Full wwPDB EM Validation Report

Aug 29, 2026 – 12:39 PM EDT

PDB ID	:	12AI / pdb_000012ai
EMDB ID	:	EMD-76264
Title	:	Structure of mammalian Type 2 Inositol 1,4,5-trisphosphate receptor (IP3R2) in the presence of IP3/Ca2+/ATP
Authors	:	Serysheva, I.I.; Baker, M.R.; Fan, G.
Deposited on	:	2026-03-23
Resolution	:	3.64 Å(reported)
Based on initial model	:	.

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 (i) 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 (1)) were used in the production of this report:

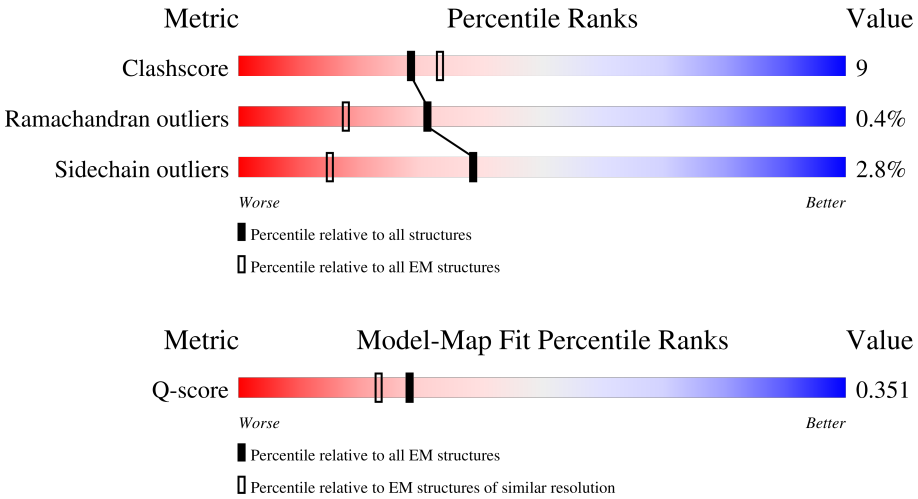
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11633 (3.14 - 4.14)

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 <=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	2701	5% 67% 18% • 14%
1	B	2701	5% 67% 18% • 14%
1	C	2701	5% 67% 18% • 14%
1	D	2701	5% 67% 17% • 14%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 72076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2310	Total 17922	C 11386	N 3130	O 3309	S 97	0	0
1	B	2310	Total 17922	C 11386	N 3130	O 3309	S 97	0	0
1	C	2310	Total 17922	C 11386	N 3130	O 3309	S 97	0	0
1	D	2310	Total 17922	C 11386	N 3130	O 3309	S 97	0	0

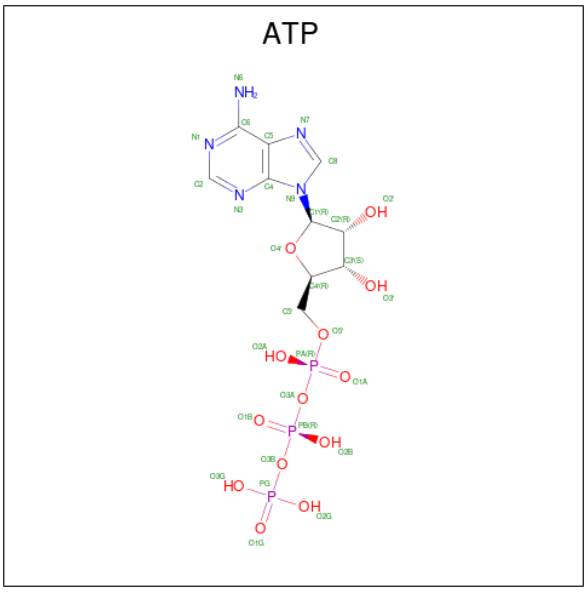
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1004	ASP	ASN	conflict	UNP Q9Z329
B	1004	ASP	ASN	conflict	UNP Q9Z329
C	1004	ASP	ASN	conflict	UNP Q9Z329
D	1004	ASP	ASN	conflict	UNP Q9Z329

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

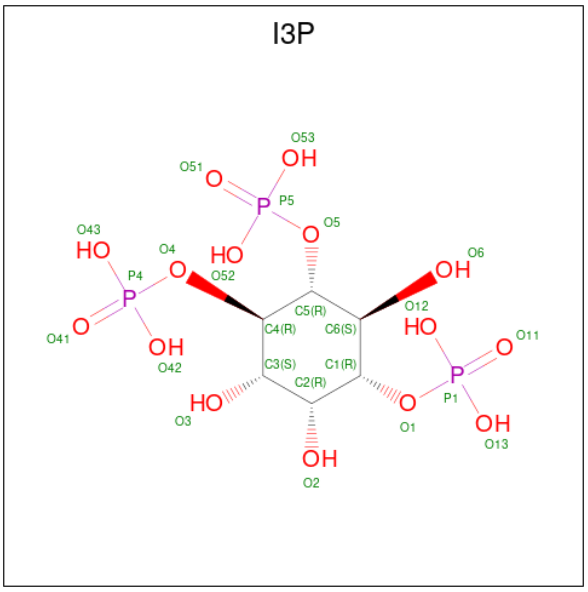
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

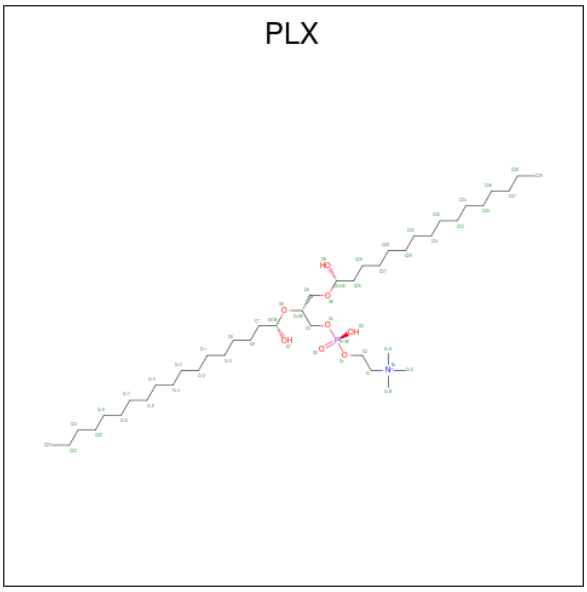


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			24	6	15	3	
4	B	1	Total	C	O	P	0
			24	6	15	3	
4	C	1	Total	C	O	P	0
			24	6	15	3	
4	D	1	Total	C	O	P	0
			24	6	15	3	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

- Molecule 6 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



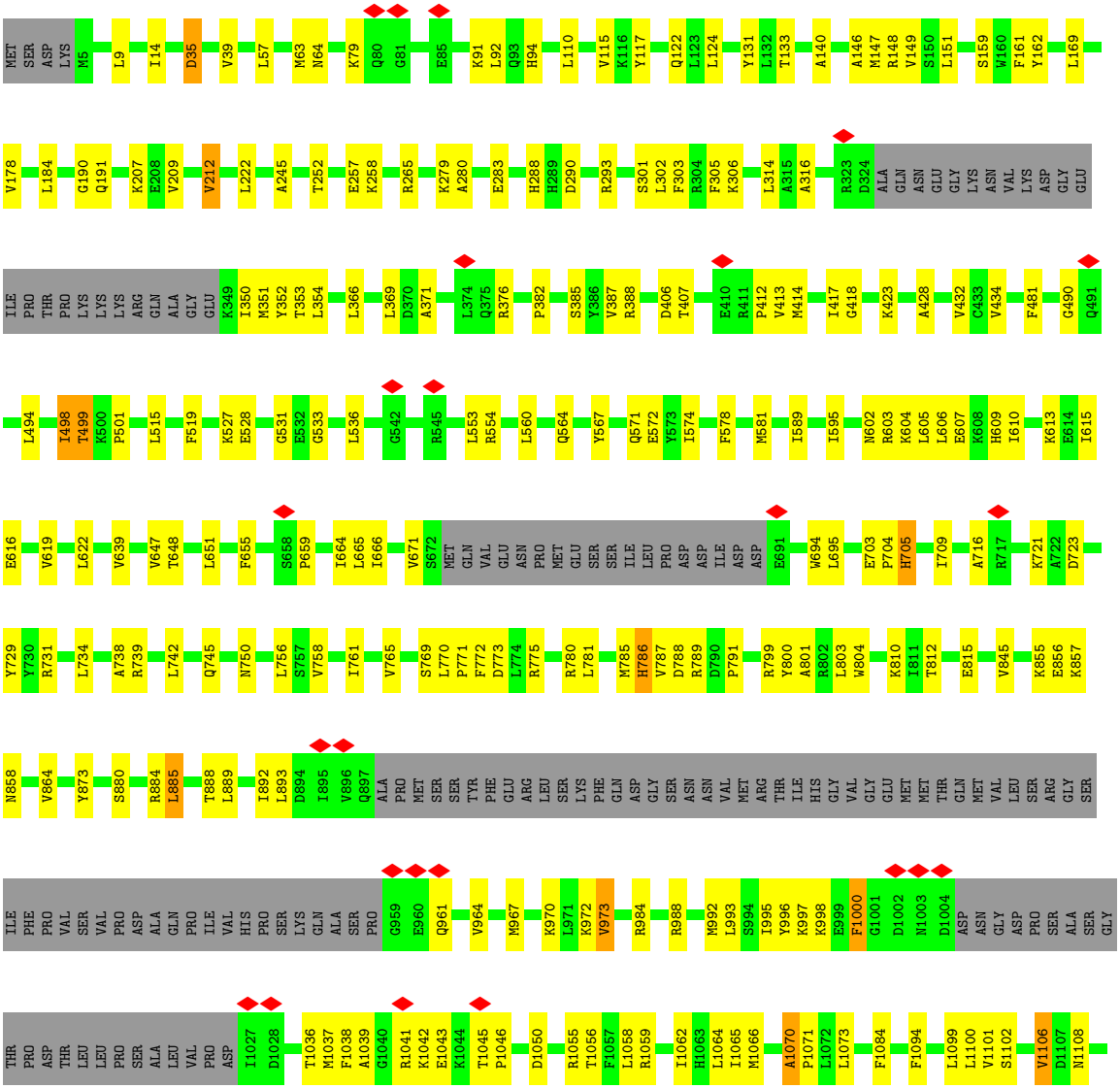
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	D	1	Total	C	N	O	P	0
			40	30	1	8	1	

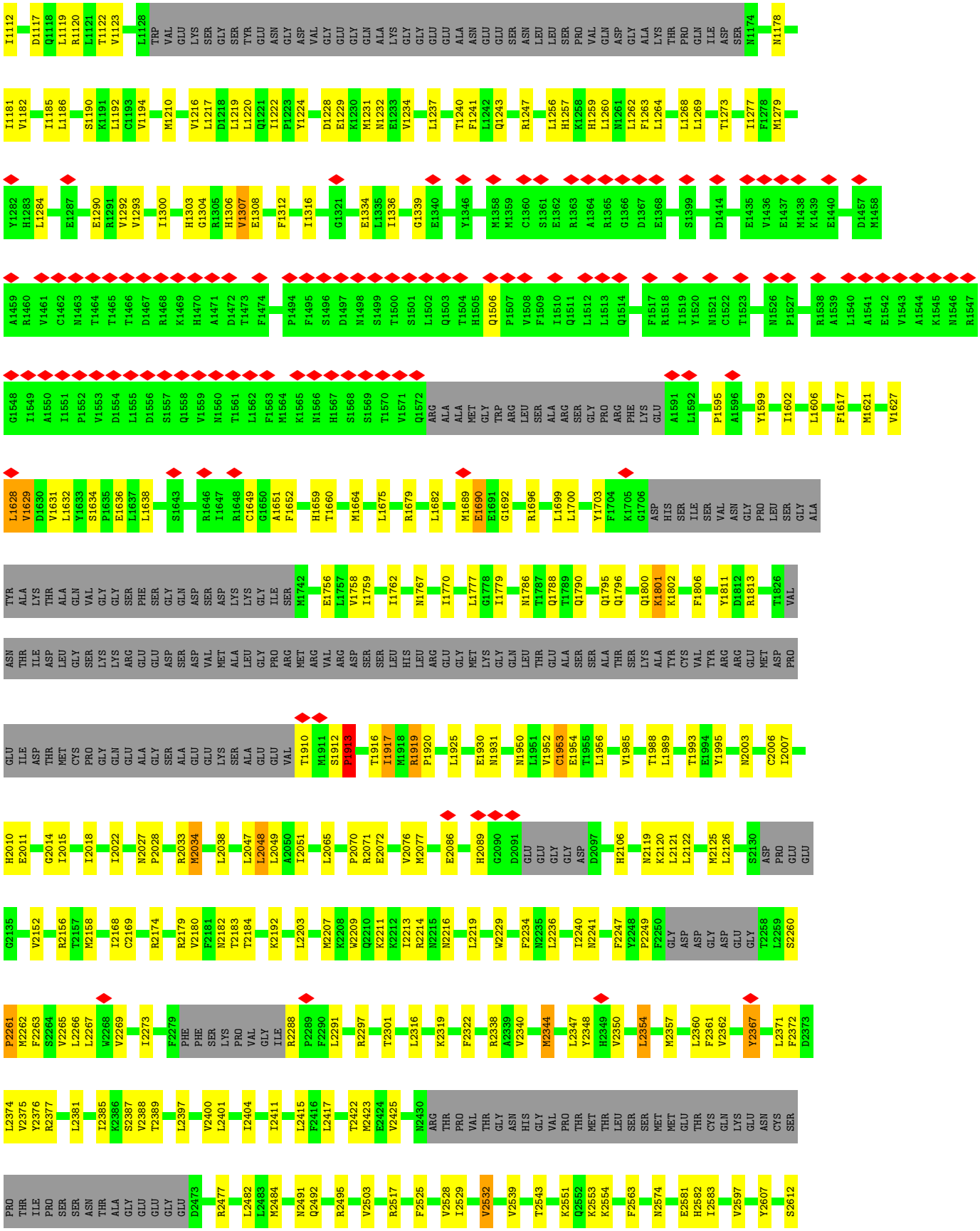
3 Residue-property plots (i)

