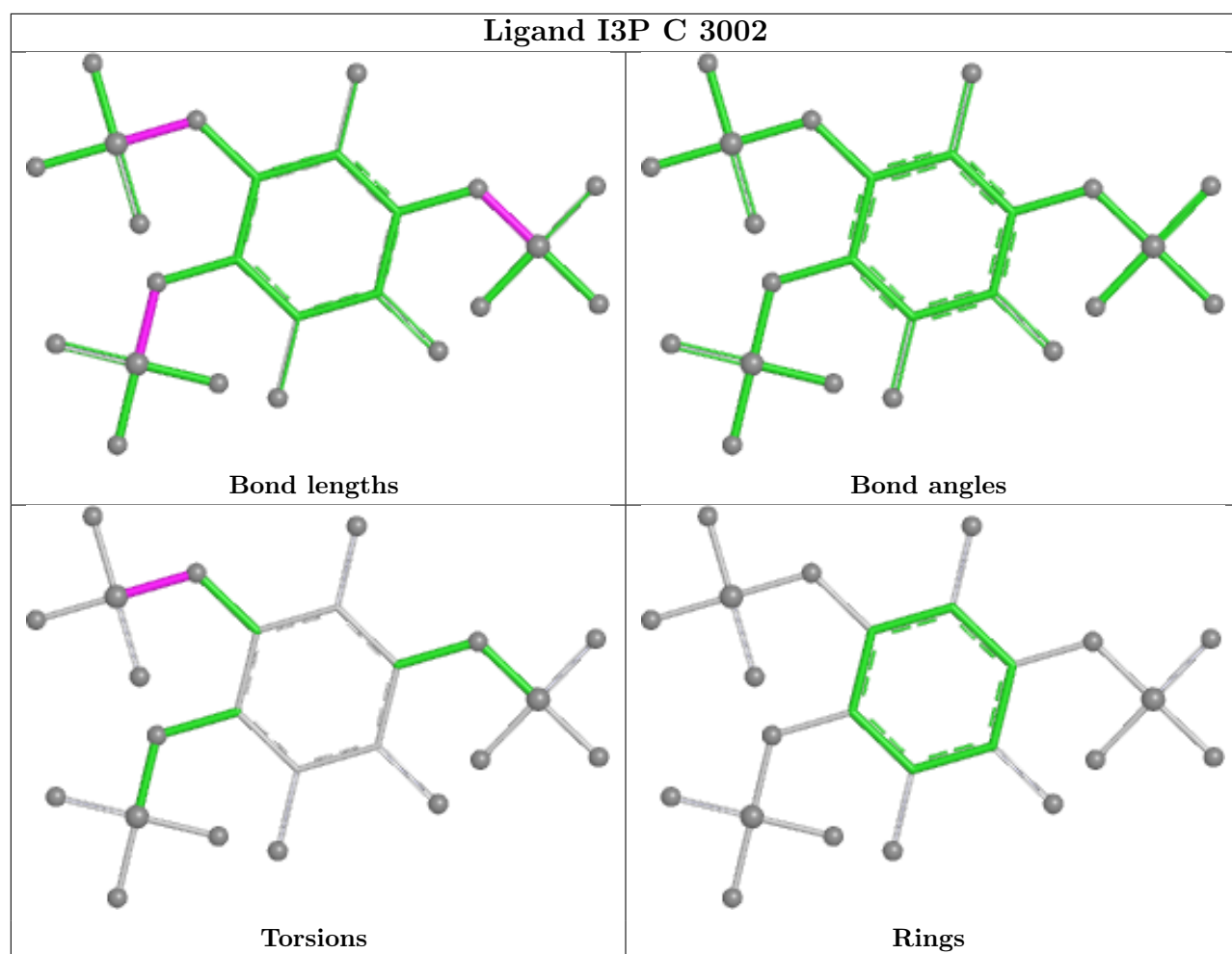


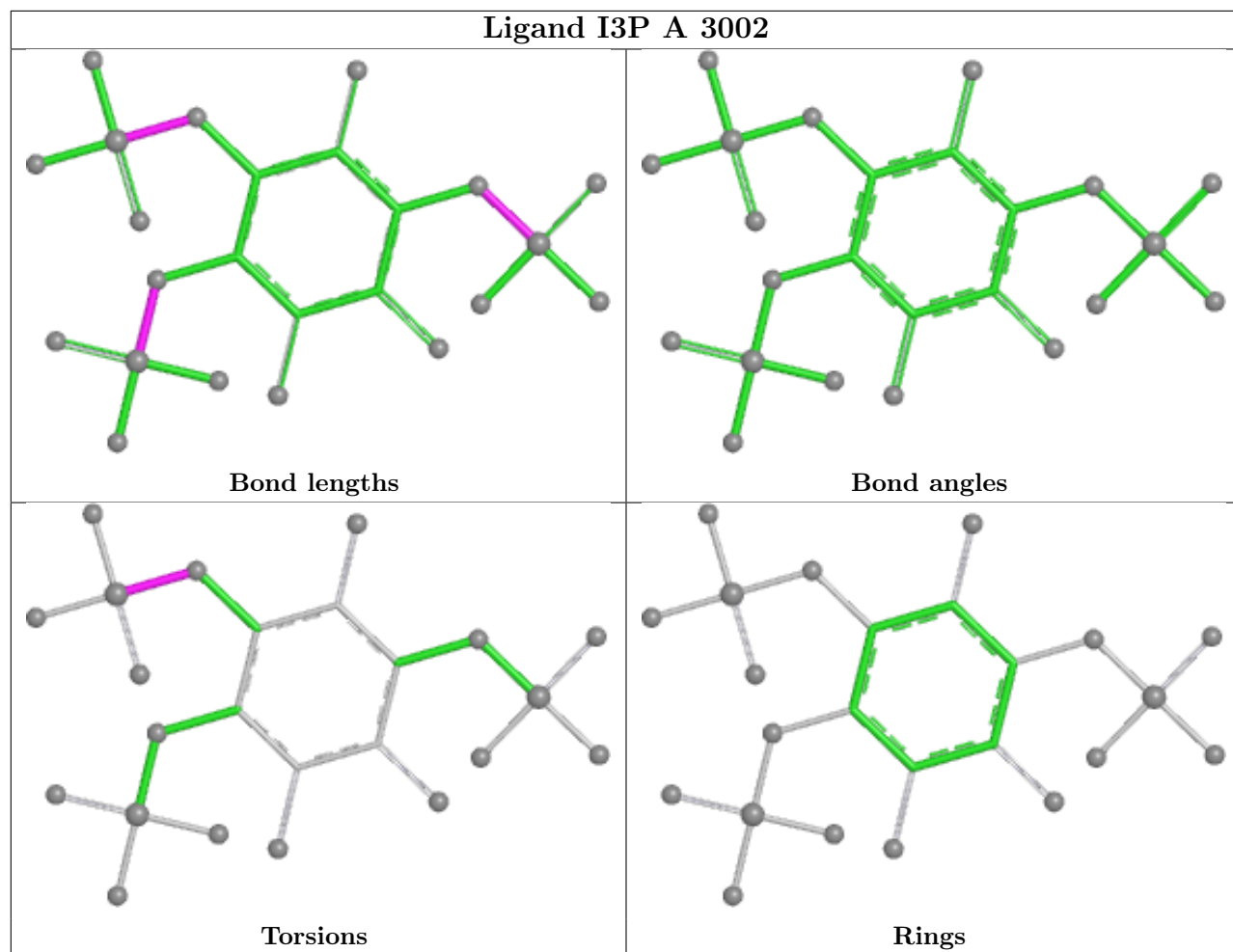


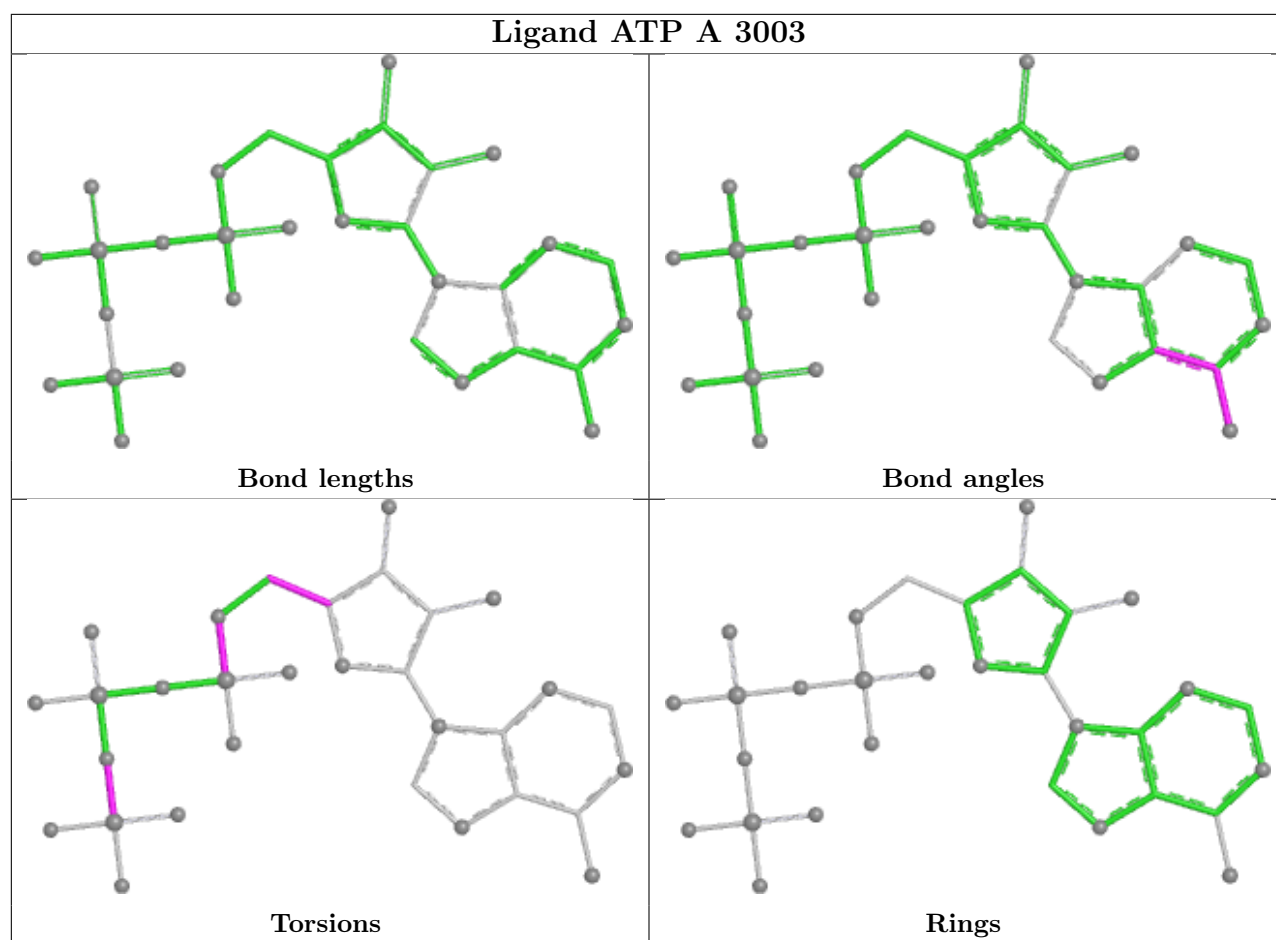












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

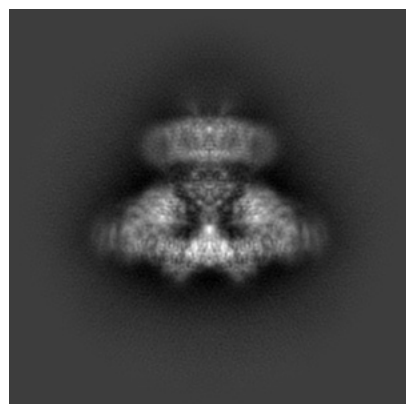
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41351. These allow visual inspection of the internal detail of the map and identification of artifacts.