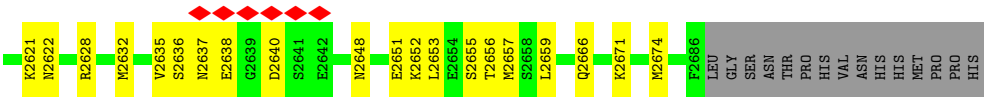
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-gated calcium channel ITPR2

Chain A:

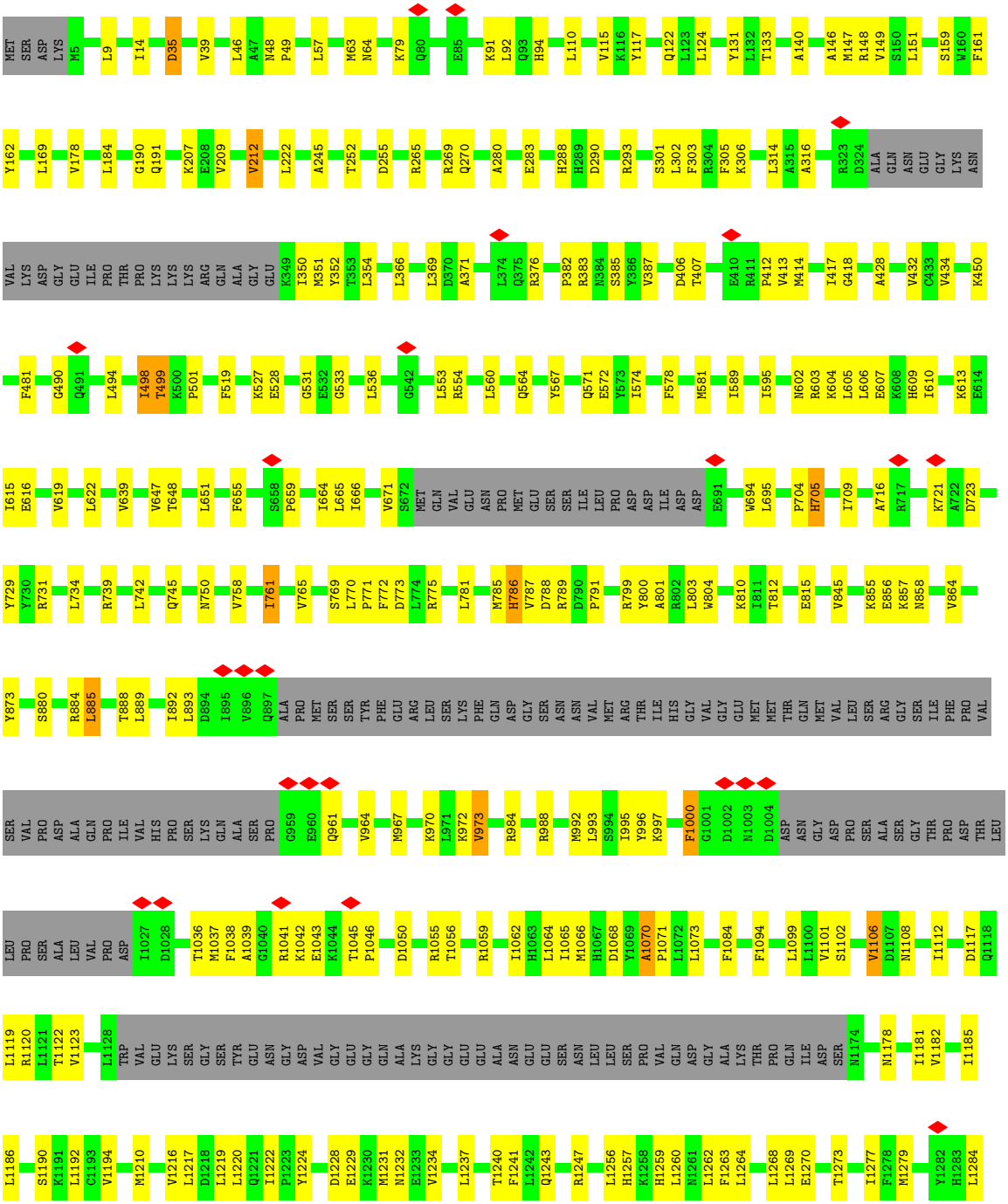


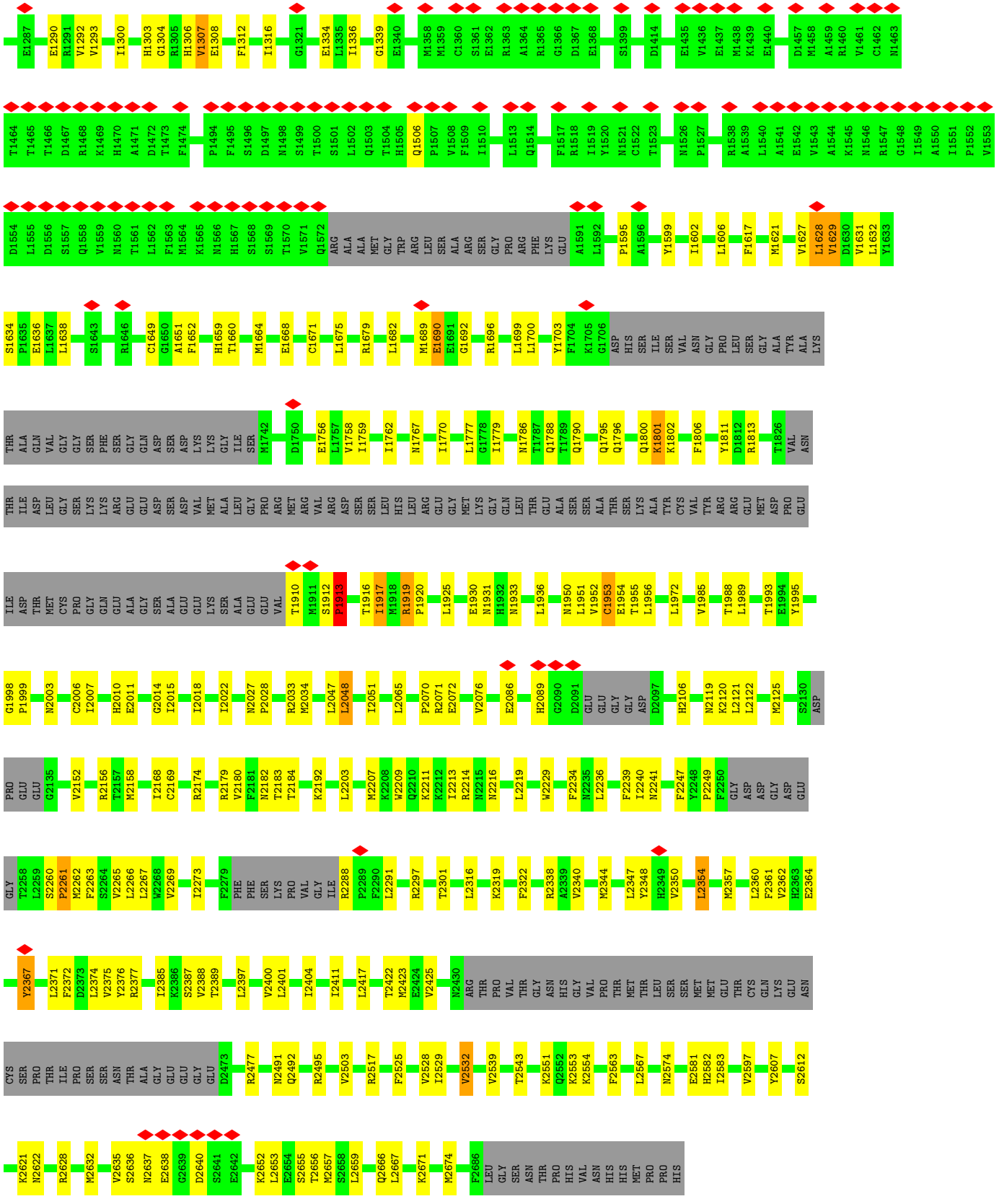




• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

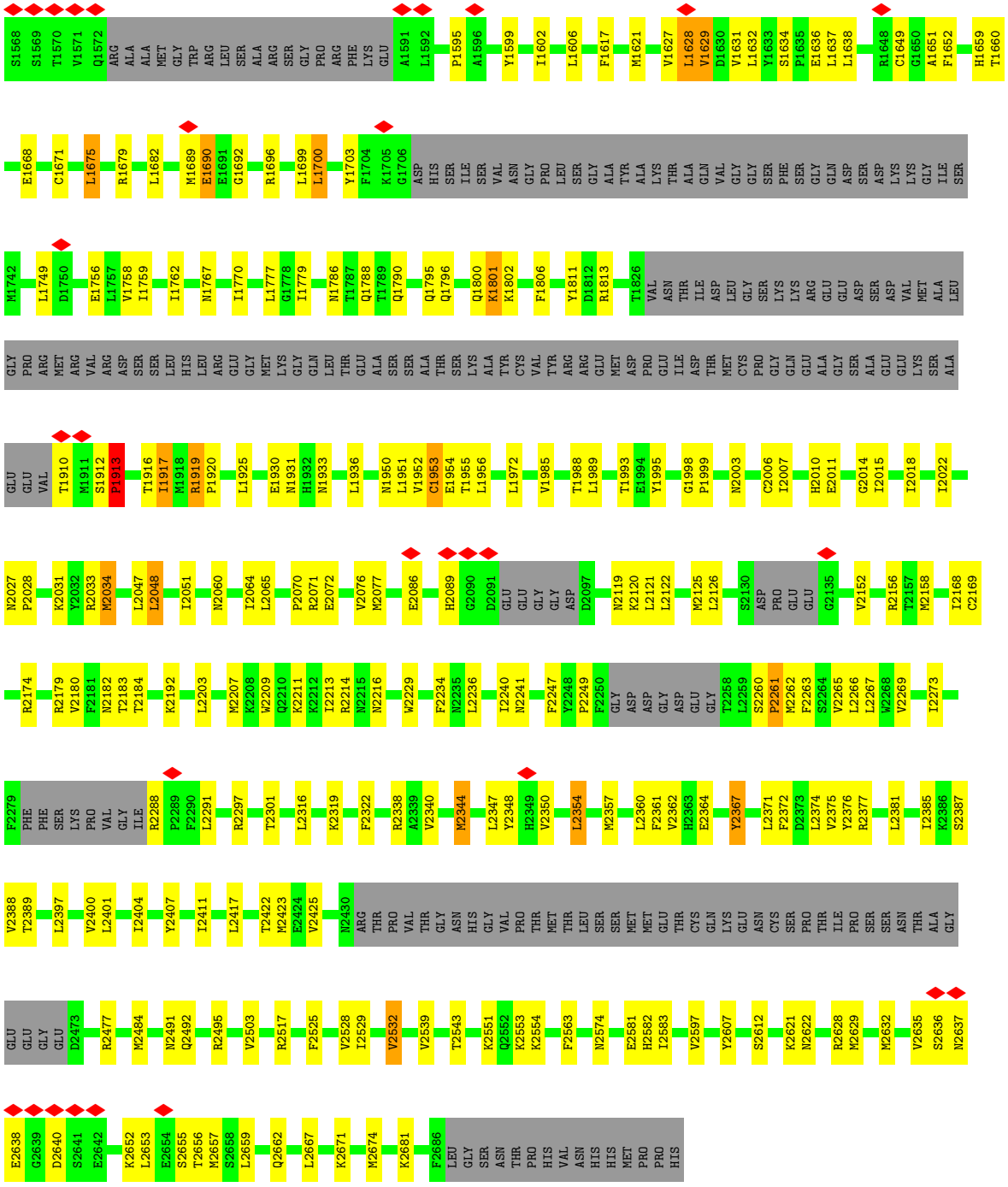
Chain B:





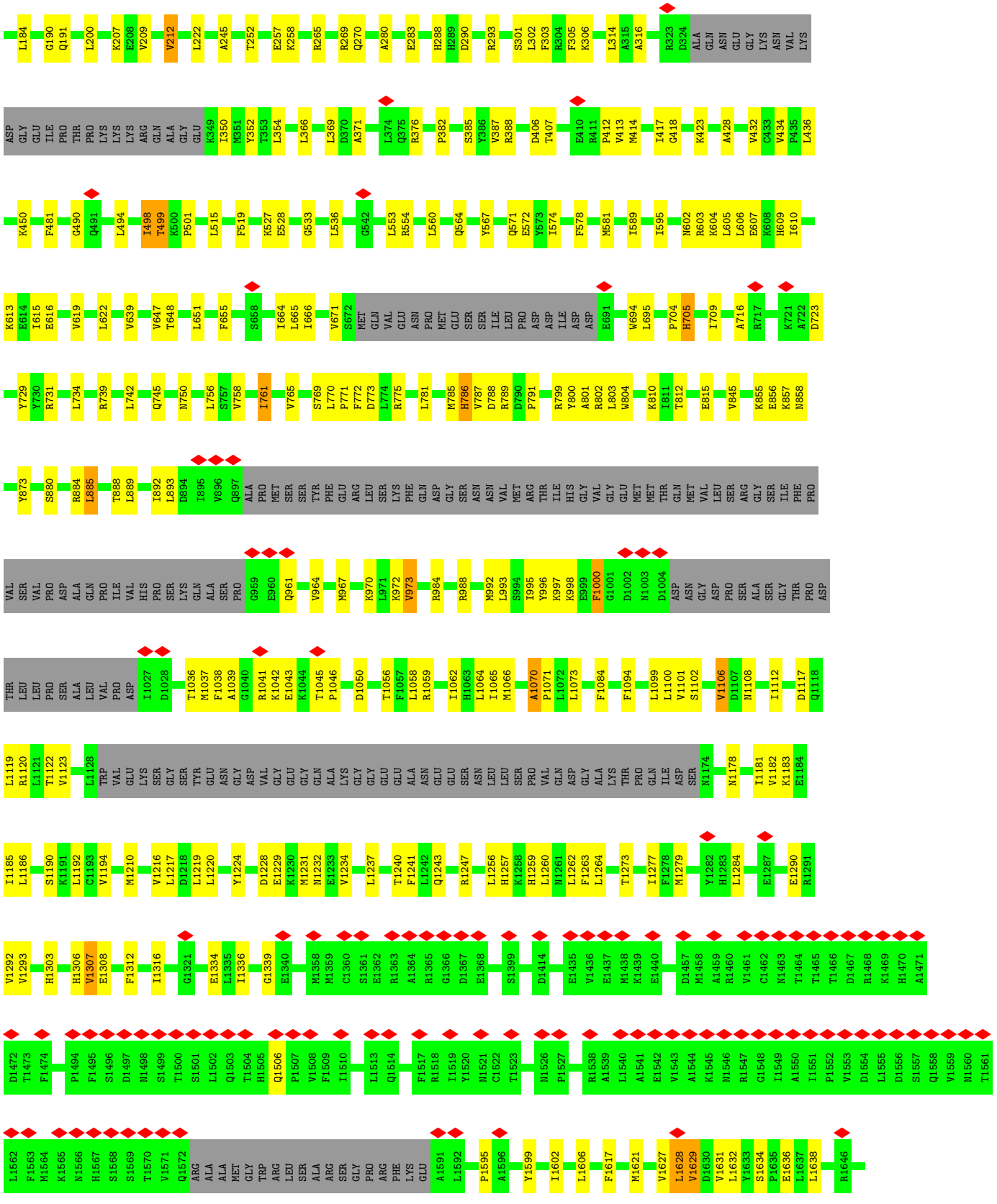
• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

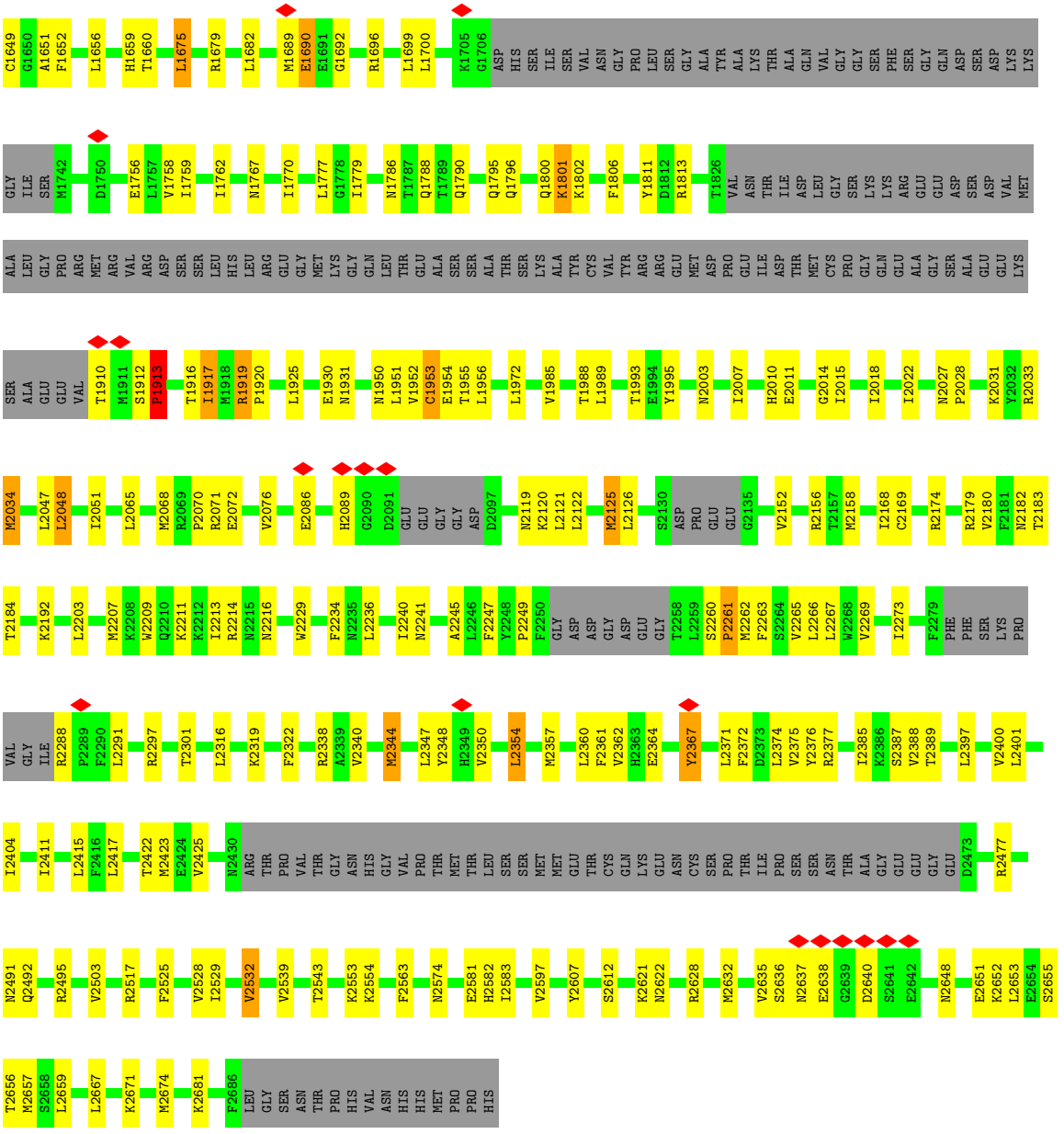
Chain C:



• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain D:




C1649 G1650 A1651 F1652 L1656 H1659 T1660 L1675 R1679 L1682 M1689 E1690 E1691 G1692 R1696 L1699 L1700 K1705 G1706
GLY ILE SER M1742 D1750 E1756 L1757 V1758 I1759 I1762 N1767 I1770 L1777 G1778 I1779 N1786 T1787 Q1788 T1789 Q1790 Q1795 Q1796 Q1800 K1801 K1802 F1806 Y1811 D1812 R1813 T1826
ALA LEU GLY PRO ARG MET ARG VAL ARG ASP SER SER LEU HIS LEU ARG GLU GLY MET LYS GLY GLN LEU THR GLU ALA SER SER ALA THR SER LYS ALA TYR CYS VAL TYR ARG ARG GLU MET ASP PRO GLU ILE ASP THR MET CYS PRO GLY GLN GLU ALA GLY SER ALA GLU GLU LYS
SER ALA GLU GLU VAL T1910 M1911 S1912 P1913 T1916 I1917 M1918 R1919 P1920 L1925 E1930 N1931 N1950 L1951 V1952 C1953 E1954 T1955 L1956 L1972 V1985 T1988 L1989 T1993 E1994 Y1995 N2003 I2007 H2010 E2011 G2014 I2015 I2018 I2022 N2027 P2028 K2031 Y2032 R2033
M2034 L2047 L2048 I2051 L2065 M2068 R2069 P2070 R2071 E2072 V2076 E2086 H2089 G2090 D2091 GLU GLU GLY GLY ASP D2097 N2119 K2120 L2121 L2122 M2125 L2126 S2130 ASP PRO GLU GLU G2135 V2152 R2156 T2157 M2158 I2168 C2169 R2174 R2179 V2180 F2181 N2182 T2183
T2184 K2192 L2203 M2207 K2208 W2209 Q2210 K2211 K2212 I2213 R2214 N2215 N2216 W2229 F2234 N2235 L2236 I2240 N2241 A2245 L2246 F2247 Y2248 P2249 F2250 GLY ASP GLY ASP GLU GLY T2268 L2259 S2260 P2261 M2262 F2263 S2264 V2265 L2266 L2267 W2268 V2269 I2273 F2279 PHE PHE SER LYS PRO
VAL GLY ILE R2288 P2289 F2290 L2291 R2297 T2301 L2316 K2319 F2322 R2338 A2339 V2340 M2344 L2347 Y2348 H2349 V2350 L2354 M2357 L2360 F2361 V2362 H2363 E2364 Y2367 L2371 F2372 D2373 L2374 V2375 Y2376 R2377 I2385 K2386 S2387 V2388 T2389 L2397 V2400 L2401
I2404 I2411 L2415 F2416 L2417 T2422 M2423 E2424 V2425 N2430 ARG THR PRO VAL THR GLY ASN HIS GLY VAL PRO THR MET THR LEU SER SER MET MET GLU THR CYS GLN LYS GLU ASN CYS SER PRO THR ILE PRO SER SER ASN THR ALA GLY GLU GLU GLY GLU D2473 R2477
N2491 Q2492 R2495 V2503 R2517 F2525 V2528 I2529 V2532 V2539 T2543 K2553 K2554 F2563 N2574 E2581 H2582 I2583 V2597 Y2607 S2612 K2621 N2622 R2628 M2632 V2635 S2636 N2637 E2638 G2639 D2640 S2641 E2642 N2648 E2651 K2652 L2653 E2654 S2655
T2656 M2657 S2658 L2659 L2667 K2671 M2674 K2681 F2686 LEU GLY SER ASN THR PRO HIS VAL ASN HIS HIS MET PRO PRO HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	151391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.43, 1.66, 1.43	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46100	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.511	Depositor
Minimum map value	-0.243	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.078	Depositor
Map size (Å)	475.2, 475.2, 475.2	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/18224	0.45	3/24654 (0.0%)
1	B	0.23	0/18224	0.45	3/24654 (0.0%)
1	C	0.23	0/18224	0.45	3/24654 (0.0%)
1	D	0.23	0/18224	0.45	3/24654 (0.0%)
All	All	0.23	0/72896	0.45	12/98616 (0.0%)

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

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1050	ASP	CB-CA-C	-6.01	109.66	116.63
1	A	1050	ASP	CB-CA-C	-6.01	109.66	116.63
1	B	1050	ASP	CB-CA-C	-5.98	109.69	116.63
1	C	1050	ASP	CB-CA-C	-5.97	109.70	116.63
1	A	2261	PRO	N-CA-C	-5.46	106.94	113.98
1	B	2261	PRO	N-CA-C	-5.46	106.94	113.98
1	D	2261	PRO	N-CA-C	-5.46	106.94	113.98
1	C	2261	PRO	N-CA-C	-5.45	106.94	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2640	ASP	CB-CA-C	-5.28	110.47	116.54
1	A	2640	ASP	CB-CA-C	-5.25	110.51	116.54
1	B	2640	ASP	CB-CA-C	-5.25	110.51	116.54
1	D	2640	ASP	CB-CA-C	-5.24	110.51	116.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2174	ARG	Sidechain
1	B	2174	ARG	Sidechain
1	C	2174	ARG	Sidechain
1	D	2174	ARG	Sidechain

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	17922	0	17381	349	0
1	B	17922	0	17381	346	0
1	C	17922	0	17381	349	0
1	D	17922	0	17381	338	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	31	0	12	2	0
3	B	31	0	12	2	0
3	C	31	0	12	2	0
3	D	31	0	12	2	0
4	A	24	0	9	0	0
4	B	24	0	9	0	0
4	C	24	0	9	0	0
4	D	24	0	9	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	A	40	0	58	1	0
6	B	40	0	58	1	0
6	C	40	0	58	1	0
6	D	40	0	58	1	0
All	All	72076	0	69840	1343	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 9.