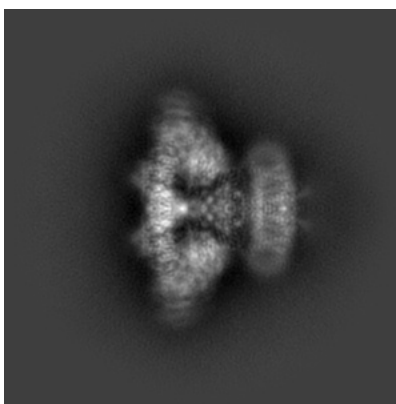
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

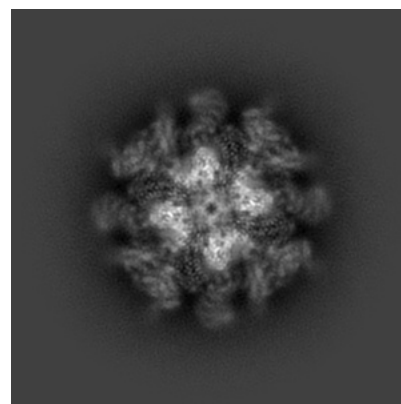
6.1.1 Primary map



X

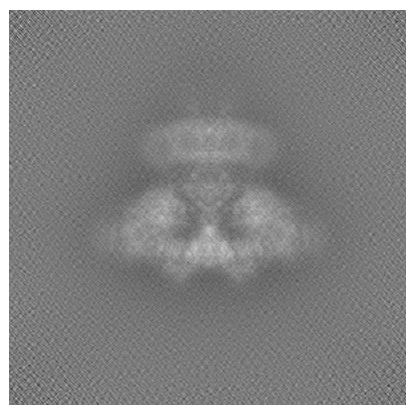


Y

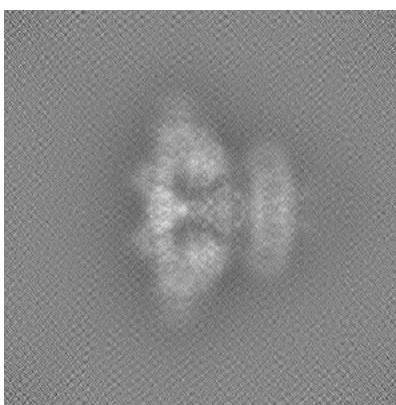


Z

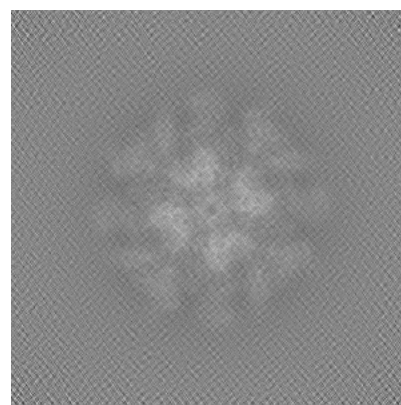
6.1.2 Raw map



X



Y

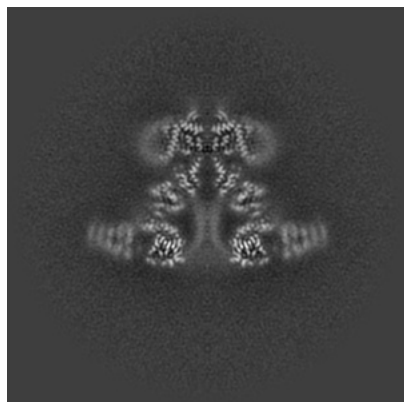


Z

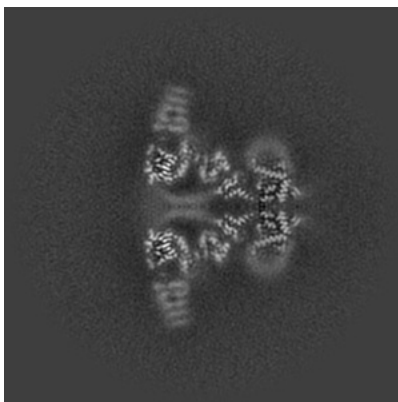
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

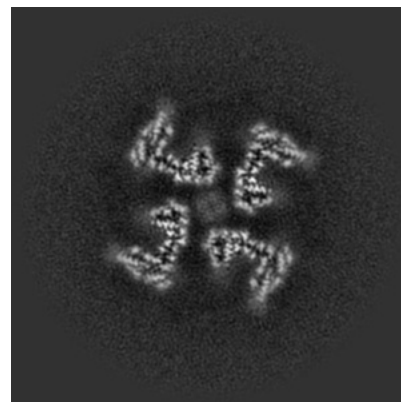
6.2.1 Primary map



X Index: 256



Y Index: 256

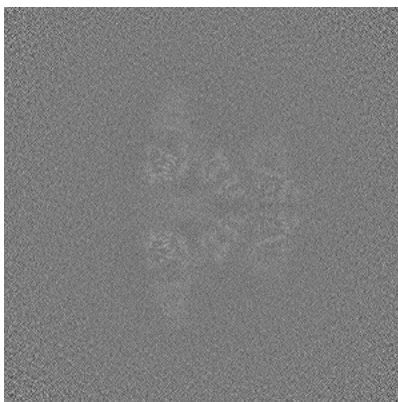


Z Index: 256

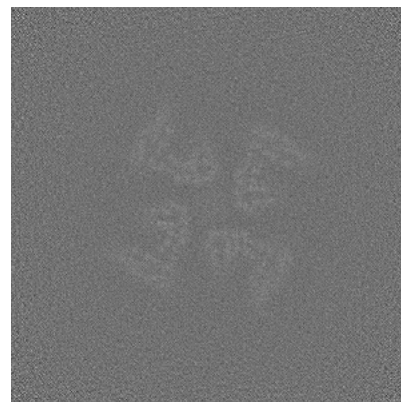
6.2.2 Raw map



X Index: 256



Y Index: 256

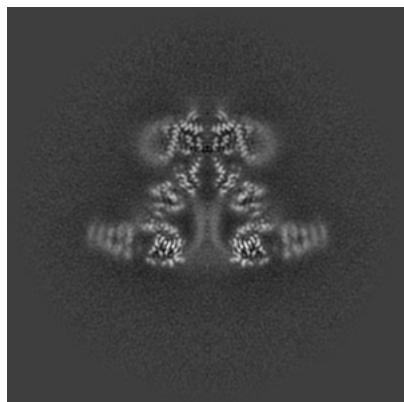


Z Index: 256

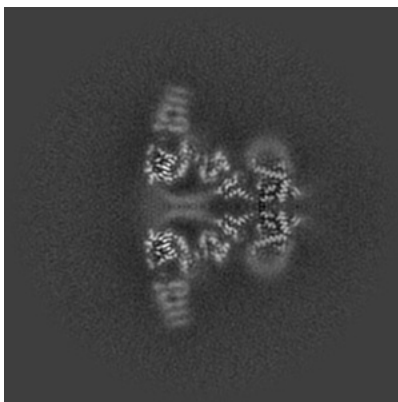
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