All (1343) 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:1913:PRO:O	1:D:1916:THR:HG22	1.65	0.97
1:C:1913:PRO:O	1:C:1916:THR:HG22	1.65	0.97
1:B:1913:PRO:O	1:B:1916:THR:HG22	1.65	0.95
1:A:1913:PRO:O	1:A:1916:THR:HG22	1.65	0.95
1:B:91:LYS:HZ2	1:C:1972:LEU:HD23	1.35	0.90
1:D:2357:MET:HA	1:D:2362:VAL:HG11	1.62	0.82
1:C:2357:MET:HA	1:C:2362:VAL:HG11	1.61	0.82
1:A:2357:MET:HA	1:A:2362:VAL:HG11	1.62	0.82
1:B:2357:MET:HA	1:B:2362:VAL:HG11	1.62	0.82
1:B:2260:SER:HB2	1:B:2262:MET:HG2	1.63	0.80
1:C:252:THR:HG22	1:C:280:ALA:HB2	1.64	0.79
1:A:2260:SER:HB2	1:A:2262:MET:HG2	1.63	0.79
1:A:2574:ASN:H	1:C:2628:ARG:HH12	1.29	0.79
1:D:2260:SER:HB2	1:D:2262:MET:HG2	1.63	0.79
1:D:252:THR:HG22	1:D:280:ALA:HB2	1.64	0.78
1:C:2260:SER:HB2	1:C:2262:MET:HG2	1.63	0.78
1:A:252:THR:HG22	1:A:280:ALA:HB2	1.64	0.77
1:A:1916:THR:O	1:A:1920:PRO:HD2	1.85	0.77
1:C:1916:THR:O	1:C:1920:PRO:HD2	1.85	0.77
1:B:252:THR:HG22	1:B:280:ALA:HB2	1.64	0.77
1:D:1916:THR:O	1:D:1920:PRO:HD2	1.85	0.77
1:B:1916:THR:O	1:B:1920:PRO:HD2	1.85	0.77
1:C:1101:VAL:HG13	1:C:1102:SER:H	1.50	0.77
1:A:1101:VAL:HG13	1:A:1102:SER:H	1.50	0.76
1:D:1101:VAL:HG13	1:D:1102:SER:H	1.50	0.75
1:B:1101:VAL:HG13	1:B:1102:SER:H	1.50	0.75
1:B:2492:GLN:HB3	1:B:2503:VAL:HG21	1.70	0.74
1:C:2492:GLN:HB3	1:C:2503:VAL:HG21	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ILE:O	1:B:578:PHE:HB3	1.88	0.73
1:A:2492:GLN:HB3	1:A:2503:VAL:HG21	1.70	0.73
1:D:2070:PRO:HB3	1:D:2122:LEU:HD22	1.71	0.73
1:C:2070:PRO:HB3	1:C:2122:LEU:HD22	1.71	0.73
1:A:2070:PRO:HB3	1:A:2122:LEU:HD22	1.71	0.73
1:D:2492:GLN:HB3	1:D:2503:VAL:HG21	1.70	0.73
1:B:2070:PRO:HB3	1:B:2122:LEU:HD22	1.71	0.72
1:A:574:ILE:O	1:A:578:PHE:HB3	1.88	0.72
1:D:574:ILE:O	1:D:578:PHE:HB3	1.88	0.72
1:C:574:ILE:O	1:C:578:PHE:HB3	1.88	0.72
1:D:803:LEU:HD23	1:D:1101:VAL:HG23	1.71	0.71
1:B:803:LEU:HD23	1:B:1101:VAL:HG23	1.71	0.70
1:B:2574:ASN:H	1:D:2628:ARG:HH12	1.39	0.70
1:A:803:LEU:HD23	1:A:1101:VAL:HG23	1.72	0.70
1:A:1066:MET:HE1	1:A:1652:PHE:HB2	1.74	0.70
1:A:2234:PHE:HE1	1:A:2374:LEU:HD13	1.57	0.70
1:D:1066:MET:HE1	1:D:1652:PHE:HB2	1.74	0.70
1:C:1066:MET:HE1	1:C:1652:PHE:HB2	1.74	0.70
1:C:803:LEU:HD23	1:C:1101:VAL:HG23	1.72	0.70
1:D:2234:PHE:HE1	1:D:2374:LEU:HD13	1.57	0.69
1:B:428:ALA:HB2	1:D:169:LEU:HD22	1.74	0.69
1:B:1066:MET:HE1	1:B:1652:PHE:HB2	1.74	0.69
1:C:2234:PHE:HE1	1:C:2374:LEU:HD13	1.57	0.69
1:B:810:LYS:HE2	1:B:810:LYS:HA	1.75	0.69
1:B:639:VAL:HG21	1:B:742:LEU:HD21	1.75	0.69
1:D:639:VAL:HG21	1:D:742:LEU:HD21	1.75	0.68
1:B:2234:PHE:HE1	1:B:2374:LEU:HD13	1.57	0.68
1:A:639:VAL:HG21	1:A:742:LEU:HD21	1.75	0.68
1:C:639:VAL:HG21	1:C:742:LEU:HD21	1.75	0.68
1:D:810:LYS:HA	1:D:810:LYS:HE2	1.75	0.68
1:C:1240:THR:HA	1:C:1243:GLN:HG2	1.76	0.68
1:A:2180:VAL:HG21	1:A:2203:LEU:HD11	1.76	0.67
1:A:810:LYS:HE2	1:A:810:LYS:HA	1.75	0.67
1:C:810:LYS:HE2	1:C:810:LYS:HA	1.75	0.67
1:B:2180:VAL:HG21	1:B:2203:LEU:HD11	1.76	0.67
1:D:1240:THR:HA	1:D:1243:GLN:HG2	1.76	0.67
1:D:63:MET:HE2	1:D:63:MET:HA	1.77	0.67
1:A:428:ALA:HB2	1:C:169:LEU:HD22	1.77	0.67
1:B:63:MET:HE2	1:B:63:MET:HA	1.77	0.67
1:A:845:VAL:HG23	1:A:857:LYS:HE2	1.77	0.66
1:A:1240:THR:HA	1:A:1243:GLN:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2180:VAL:HG21	1:D:2203:LEU:HD11	1.76	0.66
1:C:845:VAL:HG23	1:C:857:LYS:HE2	1.77	0.66
1:A:63:MET:HA	1:A:63:MET:HE2	1.77	0.66
1:A:2628:ARG:HH12	1:D:2574:ASN:H	1.44	0.66
1:C:2180:VAL:HG21	1:C:2203:LEU:HD11	1.76	0.66
1:A:622:LEU:HD12	1:A:664:ILE:HG21	1.78	0.66
1:B:1240:THR:HA	1:B:1243:GLN:HG2	1.76	0.66
1:D:622:LEU:HD12	1:D:664:ILE:HG21	1.78	0.66
1:A:14:ILE:HG22	1:A:57:LEU:HD12	1.78	0.65
1:A:2241:ASN:HD22	1:A:2371:LEU:HD22	1.61	0.65
1:C:63:MET:HE2	1:C:63:MET:HA	1.77	0.65
1:D:2241:ASN:HD22	1:D:2371:LEU:HD22	1.61	0.65
1:D:369:LEU:HD12	1:D:387:VAL:HG21	1.79	0.65
1:C:1056:THR:HA	1:C:1059:ARG:HD3	1.79	0.65
1:D:845:VAL:HG23	1:D:857:LYS:HE2	1.77	0.65
1:A:606:LEU:O	1:A:610:ILE:HG13	1.97	0.65
1:A:885:LEU:HD13	1:A:889:LEU:HD13	1.78	0.65
1:C:885:LEU:HD13	1:C:889:LEU:HD13	1.78	0.65
1:B:622:LEU:HD12	1:B:664:ILE:HG21	1.78	0.65
1:C:606:LEU:O	1:C:610:ILE:HG13	1.97	0.65
1:A:2354:LEU:HA	1:A:2357:MET:HB2	1.79	0.65
1:D:606:LEU:O	1:D:610:ILE:HG13	1.97	0.65
1:A:1800:GLN:O	1:A:1801:LYS:C	2.40	0.65
1:B:845:VAL:HG23	1:B:857:LYS:HE2	1.77	0.65
1:B:1800:GLN:O	1:B:1801:LYS:C	2.40	0.65
1:B:14:ILE:HG22	1:B:57:LEU:HD12	1.78	0.65
1:B:369:LEU:HD12	1:B:387:VAL:HG21	1.79	0.65
1:C:622:LEU:HD12	1:C:664:ILE:HG21	1.78	0.65
1:A:1056:THR:HA	1:A:1059:ARG:HD3	1.79	0.64
1:C:14:ILE:HG22	1:C:57:LEU:HD12	1.78	0.64
1:A:2652:LYS:HB2	1:C:2653:LEU:HD12	1.79	0.64
1:B:885:LEU:HD13	1:B:889:LEU:HD13	1.78	0.64
1:B:2241:ASN:HD22	1:B:2371:LEU:HD22	1.61	0.64
1:D:14:ILE:HG22	1:D:57:LEU:HD12	1.78	0.64
1:D:1800:GLN:O	1:D:1801:LYS:C	2.40	0.64
1:D:885:LEU:HD13	1:D:889:LEU:HD13	1.78	0.64
1:B:1056:THR:HA	1:B:1059:ARG:HD3	1.79	0.64
1:D:2120:LYS:HE2	1:D:2120:LYS:HA	1.80	0.64
1:B:606:LEU:O	1:B:610:ILE:HG13	1.97	0.64
1:C:2241:ASN:HD22	1:C:2371:LEU:HD22	1.61	0.64
1:A:369:LEU:HD12	1:A:387:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2574:ASN:HA	1:C:2628:ARG:HH22	1.63	0.64
1:B:2354:LEU:HA	1:B:2357:MET:HB2	1.79	0.64
1:C:369:LEU:HD12	1:C:387:VAL:HG21	1.79	0.64
1:A:799:ARG:HD2	1:A:800:TYR:H	1.63	0.64
1:C:799:ARG:HD2	1:C:800:TYR:H	1.63	0.64
1:C:1800:GLN:O	1:C:1801:LYS:C	2.40	0.64
1:D:2354:LEU:HA	1:D:2357:MET:HB2	1.79	0.63
1:B:799:ARG:HD2	1:B:800:TYR:H	1.63	0.63
1:A:1627:VAL:HG21	1:A:1696:ARG:HG2	1.81	0.63
1:D:1627:VAL:HG21	1:D:1696:ARG:HG2	1.80	0.63
1:C:1627:VAL:HG21	1:C:1696:ARG:HG2	1.81	0.63
1:A:1037:MET:HE2	1:A:1037:MET:HA	1.81	0.63
1:A:169:LEU:HD22	1:D:428:ALA:HB2	1.79	0.63
1:B:2120:LYS:HE2	1:B:2120:LYS:HA	1.80	0.63
1:C:2354:LEU:HA	1:C:2357:MET:HB2	1.79	0.63
1:A:2120:LYS:HA	1:A:2120:LYS:HE2	1.80	0.62
1:D:1056:THR:HA	1:D:1059:ARG:HD3	1.79	0.62
1:B:1627:VAL:HG21	1:B:1696:ARG:HG2	1.81	0.62
1:D:786:HIS:O	1:D:787:VAL:HG22	2.00	0.62
1:A:2065:LEU:HD13	1:A:2119:ASN:HD22	1.64	0.62
1:B:1037:MET:HA	1:B:1037:MET:HE2	1.81	0.62
1:C:1217:LEU:HD12	1:C:1262:LEU:HD23	1.82	0.62
1:B:1217:LEU:HD12	1:B:1262:LEU:HD23	1.82	0.62
1:C:2120:LYS:HE2	1:C:2120:LYS:HA	1.80	0.62
1:A:786:HIS:O	1:A:787:VAL:HG22	2.00	0.62
1:C:2065:LEU:HD13	1:C:2119:ASN:HD22	1.64	0.62
1:A:1217:LEU:HD12	1:A:1262:LEU:HD23	1.82	0.62
1:D:1217:LEU:HD12	1:D:1262:LEU:HD23	1.82	0.62
1:D:799:ARG:HD2	1:D:800:TYR:H	1.63	0.62
1:B:786:HIS:O	1:B:787:VAL:HG22	1.99	0.61
1:B:2065:LEU:HD13	1:B:2119:ASN:HD22	1.64	0.61
1:C:1037:MET:HE2	1:C:1037:MET:HA	1.81	0.61
1:C:786:HIS:O	1:C:787:VAL:HG22	2.00	0.61
1:C:2260:SER:HB3	1:C:2261:PRO:HD2	1.82	0.61
1:D:1037:MET:HA	1:D:1037:MET:HE2	1.80	0.61
1:A:1952:VAL:HG12	1:A:1995:TYR:CD2	2.36	0.61
1:C:761:ILE:O	1:C:765:VAL:HG12	2.01	0.61
1:B:2417:LEU:HD11	1:B:2517:ARG:HD3	1.82	0.61
1:D:2065:LEU:HD13	1:D:2119:ASN:HD22	1.64	0.61
1:B:1652:PHE:HD1	1:B:1652:PHE:O	1.83	0.61
1:D:564:GLN:HB3	1:D:574:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:761:ILE:O	1:D:765:VAL:HG12	2.01	0.61
1:D:1652:PHE:HD1	1:D:1652:PHE:O	1.83	0.61
1:B:1952:VAL:HG12	1:B:1995:TYR:CD2	2.36	0.61
1:C:564:GLN:HB3	1:C:574:ILE:HD12	1.82	0.61
1:C:2417:LEU:HD11	1:C:2517:ARG:HD3	1.82	0.61
1:A:761:ILE:O	1:A:765:VAL:HG12	2.01	0.61
1:A:1652:PHE:O	1:A:1652:PHE:HD1	1.83	0.61
1:B:290:ASP:HB3	1:B:293:ARG:HB2	1.83	0.61
1:B:639:VAL:HB	1:B:739:ARG:HD2	1.83	0.61
1:B:2260:SER:HB3	1:B:2261:PRO:HD2	1.83	0.61
1:C:1652:PHE:HD1	1:C:1652:PHE:O	1.83	0.61
1:C:1952:VAL:HG12	1:C:1995:TYR:CD2	2.36	0.61