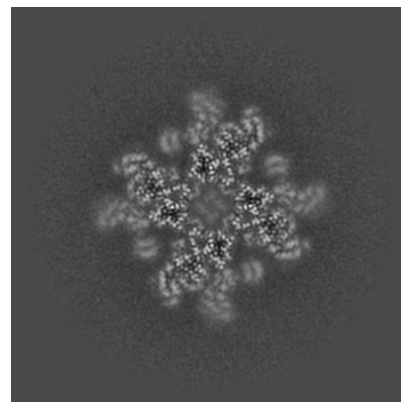
6.3.1 Primary map



X Index: 256

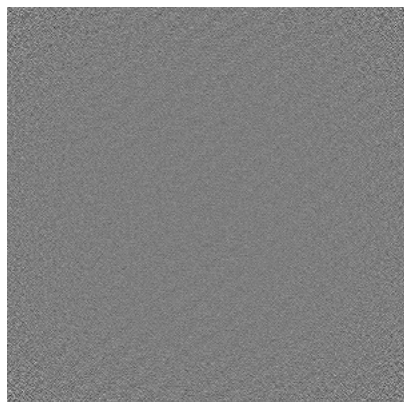


Y Index: 256

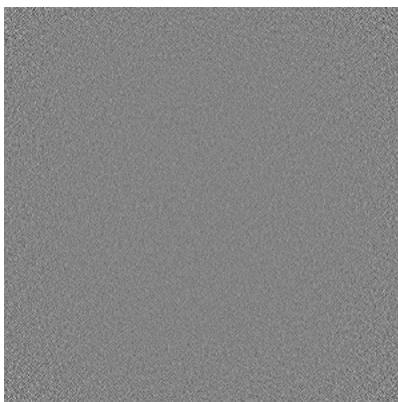


Z Index: 206

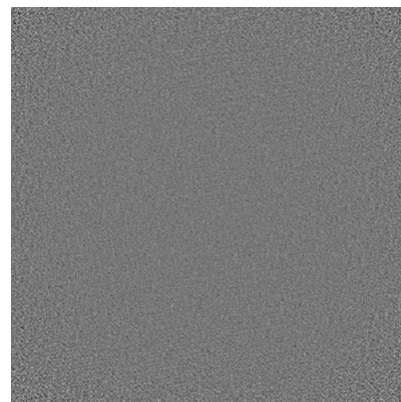
6.3.2 Raw map



X Index: 0



Y Index: 0

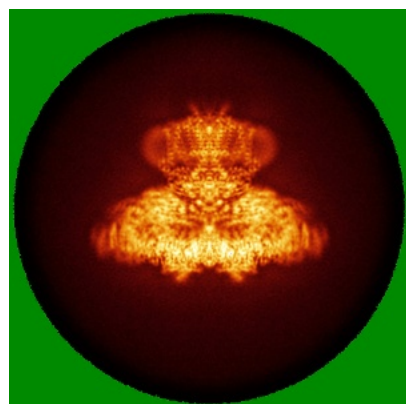


Z Index: 1

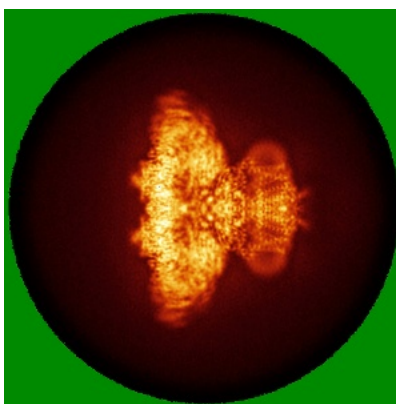
The images above show the largest variance slices of the map in three orthogonal directions.

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

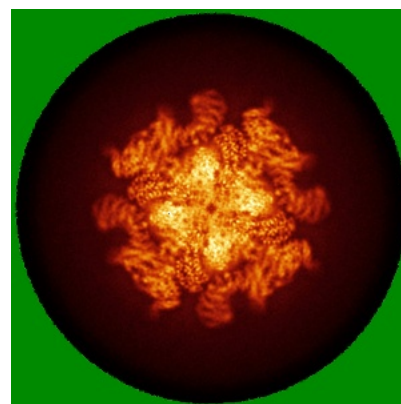
6.4.1 Primary map



X

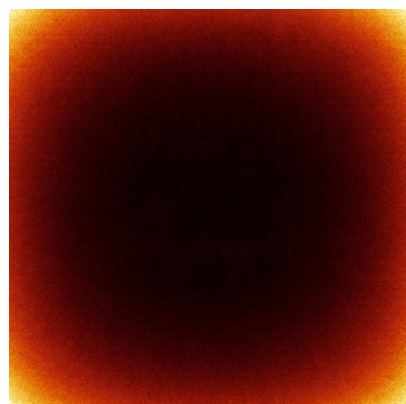


Y

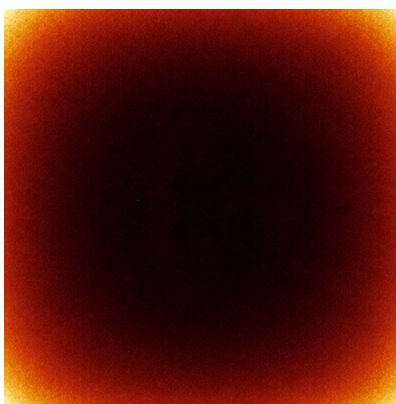


Z

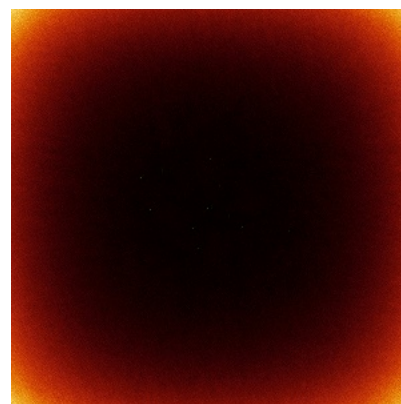
6.4.2 Raw map



X



Y

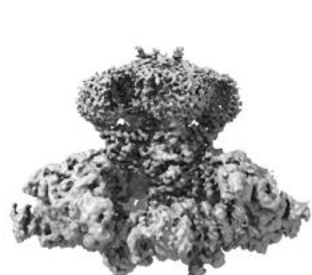


Z

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](#)

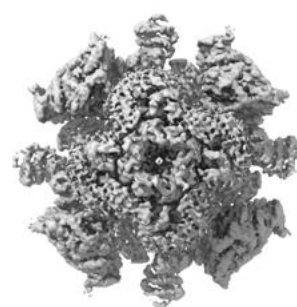
6.5.1 Primary map



X



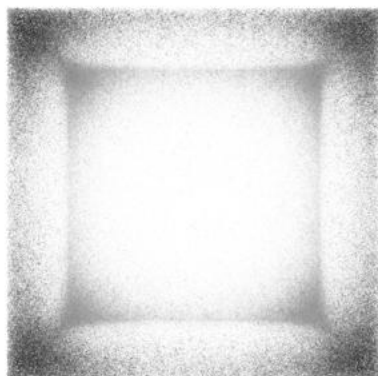
Y



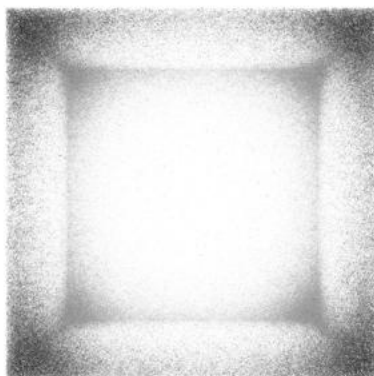
Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