1:A:290:ASP:HB3	1:A:293:ARG:HB2	1.83	0.61
1:D:1952:VAL:HG12	1:D:1995:TYR:CD2	2.36	0.61
1:D:2273:ILE:HG22	6:D:2805:PLX:H102	1.83	0.60
1:A:371:ALA:HB3	1:A:376:ARG:HD3	1.83	0.60
1:B:761:ILE:O	1:B:765:VAL:HG12	2.01	0.60
1:C:1762:ILE:HD11	1:C:1806:PHE:HE1	1.66	0.60
1:B:564:GLN:HB3	1:B:574:ILE:HD12	1.82	0.60
1:A:2417:LEU:HD11	1:A:2517:ARG:HD3	1.82	0.60
1:B:2273:ILE:HG22	6:B:2805:PLX:H102	1.83	0.60
1:A:2260:SER:HB3	1:A:2261:PRO:HD2	1.83	0.60
1:A:564:GLN:HB3	1:A:574:ILE:HD12	1.82	0.60
1:D:639:VAL:HB	1:D:739:ARG:HD2	1.83	0.60
1:A:2273:ILE:HG22	6:A:2805:PLX:H102	1.83	0.60
1:B:161:PHE:HD2	1:B:184:LEU:HB3	1.67	0.60
1:C:2273:ILE:HG22	6:C:2805:PLX:H102	1.83	0.60
1:C:1756:GLU:HA	1:C:1759:ILE:HG12	1.83	0.60
1:A:1919:ARG:HB2	1:A:1920:PRO:HD3	1.84	0.60
1:C:639:VAL:HB	1:C:739:ARG:HD2	1.83	0.60
1:D:371:ALA:HB3	1:D:376:ARG:HD3	1.83	0.60
1:D:1756:GLU:HA	1:D:1759:ILE:HG12	1.83	0.60
1:D:1762:ILE:HD11	1:D:1806:PHE:HE1	1.66	0.60
1:B:371:ALA:HB3	1:B:376:ARG:HD3	1.83	0.59
1:D:2417:LEU:HD11	1:D:2517:ARG:HD3	1.82	0.59
1:D:2260:SER:HB3	1:D:2261:PRO:HD2	1.83	0.59
1:B:1756:GLU:HA	1:B:1759:ILE:HG12	1.83	0.59
1:B:1762:ILE:HD11	1:B:1806:PHE:HE1	1.66	0.59
1:C:290:ASP:HB3	1:C:293:ARG:HB2	1.83	0.59
1:D:1919:ARG:HB2	1:D:1920:PRO:HD3	1.84	0.59
1:C:371:ALA:HB3	1:C:376:ARG:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2014:GLY:O	1:D:2018:ILE:HG22	2.02	0.59
1:B:169:LEU:HD22	1:C:428:ALA:HB2	1.84	0.59
1:C:1919:ARG:HB2	1:C:1920:PRO:HD3	1.84	0.59
1:D:161:PHE:HD2	1:D:184:LEU:HB3	1.67	0.59
1:A:161:PHE:HD2	1:A:184:LEU:HB3	1.67	0.59
1:B:1919:ARG:HB2	1:B:1920:PRO:HD3	1.84	0.59
1:B:2007:ILE:HG22	1:B:2015:ILE:HD11	1.85	0.59
1:C:2014:GLY:O	1:C:2018:ILE:HG22	2.02	0.59
1:D:622:LEU:HB3	1:D:664:ILE:HD13	1.85	0.59
1:A:639:VAL:HB	1:A:739:ARG:HD2	1.83	0.59
1:D:1913:PRO:O	1:D:1916:THR:CG2	2.48	0.59
1:C:161:PHE:HD2	1:C:184:LEU:HB3	1.67	0.59
1:D:1675:LEU:HD12	1:D:1777:LEU:HD22	1.85	0.59
1:A:91:LYS:HZ2	1:D:1972:LEU:HD23	1.68	0.58
1:C:1675:LEU:HD12	1:C:1777:LEU:HD22	1.85	0.58
1:A:622:LEU:HB3	1:A:664:ILE:HD13	1.85	0.58
1:B:2014:GLY:O	1:B:2018:ILE:HG22	2.02	0.58
1:A:1756:GLU:HA	1:A:1759:ILE:HG12	1.83	0.58
1:A:1762:ILE:HD11	1:A:1806:PHE:HE1	1.66	0.58
1:A:2014:GLY:O	1:A:2018:ILE:HG22	2.02	0.58
1:D:2007:ILE:HG22	1:D:2015:ILE:HD11	1.85	0.58
1:C:1629:VAL:O	1:C:1632:LEU:HG	2.04	0.58
1:D:290:ASP:HB3	1:D:293:ARG:HB2	1.83	0.58
1:D:734:LEU:HD22	1:D:781:LEU:HD22	1.85	0.58
1:A:1629:VAL:O	1:A:1632:LEU:HG	2.04	0.58
1:C:622:LEU:HB3	1:C:664:ILE:HD13	1.85	0.58
1:A:1675:LEU:HD12	1:A:1777:LEU:HD22	1.85	0.58
1:A:382:PRO:HG2	1:A:385:SER:HB3	1.86	0.57
1:B:622:LEU:HB3	1:B:664:ILE:HD13	1.85	0.57
1:B:734:LEU:HD22	1:B:781:LEU:HD22	1.85	0.57
1:C:2007:ILE:HG22	1:C:2015:ILE:HD11	1.85	0.57
1:A:734:LEU:HD22	1:A:781:LEU:HD22	1.85	0.57
1:C:2371:LEU:HD12	1:C:2374:LEU:HD11	1.86	0.57
1:B:382:PRO:HG2	1:B:385:SER:HB3	1.86	0.57
1:C:382:PRO:HG2	1:C:385:SER:HB3	1.86	0.57
1:B:2628:ARG:HH12	1:C:2574:ASN:H	1.52	0.57
1:D:354:LEU:HD21	1:D:417:ILE:HG13	1.86	0.57
1:D:1679:ARG:HH11	1:D:1679:ARG:HG2	1.69	0.57
1:A:2007:ILE:HG22	1:A:2015:ILE:HD11	1.85	0.57
1:B:1679:ARG:HG2	1:B:1679:ARG:HH11	1.69	0.57
1:D:1260:LEU:HD22	1:D:1263:PHE:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2319:LYS:HE3	1:A:2350:VAL:HG11	1.86	0.57
1:B:2411:ILE:HD13	1:C:2364:GLU:HG3	1.87	0.57
1:C:2319:LYS:HE3	1:C:2350:VAL:HG11	1.86	0.57
1:D:2071:ARG:HG2	1:D:2125:MET:HE1	1.87	0.57
1:A:2071:ARG:HG2	1:A:2125:MET:HE1	1.87	0.57
1:B:1629:VAL:O	1:B:1632:LEU:HG	2.04	0.57
1:B:1675:LEU:HD12	1:B:1777:LEU:HD22	1.85	0.57
1:A:2671:LYS:HA	1:A:2674:MET:HG3	1.87	0.57
1:B:1260:LEU:HD22	1:B:1263:PHE:HB2	1.87	0.57
1:B:2319:LYS:HE3	1:B:2350:VAL:HG11	1.86	0.57
1:C:354:LEU:HD21	1:C:417:ILE:HG13	1.86	0.57
1:C:734:LEU:HD22	1:C:781:LEU:HD22	1.85	0.57
1:B:2071:ARG:HG2	1:B:2125:MET:HE1	1.87	0.56
1:D:382:PRO:HG2	1:D:385:SER:HB3	1.86	0.56
1:D:1675:LEU:HD23	1:D:1770:ILE:HD11	1.87	0.56
1:A:1679:ARG:HH11	1:A:1679:ARG:HG2	1.69	0.56
1:A:2574:ASN:ND2	1:C:2629:MET:HE1	2.19	0.56
1:B:2371:LEU:HD12	1:B:2374:LEU:HD11	1.86	0.56
1:A:1925:LEU:HB3	1:A:1995:TYR:OH	2.06	0.56
1:A:2371:LEU:HD12	1:A:2374:LEU:HD11	1.86	0.56
1:B:354:LEU:HD21	1:B:417:ILE:HG13	1.86	0.56
1:C:1679:ARG:HG2	1:C:1679:ARG:HH11	1.69	0.56
1:D:772:PHE:HB2	1:D:856:GLU:HB3	1.87	0.56
1:D:1629:VAL:O	1:D:1632:LEU:HG	2.04	0.56
1:D:2671:LYS:HA	1:D:2674:MET:HG3	1.87	0.56
1:A:354:LEU:HD21	1:A:417:ILE:HG13	1.86	0.56
1:A:772:PHE:HB2	1:A:856:GLU:HB3	1.87	0.56
1:D:2319:LYS:HE3	1:D:2350:VAL:HG11	1.86	0.56
1:C:2637:ASN:O	1:C:2638:GLU:HG3	2.06	0.56
1:D:2371:LEU:HD12	1:D:2374:LEU:HD11	1.86	0.56
1:B:1627:VAL:HG13	1:B:1628:LEU:HD23	1.87	0.56
1:B:2574:ASN:HA	1:D:2628:ARG:HH22	1.69	0.56
1:C:1595:PRO:HA	1:C:1599:TYR:HB2	1.88	0.56
1:B:1660:THR:HG22	1:B:1660:THR:O	2.06	0.56
1:B:2637:ASN:O	1:B:2638:GLU:HG3	2.06	0.56
1:B:2652:LYS:HB2	1:D:2653:LEU:HD12	1.88	0.56
1:C:481:PHE:HE1	1:C:490:GLY:HA3	1.71	0.56
1:D:1925:LEU:HB3	1:D:1995:TYR:OH	2.06	0.56
1:B:481:PHE:HE1	1:B:490:GLY:HA3	1.71	0.56
1:D:1660:THR:O	1:D:1660:THR:HG22	2.06	0.56
1:A:481:PHE:HE1	1:A:490:GLY:HA3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1627:VAL:HG13	1:A:1628:LEU:HD23	1.87	0.56
1:A:1675:LEU:HD23	1:A:1770:ILE:HD11	1.87	0.56
1:A:750:ASN:HD21	1:A:789:ARG:HD2	1.71	0.56
1:B:1925:LEU:HB3	1:B:1995:TYR:OH	2.06	0.56
1:B:2671:LYS:HA	1:B:2674:MET:HG3	1.87	0.56
1:C:407:THR:HG23	1:C:412:PRO:HA	1.88	0.56
1:C:1925:LEU:HB3	1:C:1995:TYR:OH	2.06	0.56
1:C:2071:ARG:HG2	1:C:2125:MET:HE1	1.86	0.56
1:A:407:THR:HG23	1:A:412:PRO:HA	1.88	0.55
1:B:772:PHE:HB2	1:B:856:GLU:HB3	1.87	0.55
1:C:1627:VAL:HG13	1:C:1628:LEU:HD23	1.87	0.55
1:C:1913:PRO:O	1:C:1916:THR:CG2	2.48	0.55
1:B:1675:LEU:HD23	1:B:1770:ILE:HD11	1.87	0.55
1:C:1260:LEU:HD22	1:C:1263:PHE:HB2	1.87	0.55
1:C:1675:LEU:HD23	1:C:1770:ILE:HD11	1.87	0.55
1:D:481:PHE:HE1	1:D:490:GLY:HA3	1.71	0.55
1:A:1913:PRO:O	1:A:1916:THR:CG2	2.48	0.55
1:D:750:ASN:HD21	1:D:789:ARG:HD2	1.71	0.55
1:D:1595:PRO:HA	1:D:1599:TYR:HB2	1.88	0.55
1:B:572:GLU:HG2	1:B:605:LEU:HD13	1.89	0.55
1:C:1660:THR:HG22	1:C:1660:THR:O	2.06	0.55
1:B:1913:PRO:O	1:B:1916:THR:CG2	2.48	0.55
1:C:572:GLU:HG2	1:C:605:LEU:HD13	1.89	0.55
1:C:2671:LYS:HA	1:C:2674:MET:HG3	1.87	0.55
1:C:772:PHE:HB2	1:C:856:GLU:HB3	1.87	0.55
1:D:2637:ASN:O	1:D:2638:GLU:HG3	2.06	0.55
1:A:572:GLU:HG2	1:A:605:LEU:HD13	1.89	0.55
1:D:758:VAL:HG11	1:D:785:MET:HE3	1.88	0.55
1:A:758:VAL:HG11	1:A:785:MET:HE3	1.88	0.55
1:A:1260:LEU:HD22	1:A:1263:PHE:HB2	1.87	0.55
1:A:2637:ASN:O	1:A:2638:GLU:HG3	2.06	0.55
1:B:407:THR:HG23	1:B:412:PRO:HA	1.88	0.55
1:B:758:VAL:HG11	1:B:785:MET:HE3	1.88	0.55
1:B:2072:GLU:O	1:B:2076:VAL:HG12	2.07	0.55
1:D:1627:VAL:HG13	1:D:1628:LEU:HD23	1.87	0.55
1:A:1595:PRO:HA	1:A:1599:TYR:HB2	1.88	0.54
1:C:553:LEU:HD12	1:C:589:ILE:HD13	1.90	0.54
1:D:572:GLU:HG2	1:D:605:LEU:HD13	1.89	0.54
1:B:1800:GLN:O	1:B:1802:LYS:N	2.41	0.54
1:C:750:ASN:HD21	1:C:789:ARG:HD2	1.71	0.54
1:D:2072:GLU:O	1:D:2076:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1660:THR:HG22	1:A:1660:THR:O	2.06	0.54
1:B:553:LEU:HD12	1:B:589:ILE:HD13	1.90	0.54
1:B:2169:CYS:SG	1:B:2207:MET:HE1	2.47	0.54
1:B:2607:TYR:HB3	1:B:2612:SER:HB2	1.90	0.54
1:A:1070:ALA:HB3	1:A:1071:PRO:HD3	1.90	0.54
1:A:2234:PHE:CE1	1:A:2374:LEU:HD13	2.41	0.54
1:B:1595:PRO:HA	1:B:1599:TYR:HB2	1.87	0.54
1:D:407:THR:HG23	1:D:412:PRO:HA	1.88	0.54
1:A:178:VAL:HG11	1:A:222:LEU:HD13	1.90	0.54
1:C:2169:CYS:SG	1:C:2207:MET:HE1	2.47	0.54
1:D:2169:CYS:SG	1:D:2207:MET:HE1	2.47	0.54
1:B:1679:ARG:HG2	1:B:1679:ARG:NH1	2.23	0.54
1:C:2234:PHE:CE1	1:C:2374:LEU:HD13	2.41	0.54
1:D:2607:TYR:HB3	1:D:2612:SER:HB2	1.90	0.54
1:A:2072:GLU:O	1:A:2076:VAL:HG12	2.07	0.54
1:B:1056:THR:HG23	1:B:1059:ARG:NH1	2.23	0.54
1:C:178:VAL:HG11	1:C:222:LEU:HD13	1.90	0.54
1:C:758:VAL:HG11	1:C:785:MET:HE3	1.88	0.54
1:C:2072:GLU:O	1:C:2076:VAL:HG12	2.07	0.54
1:D:553:LEU:HD12	1:D:589:ILE:HD13	1.90	0.54
1:D:1070:ALA:HB3	1:D:1071:PRO:HD3	1.90	0.54
1:B:178:VAL:HG11	1:B:222:LEU:HD13	1.90	0.54
1:B:750:ASN:HD21	1:B:789:ARG:HD2	1.71	0.54
1:D:1800:GLN:O	1:D:1802:LYS:N	2.41	0.54
1:D:2635:VAL:HG22	1:D:2636:SER:H	1.73	0.54
1:D:2652:LYS:HD3	1:D:2655:SER:HB3	1.89	0.54
1:A:1800:GLN:O	1:A:1802:LYS:N	2.41	0.54
1:A:770:LEU:HB2	1:A:771:PRO:HD3	1.90	0.53
1:B:770:LEU:HB2	1:B:771:PRO:HD3	1.90	0.53
1:C:2635:VAL:HG22	1:C:2636:SER:H	1.73	0.53
1:D:992:MET:HB3	1:D:1094:PHE:HE1	1.73	0.53
1:A:35:ASP:HB2	1:A:151:LEU:HB2	1.91	0.53
1:A:1056:THR:HG23	1:A:1059:ARG:NH1	2.23	0.53
1:A:2635:VAL:HG22	1:A:2636:SER:H	1.73	0.53
1:B:35:ASP:HB2	1:B:151:LEU:HB2	1.91	0.53
1:B:2652:LYS:HD3	1:B:2655:SER:HB3	1.89	0.53
1:C:1056:THR:HG23	1:C:1059:ARG:NH1	2.23	0.53
1:C:1930:GLU:OE1	1:C:1931:ASN:HB2	2.09	0.53
1:C:2652:LYS:HD3	1:C:2655:SER:HB3	1.89	0.53
1:D:772:PHE:HA	1:D:775:ARG:HD3	1.90	0.53
1:A:2607:TYR:HB3	1:A:2612:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:992:MET:HB3	1:B:1094:PHE:HE1	1.73	0.53
1:B:1070:ALA:HB3	1:B:1071:PRO:HD3	1.90	0.53
1:B:1306:HIS:O	1:B:1307:VAL:HG12	2.09	0.53
1:A:91:LYS:NZ	1:D:1972:LEU:HD23	2.23	0.53
1:B:2635:VAL:HG22	1:B:2636:SER:H	1.73	0.53
1:C:770:LEU:HB2	1:C:771:PRO:HD3	1.90	0.53
1:A:553:LEU:HD12	1:A:589:ILE:HD13	1.90	0.53
1:A:1101:VAL:HG13	1:A:1102:SER:N	2.22	0.53
1:A:1930:GLU:OE1	1:A:1931:ASN:HB2	2.09	0.53
1:B:1930:GLU:OE1	1:B:1931:ASN:HB2	2.09	0.53
1:A:2169:CYS:SG	1:A:2207:MET:HE1	2.48	0.53
1:A:2652:LYS:HD3	1:A:2655:SER:HB3	1.89	0.53
1:A:2653:LEU:HD12	1:D:2652:LYS:HB2	1.91	0.53
1:C:35:ASP:HB2	1:C:151:LEU:HB2	1.91	0.53
1:C:1101:VAL:HG13	1:C:1102:SER:N	2.22	0.53
1:D:178:VAL:HG11	1:D:222:LEU:HD13	1.90	0.53
1:C:1062:ILE:O	1:C:1065:ILE:HG22	2.09	0.53
1:D:35:ASP:HB2	1:D:151:LEU:HB2	1.91	0.53
1:D:1056:THR:HG23	1:D:1059:ARG:NH1	2.23	0.53
1:B:2288:ARG:HB2	1:B:2291:LEU:HD23	1.91	0.53
1:C:1800:GLN:O	1:C:1802:LYS:N	2.41	0.53
1:D:1062:ILE:O	1:D:1065:ILE:HG22	2.09	0.53
1:D:1306:HIS:O	1:D:1307:VAL:HG12	2.09	0.53
1:D:1627:VAL:O	1:D:1631:VAL:HG13	2.09	0.53
1:D:2288:ARG:HB2	1:D:2291:LEU:HD23	1.91	0.53
1:A:992:MET:HB3	1:A:1094:PHE:HE1	1.73	0.53
1:B:1062:ILE:O	1:B:1065:ILE:HG22	2.09	0.53
1:B:1800:GLN:C	1:B:1802:LYS:N	2.67	0.53
1:D:1800:GLN:C	1:D:1802:LYS:N	2.67	0.53
1:C:2607:TYR:HB3	1:C:2612:SER:HB2	1.90	0.53
1:A:1062:ILE:O	1:A:1065:ILE:HG22	2.09	0.52
1:A:1679:ARG:HG2	1:A:1679:ARG:NH1	2.23	0.52
1:B:133:THR:HG22	1:B:159:SER:HB3	1.91	0.52
1:C:533:GLY:HA2	1:C:536:LEU:HD12	1.91	0.52
1:C:992:MET:HB3	1:C:1094:PHE:HE1	1.73	0.52
1:A:772:PHE:HA	1:A:775:ARG:HD3	1.90	0.52
1:A:1627:VAL:O	1:A:1631:VAL:HG13	2.09	0.52
1:C:1627:VAL:O	1:C:1631:VAL:HG13	2.09	0.52
1:D:770:LEU:HB2	1:D:771:PRO:HD3	1.90	0.52
1:C:1070:ALA:HB3	1:C:1071:PRO:HD3	1.90	0.52
1:D:1042:LYS:HD2	1:D:1046:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:THR:O	1:A:1277:ILE:HG22	2.09	0.52
1:A:1800:GLN:C	1:A:1802:LYS:N	2.67	0.52
1:B:1042:LYS:HD2	1:B:1046:PRO:HG3	1.92	0.52
1:C:133:THR:HG22	1:C:159:SER:HB3	1.91	0.52
1:C:1800:GLN:C	1:C:1802:LYS:N	2.67	0.52
1:C:2288:ARG:HB2	1:C:2291:LEU:HD23	1.91	0.52
1:A:133:THR:HG22	1:A:159:SER:HB3	1.91	0.52
1:A:533:GLY:HA2	1:A:536:LEU:HD12	1.91	0.52
1:A:2018:ILE:HD13	1:A:2047:LEU:HD12	1.91	0.52
1:B:1627:VAL:O	1:B:1631:VAL:HG13	2.09	0.52
1:B:2234:PHE:CE1	1:B:2374:LEU:HD13	2.41	0.52
1:C:772:PHE:HA	1:C:775:ARG:HD3	1.90	0.52
1:A:1306:HIS:O	1:A:1307:VAL:HG12	2.09	0.52
1:C:1123:VAL:HG22	1:C:1219:LEU:HD23	1.92	0.52
1:C:1679:ARG:HG2	1:C:1679:ARG:NH1	2.23	0.52
1:D:1273:THR:O	1:D:1277:ILE:HG22	2.09	0.52
1:A:2628:ARG:HH22	1:D:2574:ASN:HA	1.74	0.52
1:B:772:PHE:HA	1:B:775:ARG:HD3	1.90	0.52
1:C:1306:HIS:O	1:C:1307:VAL:HG12	2.09	0.52
1:D:533:GLY:HA2	1:D:536:LEU:HD12	1.91	0.52
1:D:996:TYR:CE1	1:D:1606:LEU:HD23	2.45	0.52
1:D:1930:GLU:OE1	1:D:1931:ASN:HB2	2.09	0.52
1:A:1042:LYS:HD2	1:A:1046:PRO:HG3	1.92	0.52
1:C:302:LEU:HD13	1:C:366:LEU:HD11	1.92	0.52
1:D:1101:VAL:HG13	1:D:1102:SER:N	2.22	0.52
1:C:1178:ASN:O	1:C:1181:ILE:HG13	2.10	0.52
1:C:2018:ILE:HD13	1:C:2047:LEU:HD12	1.91	0.52
1:D:1123:VAL:HG22	1:D:1219:LEU:HD23	1.92	0.52
1:A:2574:ASN:H	1:C:2628:ARG:NH1	2.04	0.52
1:B:91:LYS:NZ	1:C:1972:LEU:HD23	2.18	0.52
1:B:302:LEU:HD13	1:B:366:LEU:HD11	1.92	0.52
1:C:1042:LYS:HD2	1:C:1046:PRO:HG3	1.92	0.52
1:D:1679:ARG:HG2	1:D:1679:ARG:NH1	2.23	0.52
1:C:996:TYR:CE1	1:C:1606:LEU:HD23	2.45	0.51
1:C:1813:ARG:HG2	1:C:1917:ILE:HG21	1.92	0.51
1:A:2288:ARG:HB2	1:A:2291:LEU:HD23	1.91	0.51
1:D:2018:ILE:HD13	1:D:2047:LEU:HD12	1.91	0.51
1:B:533:GLY:HA2	1:B:536:LEU:HD12	1.91	0.51
1:C:855:LYS:HA	1:C:858:ASN:HD21	1.76	0.51
1:C:2581:GLU:OE2	1:C:2581:GLU:HA	2.11	0.51
1:D:133:THR:HG22	1:D:159:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:TYR:CE1	1:A:1606:LEU:HD23	2.45	0.51
1:B:1119:LEU:HD12	1:B:1185:ILE:HD11	1.93	0.51
1:B:1178:ASN:O	1:B:1181:ILE:HG13	2.10	0.51
1:B:1273:THR:O	1:B:1277:ILE:HG22	2.09	0.51
1:C:1273:THR:O	1:C:1277:ILE:HG22	2.09	0.51
1:C:2247:PHE:HB3	1:C:2249:PRO:HD3	1.93	0.51
1:D:302:LEU:HD13	1:D:366:LEU:HD11	1.92	0.51
1:D:1112:ILE:HD11	1:D:1192:LEU:HG	1.93	0.51
1:D:1122:THR:HG21	1:D:1182:VAL:HG12	1.93	0.51
1:A:302:LEU:HD13	1:A:366:LEU:HD11	1.92	0.51
1:A:664:ILE:O	1:A:665:LEU:HD13	2.11	0.51
1:A:855:LYS:HA	1:A:858:ASN:HD21	1.76	0.51
1:D:1119:LEU:HD12	1:D:1185:ILE:HD11	1.93	0.51
1:D:1786:ASN:O	1:D:1790:GLN:HG3	2.11	0.51
1:A:1122:THR:HG21	1:A:1182:VAL:HG12	1.93	0.51
1:A:1813:ARG:HG2	1:A:1917:ILE:HG21	1.92	0.51
1:A:2422:THR:HA	1:A:2477:ARG:HA	1.93	0.51
1:A:2666:GLN:HE21	1:C:2667:LEU:HD12	1.76	0.51
1:B:2581:GLU:HA	1:B:2581:GLU:OE2	2.11	0.51
1:C:316:ALA:HB1	1:C:352:TYR:HB3	1.93	0.51
1:C:2539:VAL:O	1:C:2543:THR:HG23	2.11	0.51
1:D:855:LYS:HA	1:D:858:ASN:HD21	1.76	0.51
1:D:2247:PHE:HB3	1:D:2249:PRO:HD3	1.93	0.51
1:A:1786:ASN:O	1:A:1790:GLN:HG3	2.11	0.51
1:C:664:ILE:O	1:C:665:LEU:HD13	2.11	0.51
1:A:1123:VAL:HG22	1:A:1219:LEU:HD23	1.92	0.51
1:A:1178:ASN:O	1:A:1181:ILE:HG13	2.10	0.51
1:A:2581:GLU:OE2	1:A:2581:GLU:HA	2.11	0.51
1:B:855:LYS:HA	1:B:858:ASN:HD21	1.76	0.51
1:B:996:TYR:CE1	1:B:1606:LEU:HD23	2.45	0.51
1:B:1786:ASN:O	1:B:1790:GLN:HG3	2.11	0.51
1:B:2018:ILE:HD13	1:B:2047:LEU:HD12	1.91	0.51
1:B:1112:ILE:HD11	1:B:1192:LEU:HG	1.93	0.51
1:B:1122:THR:HG21	1:B:1182:VAL:HG12	1.93	0.51
1:C:1119:LEU:HD12	1:C:1185:ILE:HD11	1.93	0.51
1:C:1122:THR:HG21	1:C:1182:VAL:HG12	1.93	0.51
1:D:1178:ASN:O	1:D:1181:ILE:HG13	2.10	0.51
1:D:1767:ASN:HB3	1:D:1770:ILE:HG22	1.93	0.51
1:A:316:ALA:HB1	1:A:352:TYR:HB3	1.93	0.50
1:A:2539:VAL:O	1:A:2543:THR:HG23	2.11	0.50
1:B:1257:HIS:HD2	1:B:1284:LEU:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:PHE:HE1	1:A:560:LEU:HD21	1.76	0.50
1:A:2018:ILE:O	1:A:2022:ILE:HG22	2.11	0.50
1:C:519:PHE:HE1	1:C:560:LEU:HD21	1.76	0.50
1:C:1257:HIS:HD2	1:C:1284:LEU:HD11	1.77	0.50
1:D:2539:VAL:O	1:D:2543:THR:HG23	2.11	0.50
1:A:1119:LEU:HD12	1:A:1185:ILE:HD11	1.93	0.50
1:C:527:LYS:HG3	1:C:528:GLU:H	1.76	0.50
1:C:2184:THR:HG21	1:C:2563:PHE:HZ	1.77	0.50
1:B:527:LYS:HG3	1:B:528:GLU:H	1.76	0.50
1:B:2018:ILE:O	1:B:2022:ILE:HG22	2.11	0.50