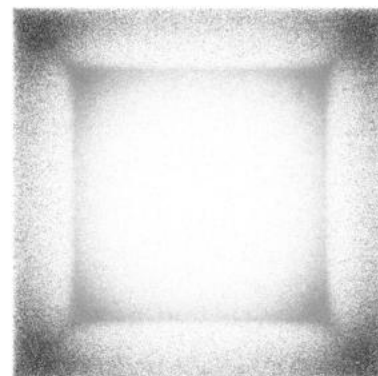
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

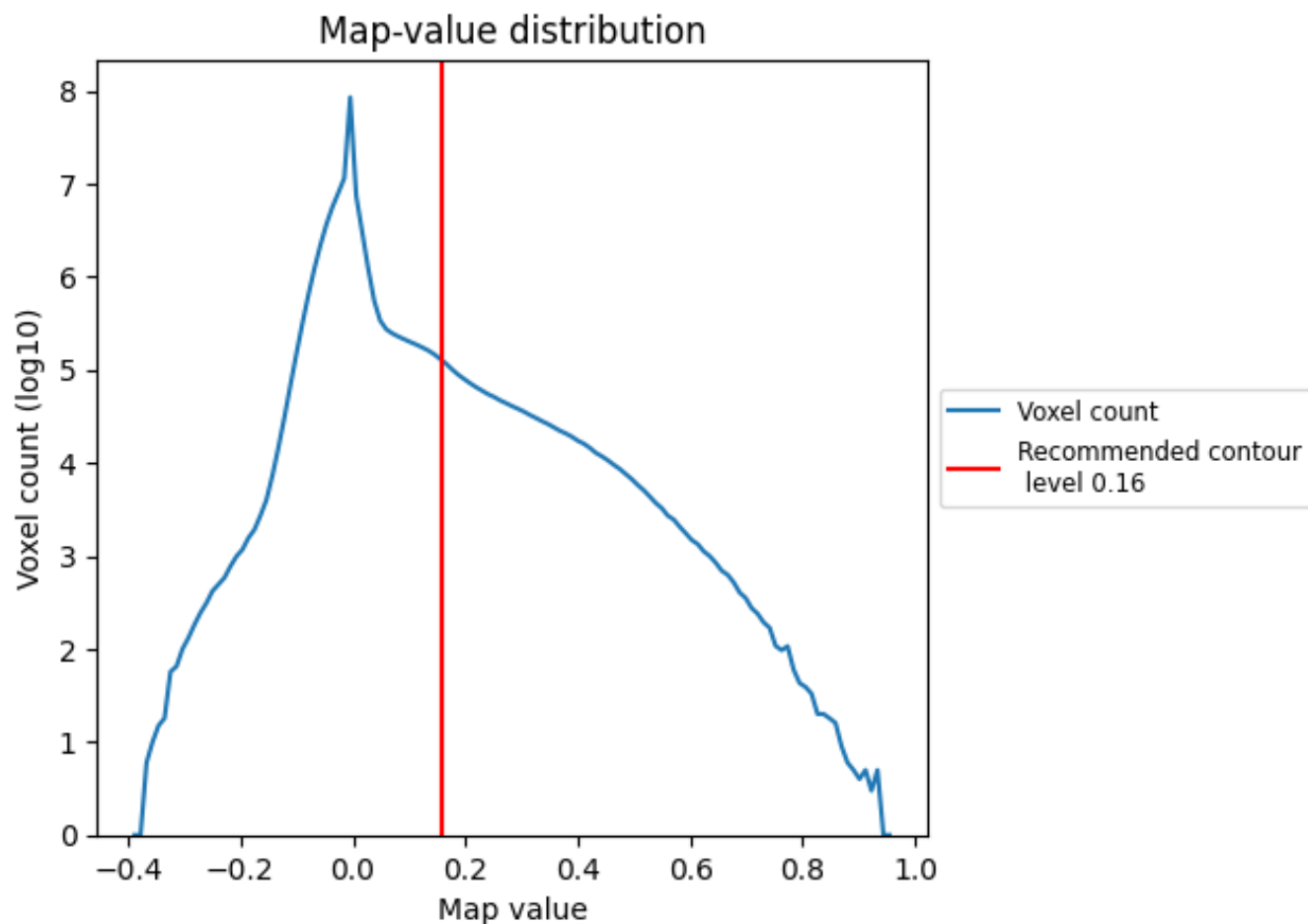
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