1:B:2247:PHE:HB3	1:B:2249:PRO:HD3	1.93	0.50
1:C:1786:ASN:O	1:C:1790:GLN:HG3	2.11	0.50
1:D:1290:GLU:CD	1:D:1290:GLU:H	2.20	0.50
1:D:1989:LEU:O	1:D:1993:THR:HG22	2.12	0.50
1:D:2018:ILE:O	1:D:2022:ILE:HG22	2.11	0.50
1:D:2656:THR:HA	1:D:2659:LEU:HB3	1.93	0.50
1:A:2267:LEU:C	1:A:2269:VAL:H	2.20	0.50
1:B:1123:VAL:HG22	1:B:1219:LEU:HD23	1.92	0.50
1:A:2574:ASN:HA	1:C:2628:ARG:NH2	2.25	0.50
1:C:1112:ILE:HD11	1:C:1192:LEU:HG	1.93	0.50
1:C:2525:PHE:HA	1:C:2529:ILE:HD13	1.93	0.50
1:D:1257:HIS:HD2	1:D:1284:LEU:HD11	1.77	0.50
1:D:2422:THR:HA	1:D:2477:ARG:HA	1.93	0.50
1:D:2525:PHE:HA	1:D:2529:ILE:HD13	1.93	0.50
1:A:2184:THR:HG21	1:A:2563:PHE:HZ	1.77	0.50
1:A:2367:TYR:CE1	1:C:2407:TYR:CE1	2.99	0.50
1:A:2367:TYR:HE1	1:A:2371:LEU:HD23	1.77	0.50
1:B:316:ALA:HB1	1:B:352:TYR:HB3	1.93	0.50
1:B:664:ILE:O	1:B:665:LEU:HD13	2.11	0.50
1:D:1956:LEU:HD23	1:D:2010:HIS:HD2	1.77	0.50
1:D:2184:THR:HG21	1:D:2563:PHE:HZ	1.77	0.50
1:A:1290:GLU:CD	1:A:1290:GLU:H	2.20	0.50
1:B:1813:ARG:HG2	1:B:1917:ILE:HG21	1.92	0.50
1:B:1956:LEU:HD23	1:B:2010:HIS:HD2	1.77	0.50
1:A:1257:HIS:HD2	1:A:1284:LEU:HD11	1.77	0.50
1:A:1767:ASN:HB3	1:A:1770:ILE:HG22	1.93	0.50
1:B:2184:THR:HG21	1:B:2563:PHE:HZ	1.77	0.50
1:B:2229:TRP:HB2	1:B:2322:PHE:HD1	1.76	0.50
1:C:615:ILE:HD11	1:C:655:PHE:CG	2.47	0.50
1:D:1813:ARG:HG2	1:D:1917:ILE:HG21	1.92	0.50
1:A:1065:ILE:HD12	1:A:1073:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2539:VAL:O	1:B:2543:THR:HG23	2.11	0.49
1:C:1956:LEU:HD23	1:C:2010:HIS:HD2	1.77	0.49
1:C:1989:LEU:O	1:C:1993:THR:HG22	2.12	0.49
1:C:2263:PHE:O	1:C:2266:LEU:HG	2.12	0.49
1:D:664:ILE:O	1:D:665:LEU:HD13	2.11	0.49
1:B:2422:THR:HA	1:B:2477:ARG:HA	1.93	0.49
1:C:1065:ILE:HD12	1:C:1073:LEU:CD1	2.42	0.49
1:C:2367:TYR:HE1	1:C:2371:LEU:HD23	1.77	0.49
1:D:2229:TRP:HB2	1:D:2322:PHE:HD1	1.76	0.49
1:A:1112:ILE:HD11	1:A:1192:LEU:HG	1.93	0.49
1:A:2263:PHE:O	1:A:2266:LEU:HG	2.12	0.49
1:A:2656:THR:HA	1:A:2659:LEU:HB3	1.93	0.49
1:B:1989:LEU:O	1:B:1993:THR:HG22	2.12	0.49
1:C:2267:LEU:C	1:C:2269:VAL:H	2.20	0.49
1:D:316:ALA:HB1	1:D:352:TYR:HB3	1.93	0.49
1:D:1065:ILE:HD12	1:D:1073:LEU:CD1	2.42	0.49
1:D:2581:GLU:HA	1:D:2581:GLU:OE2	2.11	0.49
1:A:2247:PHE:HB3	1:A:2249:PRO:HD3	1.93	0.49
1:B:615:ILE:HD11	1:B:655:PHE:CG	2.47	0.49
1:B:1767:ASN:HB3	1:B:1770:ILE:HG22	1.93	0.49
1:B:2263:PHE:O	1:B:2266:LEU:HG	2.12	0.49
1:C:716:ALA:HB2	1:C:723:ASP:HB3	1.93	0.49
1:C:2018:ILE:O	1:C:2022:ILE:HG22	2.11	0.49
1:A:388:ARG:HH21	1:A:423:LYS:HZ2	1.60	0.49
1:A:1956:LEU:HD23	1:A:2010:HIS:HD2	1.77	0.49
1:A:1989:LEU:O	1:A:1993:THR:HG22	2.12	0.49
1:B:2267:LEU:C	1:B:2269:VAL:H	2.20	0.49
1:C:2229:TRP:HB2	1:C:2322:PHE:HD1	1.76	0.49
1:C:2422:THR:HA	1:C:2477:ARG:HA	1.93	0.49
1:D:527:LYS:HG3	1:D:528:GLU:H	1.76	0.49
1:D:2267:LEU:C	1:D:2269:VAL:H	2.20	0.49
1:B:519:PHE:HE1	1:B:560:LEU:HD21	1.76	0.49
1:B:716:ALA:HB2	1:B:723:ASP:HB3	1.94	0.49
1:B:1065:ILE:HD12	1:B:1073:LEU:CD1	2.42	0.49
1:B:1290:GLU:H	1:B:1290:GLU:CD	2.20	0.49
1:B:2367:TYR:HE1	1:B:2371:LEU:HD23	1.77	0.49
1:C:1767:ASN:HB3	1:C:1770:ILE:HG22	1.93	0.49
1:C:2656:THR:HA	1:C:2659:LEU:HB3	1.93	0.49
1:D:519:PHE:HE1	1:D:560:LEU:HD21	1.76	0.49
1:D:2033:ARG:O	1:D:2034:MET:HE2	2.13	0.49
1:D:2367:TYR:HE1	1:D:2371:LEU:HD23	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LYS:HG3	1:A:528:GLU:H	1.76	0.49
1:A:2525:PHE:HA	1:A:2529:ILE:HD13	1.93	0.49
1:C:2065:LEU:CD1	1:C:2119:ASN:HD22	2.26	0.49
1:D:716:ALA:HB2	1:D:723:ASP:HB3	1.94	0.49
1:D:787:VAL:HG23	1:D:787:VAL:O	2.13	0.49
1:A:615:ILE:HD11	1:A:655:PHE:CG	2.47	0.49
1:A:1758:VAL:O	1:A:1762:ILE:HG23	2.13	0.49
1:B:2656:THR:HA	1:B:2659:LEU:HB3	1.93	0.49
1:A:787:VAL:HG23	1:A:787:VAL:O	2.13	0.49
1:A:2065:LEU:CD1	1:A:2119:ASN:HD22	2.26	0.49
1:A:2229:TRP:HB2	1:A:2322:PHE:HD1	1.76	0.49
1:A:2316:LEU:HD13	1:A:2354:LEU:HD23	1.94	0.49
1:C:1652:PHE:O	1:C:1652:PHE:CD1	2.65	0.49
1:D:2234:PHE:CE1	1:D:2374:LEU:HD13	2.42	0.49
1:D:2316:LEU:HD13	1:D:2354:LEU:HD23	1.94	0.49
1:B:2525:PHE:HA	1:B:2529:ILE:HD13	1.94	0.49
1:C:787:VAL:HG23	1:C:787:VAL:O	2.13	0.49
1:C:2086:GLU:HA	1:C:2089:HIS:CD2	2.48	0.49
1:A:2033:ARG:O	1:A:2034:MET:HE2	2.13	0.48
1:B:2156:ARG:HH22	1:B:2628:ARG:HH21	1.60	0.48
1:C:1290:GLU:CD	1:C:1290:GLU:H	2.20	0.48
1:C:2033:ARG:O	1:C:2034:MET:HE2	2.13	0.48
1:D:2086:GLU:HA	1:D:2089:HIS:CD2	2.48	0.48
1:D:2263:PHE:O	1:D:2266:LEU:HG	2.12	0.48
1:B:190:GLY:C	1:B:191:GLN:HG2	2.38	0.48
1:B:2086:GLU:HA	1:B:2089:HIS:CD2	2.48	0.48
1:B:2316:LEU:HD13	1:B:2354:LEU:HD23	1.94	0.48
1:D:615:ILE:HD11	1:D:655:PHE:CG	2.47	0.48
1:A:716:ALA:HB2	1:A:723:ASP:HB3	1.94	0.48
1:A:995:ILE:HD13	1:A:998:LYS:HZ3	1.77	0.48
1:B:1228:ASP:HB3	1:B:1231:MET:SD	2.53	0.48
1:B:2033:ARG:O	1:B:2034:MET:HE2	2.13	0.48
1:C:190:GLY:C	1:C:191:GLN:HG2	2.38	0.48
1:D:1758:VAL:O	1:D:1762:ILE:HG23	2.13	0.48
1:B:787:VAL:O	1:B:787:VAL:HG23	2.13	0.48
1:B:1652:PHE:O	1:B:1652:PHE:CD1	2.65	0.48
1:D:1084:PHE:CE1	1:D:1628:LEU:HD12	2.49	0.48
1:B:2065:LEU:CD1	1:B:2119:ASN:HD22	2.26	0.48
1:C:1758:VAL:O	1:C:1762:ILE:HG23	2.13	0.48
1:C:2156:ARG:HH22	1:C:2628:ARG:HH21	1.60	0.48
1:D:1652:PHE:O	1:D:1652:PHE:CD1	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2297:ARG:O	1:D:2301:THR:HG23	2.14	0.48
1:B:995:ILE:HG21	1:B:1036:THR:HG21	1.96	0.48
1:B:1084:PHE:CE1	1:B:1628:LEU:HD12	2.49	0.48
1:B:1101:VAL:HG13	1:B:1102:SER:N	2.22	0.48
1:C:995:ILE:HG21	1:C:1036:THR:HG21	1.96	0.48
1:A:1617:PHE:O	1:A:1621:MET:HB2	2.14	0.48
1:A:2156:ARG:HH22	1:A:2628:ARG:HH21	1.60	0.48
1:C:1228:ASP:HB3	1:C:1231:MET:SD	2.53	0.48
1:C:1617:PHE:O	1:C:1621:MET:HB2	2.14	0.48
1:D:695:LEU:HG	1:D:709:ILE:HB	1.96	0.48
1:D:2065:LEU:CD1	1:D:2119:ASN:HD22	2.26	0.48
1:B:2297:ARG:O	1:B:2301:THR:HG23	2.14	0.48
1:C:2297:ARG:O	1:C:2301:THR:HG23	2.14	0.48
1:C:2316:LEU:HD13	1:C:2354:LEU:HD23	1.94	0.48
1:A:695:LEU:HG	1:A:709:ILE:HB	1.96	0.48
1:A:2086:GLU:HA	1:A:2089:HIS:CD2	2.48	0.48
1:A:2297:ARG:O	1:A:2301:THR:HG23	2.14	0.48
1:B:2583:ILE:HD12	3:B:2802:ATP:C6	2.49	0.48
1:D:245:ALA:HB3	1:D:428:ALA:HB3	1.96	0.48
1:D:655:PHE:CD1	1:D:655:PHE:C	2.92	0.48
1:D:1228:ASP:HB3	1:D:1231:MET:SD	2.53	0.48
1:A:1084:PHE:CE1	1:A:1628:LEU:HD12	2.49	0.48
1:C:2203:LEU:O	1:C:2207:MET:HG2	2.14	0.48
1:A:190:GLY:C	1:A:191:GLN:HG2	2.38	0.47
1:A:1228:ASP:HB3	1:A:1231:MET:SD	2.53	0.47
1:A:1652:PHE:O	1:A:1652:PHE:CD1	2.65	0.47
1:B:1617:PHE:O	1:B:1621:MET:HB2	2.14	0.47
1:C:1084:PHE:CE1	1:C:1628:LEU:HD12	2.49	0.47
1:C:2236:LEU:O	1:C:2240:ILE:HG22	2.14	0.47
1:D:190:GLY:C	1:D:191:GLN:HG2	2.38	0.47
1:D:388:ARG:HH21	1:D:423:LYS:HZ2	1.62	0.47
1:D:855:LYS:HE2	1:D:855:LYS:HB2	1.69	0.47
1:D:1617:PHE:O	1:D:1621:MET:HB2	2.14	0.47
1:D:2156:ARG:HH22	1:D:2628:ARG:HH21	1.60	0.47
1:D:2583:ILE:HD12	3:D:2802:ATP:C6	2.49	0.47
1:A:2203:LEU:O	1:A:2207:MET:HG2	2.14	0.47
1:B:1758:VAL:O	1:B:1762:ILE:HG23	2.13	0.47
1:D:2203:LEU:O	1:D:2207:MET:HG2	2.14	0.47
1:A:245:ALA:HB3	1:A:428:ALA:HB3	1.96	0.47
1:A:2583:ILE:HD12	3:A:2802:ATP:C6	2.49	0.47
1:B:655:PHE:CD1	1:B:655:PHE:C	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2214:ARG:HA	1:B:2214:ARG:NE	2.29	0.47
1:C:2583:ILE:HD12	3:C:2802:ATP:C6	2.49	0.47
1:A:1690:GLU:C	1:A:1692:GLY:H	2.23	0.47
1:A:2236:LEU:O	1:A:2240:ILE:HG22	2.14	0.47
1:A:2657:MET:HE2	1:A:2657:MET:HA	1.96	0.47
1:B:2203:LEU:O	1:B:2207:MET:HG2	2.14	0.47
1:A:995:ILE:HG21	1:A:1036:THR:HG21	1.96	0.47
1:B:2364:GLU:HG3	1:D:2411:ILE:HD13	1.96	0.47
1:C:1690:GLU:C	1:C:1692:GLY:H	2.23	0.47
1:D:581:MET:HE1	1:D:595:ILE:HB	1.96	0.47
1:A:316:ALA:HA	1:A:354:LEU:HA	1.96	0.47