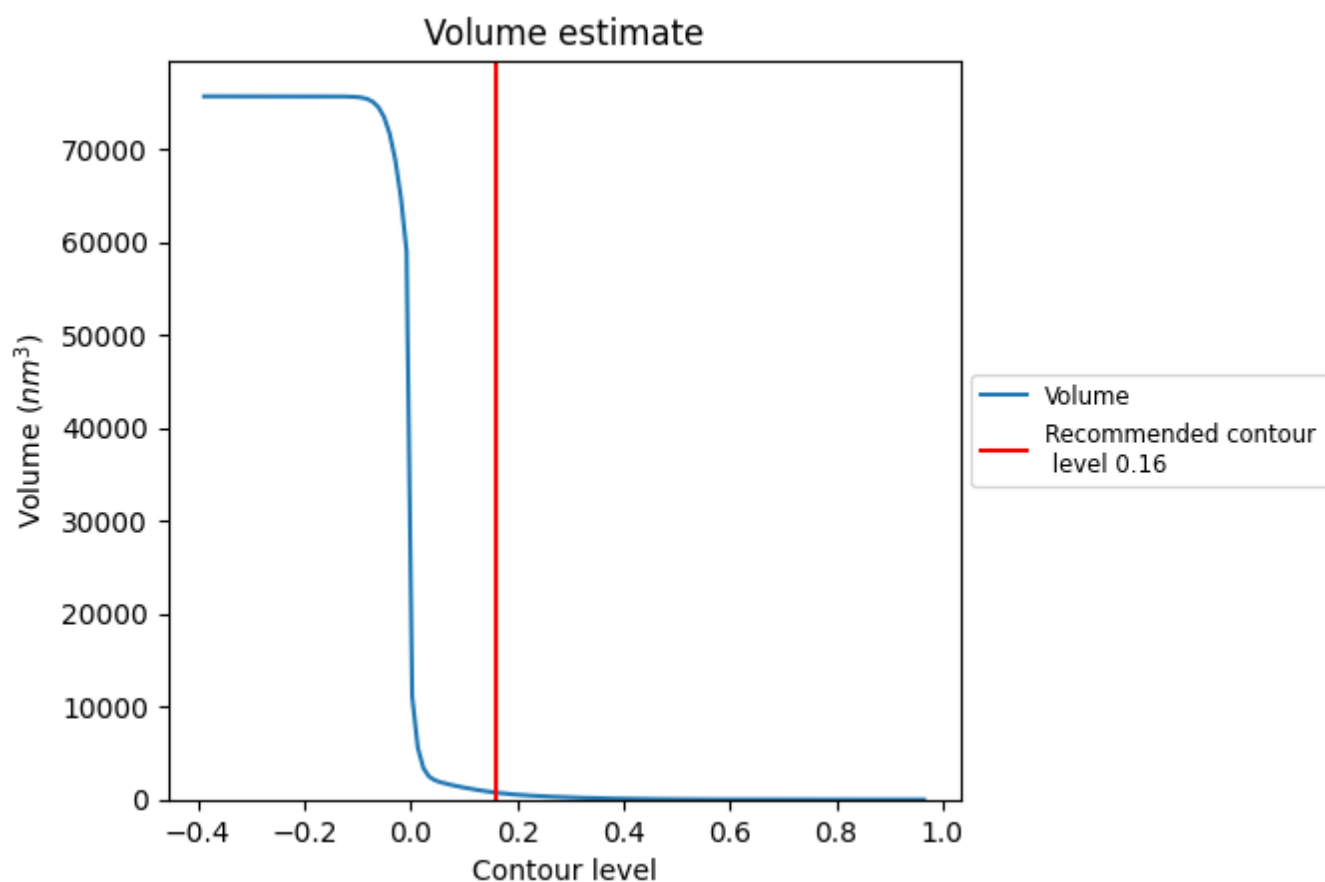
This section contains the results of statistical analysis of the map.

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.

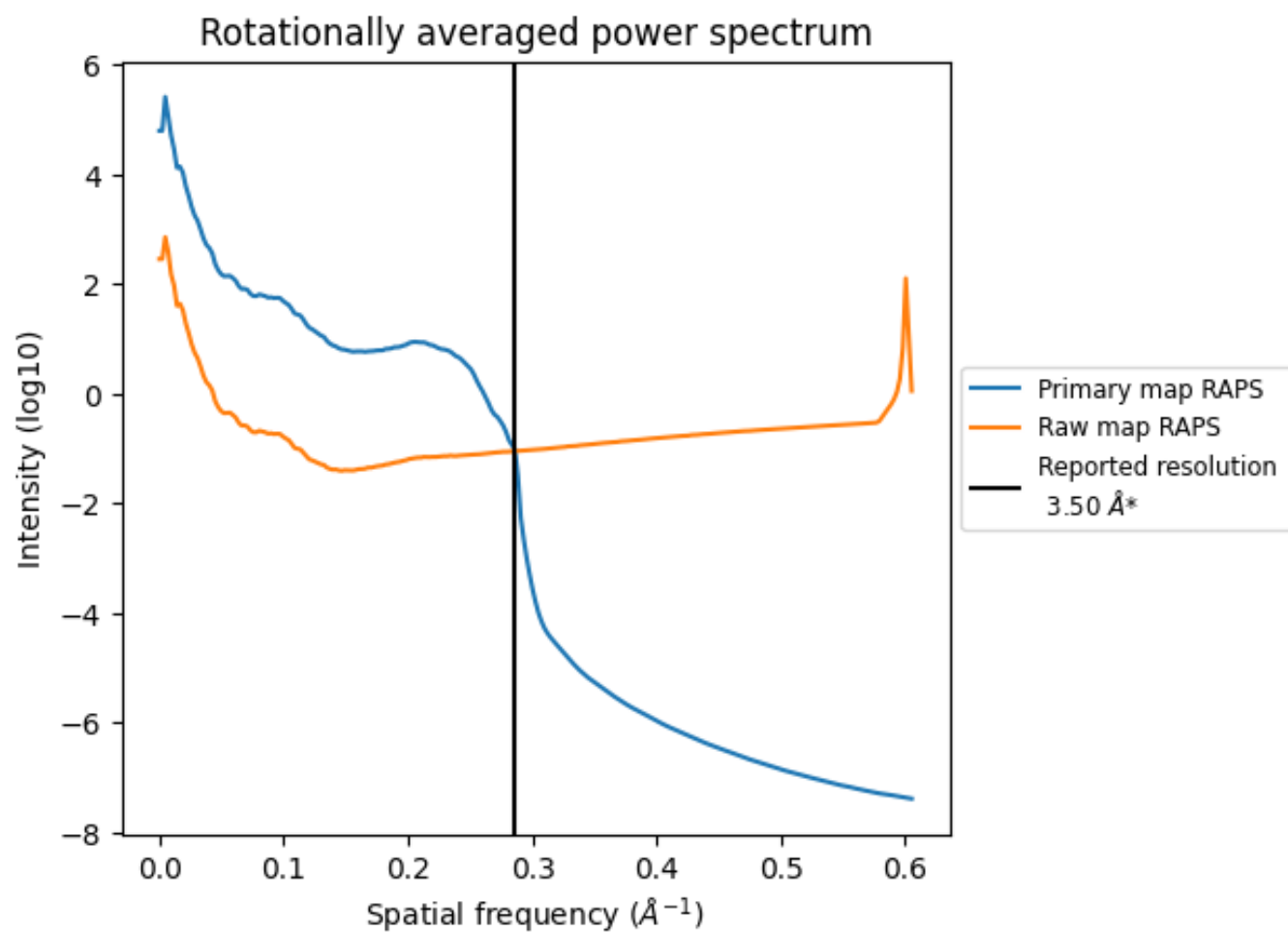
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm³; this corresponds to an approximate mass of 675 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 ⓘ

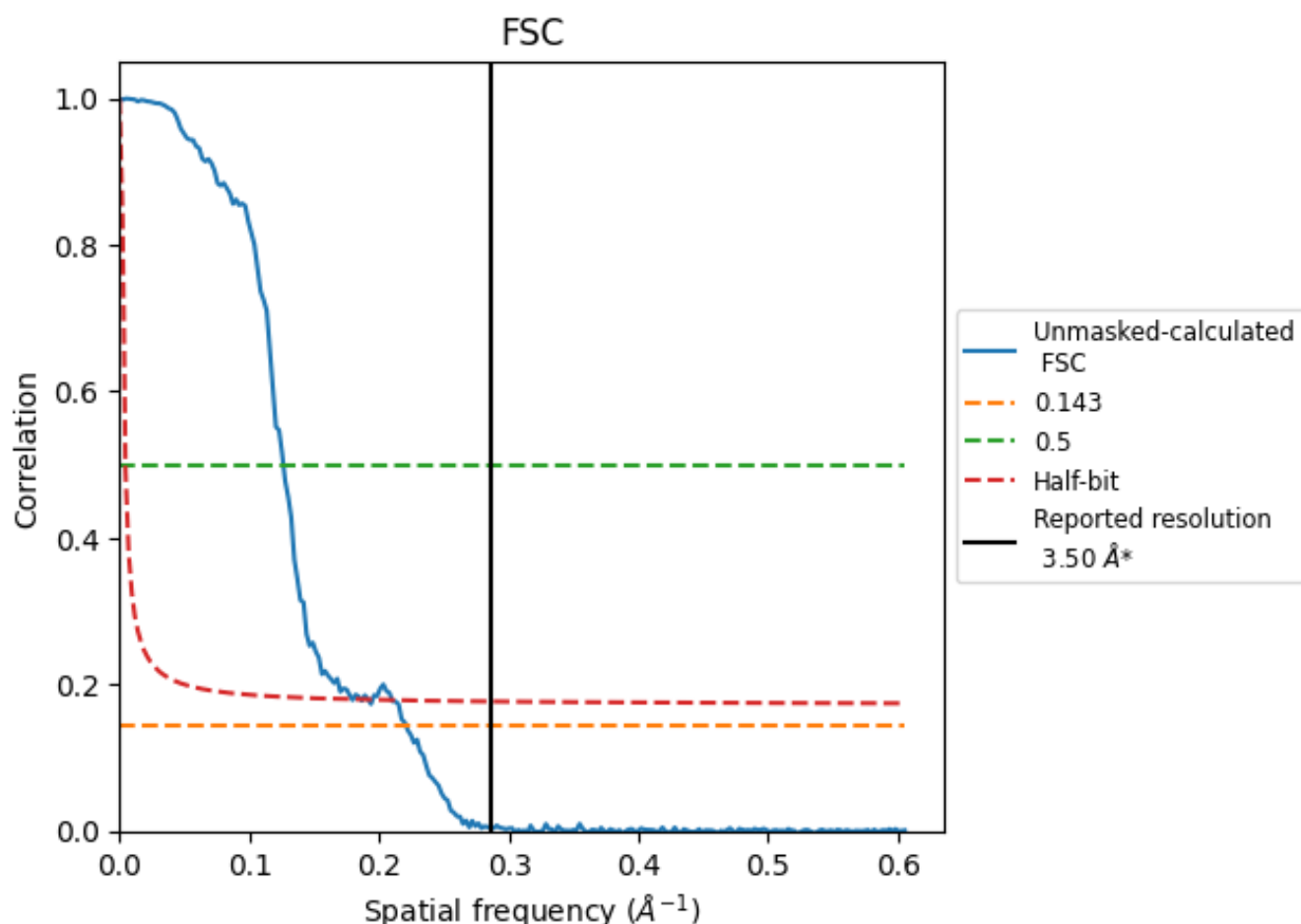


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

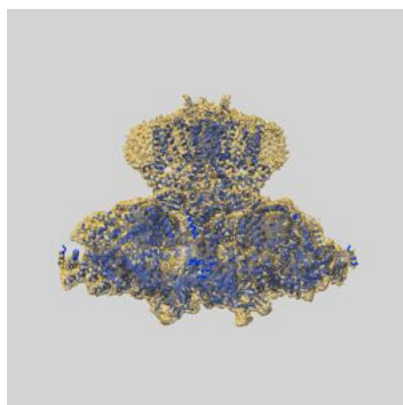
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.53	7.92	5.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.53 differs from the reported value 3.5 by more than 10 %

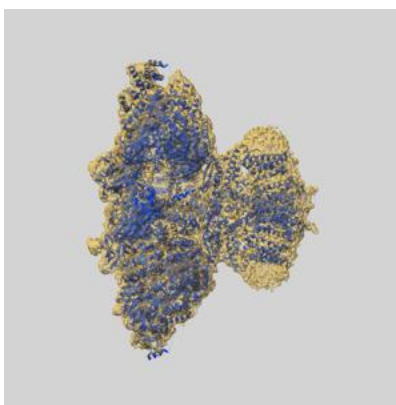
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41351 and PDB model 8TKH. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

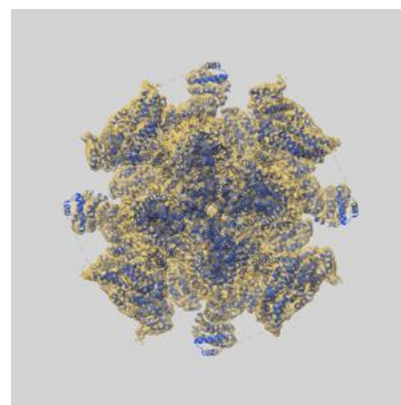
9.1 Map-model overlay [i](#)



X



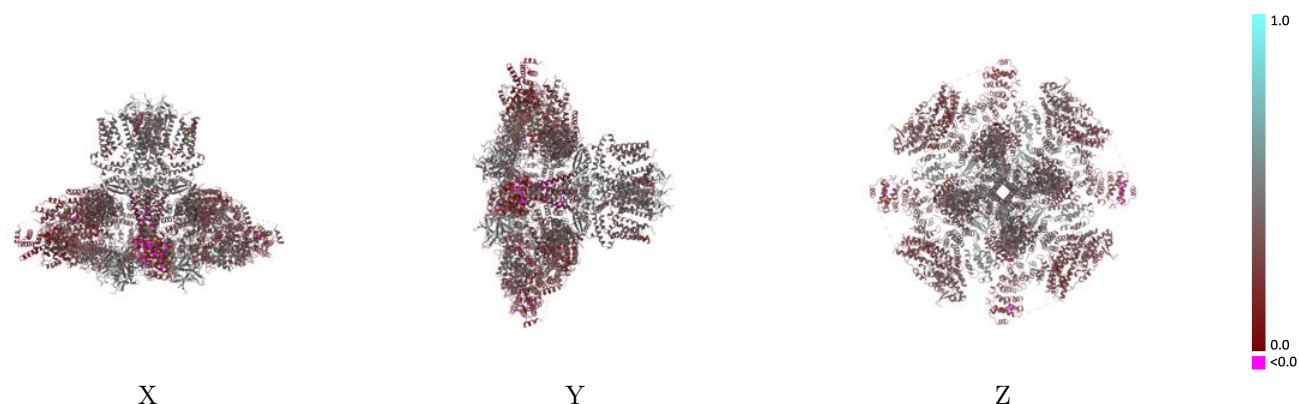
Y



Z

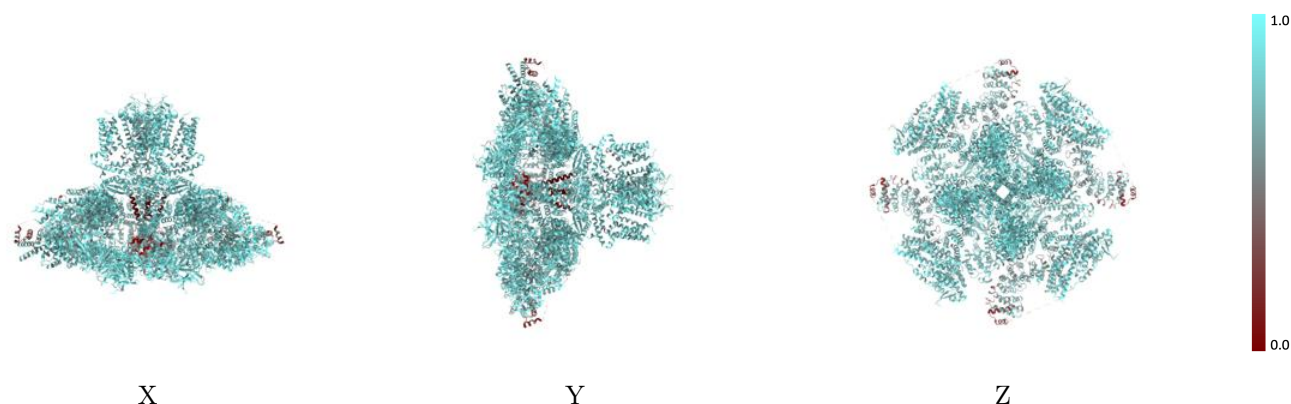
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



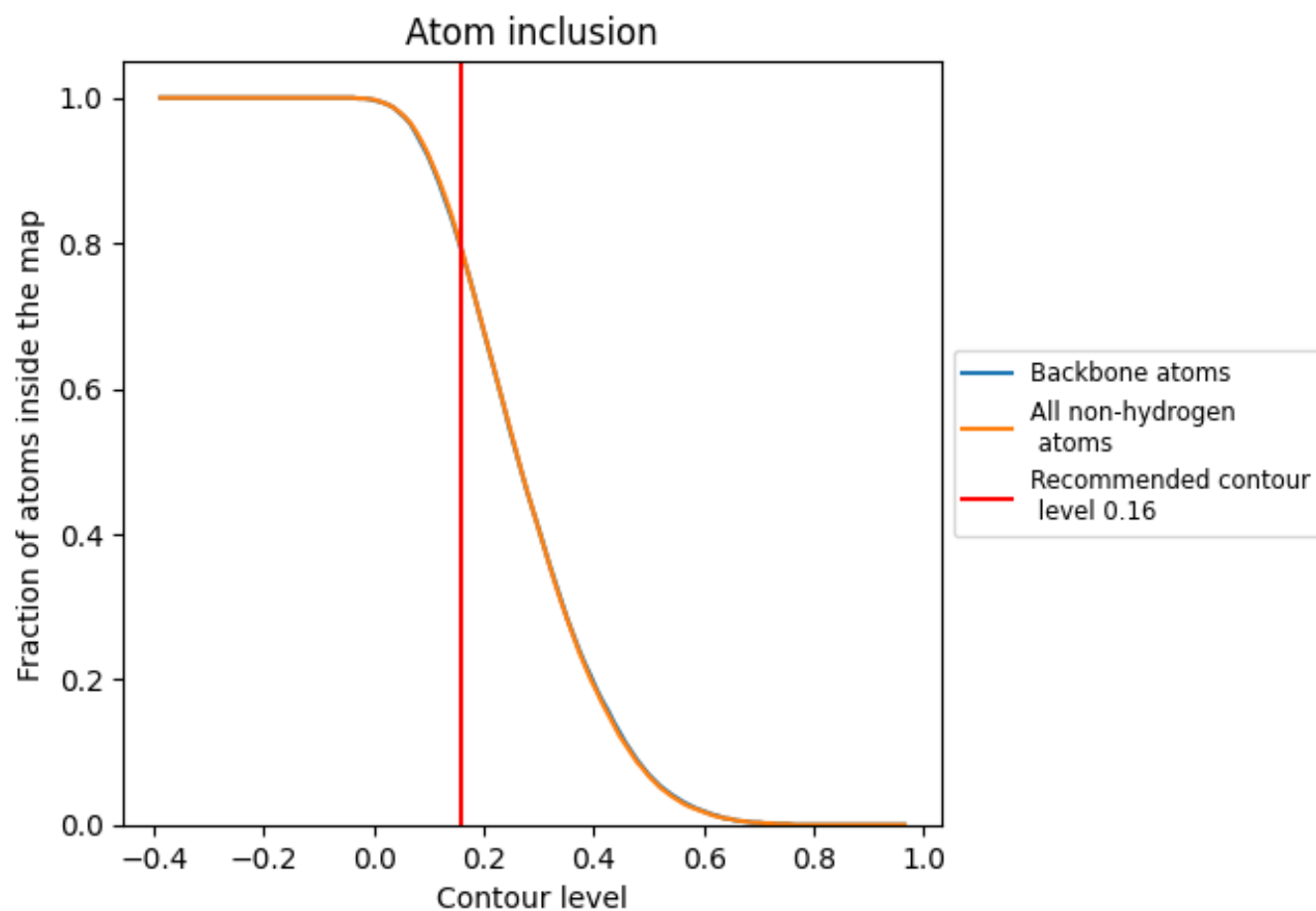
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7900	<div></div> 0.3620
A	<div></div> 0.7990	<div></div> 0.3680
B	<div></div> 0.7960	<div></div> 0.3580
C	<div></div> 0.7960	<div></div> 0.3650
D	<div></div> 0.7880	<div></div> 0.3560