1:A:655:PHE:CD1	1:A:655:PHE:C	2.92	0.47
1:A:2214:ARG:NE	1:A:2214:ARG:HA	2.29	0.47
1:A:2411:ILE:HD13	1:D:2364:GLU:HG3	1.94	0.47
1:B:2236:LEU:O	1:B:2240:ILE:HG22	2.14	0.47
1:C:2657:MET:HE2	1:C:2657:MET:HA	1.96	0.47
1:D:1690:GLU:C	1:D:1692:GLY:H	2.23	0.47
1:A:581:MET:HE1	1:A:595:ILE:HB	1.96	0.47
1:B:316:ALA:HA	1:B:354:LEU:HA	1.96	0.47
1:B:494:LEU:HD11	1:B:554:ARG:HB3	1.97	0.47
1:C:316:ALA:HA	1:C:354:LEU:HA	1.96	0.47
1:C:695:LEU:HG	1:C:709:ILE:HB	1.96	0.47
1:C:1953:CYS:HB3	1:C:2006:CYS:HB3	1.74	0.47
1:C:2214:ARG:HA	1:C:2214:ARG:NE	2.29	0.47
1:D:995:ILE:HD13	1:D:998:LYS:HZ3	1.80	0.47
1:D:2214:ARG:HA	1:D:2214:ARG:NE	2.29	0.47
1:C:1952:VAL:HG12	1:C:1995:TYR:HD2	1.80	0.47
1:A:2077:MET:HE2	1:A:2077:MET:HB3	1.70	0.47
1:D:265:ARG:HA	1:D:265:ARG:HD2	1.69	0.47
1:B:245:ALA:HB3	1:B:428:ALA:HB3	1.96	0.47
1:B:1690:GLU:C	1:B:1692:GLY:H	2.23	0.47
1:C:494:LEU:HD11	1:C:554:ARG:HB3	1.97	0.47
1:D:316:ALA:HA	1:D:354:LEU:HA	1.96	0.47
1:D:995:ILE:HG21	1:D:1036:THR:HG21	1.96	0.47
1:A:301:SER:HB2	1:A:303:PHE:HE1	1.80	0.46
1:A:494:LEU:HD11	1:A:554:ARG:HB3	1.97	0.46
1:D:301:SER:HB2	1:D:303:PHE:HE1	1.80	0.46
1:D:567:TYR:O	1:D:571:GLN:HG2	2.15	0.46
1:D:2236:LEU:O	1:D:2240:ILE:HG22	2.14	0.46
1:A:567:TYR:O	1:A:571:GLN:HG2	2.15	0.46
1:A:1811:TYR:CE1	1:A:1954:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ARG:O	1:B:607:GLU:CB	2.64	0.46
1:D:758:VAL:HA	1:D:761:ILE:HG23	1.98	0.46
1:A:305:PHE:HB2	1:A:314:LEU:HD22	1.97	0.46
1:C:64:ASN:HB2	1:C:122:GLN:NE2	2.31	0.46
1:C:655:PHE:CD1	1:C:655:PHE:C	2.92	0.46
1:C:988:ARG:NH1	1:C:1043:GLU:HB3	2.31	0.46
1:C:1913:PRO:C	1:C:1916:THR:HG22	2.39	0.46
1:D:603:ARG:O	1:D:607:GLU:CB	2.64	0.46
1:A:603:ARG:O	1:A:607:GLU:CB	2.64	0.46
1:B:1972:LEU:HD23	1:D:91:LYS:NZ	2.30	0.46
1:C:245:ALA:HB3	1:C:428:ALA:HB3	1.96	0.46
1:C:567:TYR:O	1:C:571:GLN:HG2	2.15	0.46
1:C:758:VAL:HA	1:C:761:ILE:HG23	1.98	0.46
1:C:2632:MET:HA	1:C:2635:VAL:HG12	1.98	0.46
1:D:888:THR:O	1:D:892:ILE:HG22	2.16	0.46
1:D:1811:TYR:CE1	1:D:1954:GLU:HG3	2.50	0.46
1:B:305:PHE:HB2	1:B:314:LEU:HD22	1.97	0.46
1:B:581:MET:HE1	1:B:595:ILE:HB	1.96	0.46
1:B:758:VAL:HA	1:B:761:ILE:HG23	1.98	0.46
1:C:581:MET:HE1	1:C:595:ILE:HB	1.96	0.46
1:C:1811:TYR:CE1	1:C:1954:GLU:HG3	2.50	0.46
1:D:2376:TYR:HD1	1:D:2377:ARG:HD2	1.81	0.46
1:B:269:ARG:HB3	1:B:270:GLN:H	1.54	0.46
1:B:695:LEU:HG	1:B:709:ILE:HB	1.96	0.46
1:B:2376:TYR:HD1	1:B:2377:ARG:HD2	1.81	0.46
1:D:671:VAL:HG21	1:D:694:TRP:HB2	1.98	0.46
1:D:1779:ILE:HD11	1:D:1920:PRO:O	2.16	0.46
1:A:758:VAL:HA	1:A:761:ILE:HG23	1.98	0.46
1:A:988:ARG:NH1	1:A:1043:GLU:HB3	2.31	0.46
1:A:2169:CYS:SG	1:A:2597:VAL:HG11	2.56	0.46
1:A:2209:TRP:O	1:A:2213:ILE:HG22	2.16	0.46
1:B:2632:MET:HA	1:B:2635:VAL:HG12	1.98	0.46
1:D:2657:MET:HE2	1:D:2657:MET:HA	1.96	0.46
1:A:64:ASN:HB2	1:A:122:GLN:NE2	2.31	0.46
1:A:1237:LEU:O	1:A:1240:THR:HG22	2.16	0.46
1:A:2372:PHE:HA	1:A:2375:VAL:HG12	1.98	0.46
1:A:2632:MET:HA	1:A:2635:VAL:HG12	1.98	0.46
1:B:799:ARG:HH21	1:B:801:ALA:HB3	1.81	0.46
1:B:1811:TYR:CE1	1:B:1954:GLU:HG3	2.50	0.46
1:B:2621:LYS:HA	1:B:2621:LYS:HE3	1.98	0.46
1:B:2666:GLN:HE21	1:D:2667:LEU:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:SER:HB2	1:C:303:PHE:HE1	1.80	0.46
1:C:603:ARG:O	1:C:607:GLU:CB	2.64	0.46
1:C:961:GLN:H	1:C:961:GLN:HG2	1.57	0.46
1:C:2621:LYS:HE3	1:C:2621:LYS:HA	1.98	0.46
1:D:2372:PHE:HA	1:D:2375:VAL:HG12	1.98	0.46
1:D:2491:ASN:O	1:D:2495:ARG:HG2	2.16	0.46
1:A:606:LEU:HA	1:A:609:HIS:HB2	1.98	0.45
1:A:961:GLN:H	1:A:961:GLN:HG2	1.57	0.45
1:A:1181:ILE:O	1:A:1185:ILE:HG23	2.17	0.45
1:B:671:VAL:HG21	1:B:694:TRP:HB2	1.98	0.45
1:B:888:THR:O	1:B:892:ILE:HG22	2.16	0.45
1:B:1952:VAL:HG12	1:B:1995:TYR:HD2	1.80	0.45
1:B:2209:TRP:O	1:B:2213:ILE:HG22	2.16	0.45
1:B:2528:VAL:O	1:B:2532:VAL:HG22	2.16	0.45
1:B:2657:MET:HA	1:B:2657:MET:HE2	1.96	0.45
1:C:799:ARG:HH21	1:C:801:ALA:HB3	1.81	0.45
1:D:788:ASP:O	1:D:791:PRO:HD3	2.16	0.45
1:D:799:ARG:HH21	1:D:801:ALA:HB3	1.81	0.45
1:D:2209:TRP:O	1:D:2213:ILE:HG22	2.16	0.45
1:A:498:ILE:HD11	1:A:501:PRO:HA	1.98	0.45
1:A:888:THR:O	1:A:892:ILE:HG22	2.16	0.45
1:B:498:ILE:HD11	1:B:501:PRO:HA	1.98	0.45
1:B:567:TYR:O	1:B:571:GLN:HG2	2.15	0.45
1:B:1953:CYS:HB3	1:B:2006:CYS:HB3	1.74	0.45
1:C:1779:ILE:HD11	1:C:1920:PRO:O	2.16	0.45
1:D:64:ASN:HB2	1:D:122:GLN:NE2	2.31	0.45
1:D:1062:ILE:HA	1:D:1065:ILE:HG22	1.98	0.45
1:B:616:GLU:HA	1:B:619:VAL:HG12	1.98	0.45
1:C:888:THR:O	1:C:892:ILE:HG22	2.16	0.45
1:A:703:GLU:HA	1:A:704:PRO:HD3	1.84	0.45
1:B:2169:CYS:SG	1:B:2597:VAL:HG11	2.56	0.45
1:C:671:VAL:HG21	1:C:694:TRP:HB2	1.98	0.45
1:C:1237:LEU:O	1:C:1240:THR:HG22	2.16	0.45
1:D:269:ARG:HB3	1:D:270:GLN:H	1.54	0.45
1:D:1237:LEU:O	1:D:1240:THR:HG22	2.16	0.45
1:D:2169:CYS:SG	1:D:2597:VAL:HG11	2.56	0.45
1:D:2554:LYS:HE2	1:D:2554:LYS:HB3	1.79	0.45
1:A:788:ASP:O	1:A:791:PRO:HD3	2.16	0.45
1:A:2344:MET:HE2	1:A:2344:MET:HB3	1.81	0.45
1:A:2491:ASN:O	1:A:2495:ARG:HG2	2.16	0.45
1:A:2528:VAL:O	1:A:2532:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:HG11	1:B:209:VAL:HG23	1.99	0.45
1:B:2628:ARG:HH22	1:C:2574:ASN:HA	1.82	0.45
1:C:606:LEU:HA	1:C:609:HIS:HB2	1.98	0.45
1:C:1181:ILE:O	1:C:1185:ILE:HG23	2.17	0.45
1:C:2209:TRP:O	1:C:2213:ILE:HG22	2.16	0.45
1:C:2357:MET:HA	1:C:2362:VAL:HG21	1.99	0.45
1:C:2528:VAL:O	1:C:2532:VAL:HG22	2.17	0.45
1:D:305:PHE:HB2	1:D:314:LEU:HD22	1.97	0.45
1:D:756:LEU:HD23	1:D:756:LEU:HA	1.85	0.45
1:D:988:ARG:NH1	1:D:1043:GLU:HB3	2.31	0.45
1:D:1181:ILE:O	1:D:1185:ILE:HG23	2.16	0.45
1:B:265:ARG:HA	1:B:265:ARG:HD2	1.69	0.45
1:B:788:ASP:O	1:B:791:PRO:HD3	2.16	0.45
1:B:1181:ILE:O	1:B:1185:ILE:HG23	2.16	0.45
1:B:1237:LEU:O	1:B:1240:THR:HG22	2.15	0.45
1:B:2491:ASN:O	1:B:2495:ARG:HG2	2.16	0.45
1:C:603:ARG:O	1:C:607:GLU:HB2	2.17	0.45
1:C:769:SER:HB2	1:C:775:ARG:HH11	1.82	0.45
1:D:494:LEU:HD11	1:D:554:ARG:HB3	1.97	0.45
1:D:648:THR:O	1:D:651:LEU:HG	2.17	0.45
1:A:1062:ILE:HA	1:A:1065:ILE:HG22	1.98	0.45
1:A:1651:ALA:O	1:A:1652:PHE:HB3	2.17	0.45
1:B:1264:LEU:HD11	1:B:1292:VAL:HG22	1.99	0.45
1:B:1651:ALA:O	1:B:1652:PHE:HB3	2.17	0.45
1:B:1779:ILE:HD11	1:B:1920:PRO:O	2.16	0.45
1:B:1795:GLN:O	1:B:1796:GLN:C	2.60	0.45
1:D:1651:ALA:O	1:D:1652:PHE:HB3	2.17	0.45
1:D:2621:LYS:HE3	1:D:2621:LYS:HA	1.98	0.45
1:A:1264:LEU:HD11	1:A:1292:VAL:HG22	1.99	0.45
1:A:1779:ILE:HD11	1:A:1920:PRO:O	2.16	0.45
1:A:1985:VAL:HA	1:A:1988:THR:HG22	1.99	0.45
1:B:64:ASN:HB2	1:B:122:GLN:NE2	2.31	0.45
1:B:110:LEU:O	1:B:110:LEU:HD13	2.16	0.45
1:B:648:THR:O	1:B:651:LEU:HG	2.17	0.45
1:B:1985:VAL:HA	1:B:1988:THR:HG22	1.99	0.45
1:C:305:PHE:HB2	1:C:314:LEU:HD22	1.97	0.45
1:C:1279:MET:HE3	1:C:1279:MET:O	2.17	0.45
1:A:265:ARG:HD2	1:A:265:ARG:HA	1.69	0.45
1:A:1178:ASN:O	1:A:1182:VAL:HG13	2.16	0.45
1:B:301:SER:HB2	1:B:303:PHE:HE1	1.80	0.45
1:B:1101:VAL:CG1	1:B:1102:SER:H	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:ASN:O	1:B:1182:VAL:HG13	2.16	0.45
1:B:1303:HIS:HB3	1:B:1306:HIS:HE1	1.82	0.45
1:B:1913:PRO:C	1:B:1916:THR:HG22	2.39	0.45
1:B:2411:ILE:HG23	1:C:2364:GLU:HG2	1.98	0.45
1:C:1264:LEU:HD11	1:C:1292:VAL:HG22	1.99	0.45
1:C:1303:HIS:HB3	1:C:1306:HIS:HE1	1.82	0.45
1:C:2169:CYS:SG	1:C:2597:VAL:HG11	2.56	0.45
1:C:2491:ASN:O	1:C:2495:ARG:HG2	2.16	0.45
1:D:149:VAL:HG11	1:D:209:VAL:HG23	1.99	0.45
1:D:498:ILE:HD11	1:D:501:PRO:HA	1.98	0.45
1:D:1264:LEU:HD11	1:D:1292:VAL:HG22	1.99	0.45
1:D:1985:VAL:HA	1:D:1988:THR:HG22	1.99	0.45
1:A:2376:TYR:HD1	1:A:2377:ARG:HD2	1.81	0.45
1:B:1073:LEU:HD23	1:B:1659:HIS:ND1	2.32	0.45
1:B:1972:LEU:HD23	1:D:91:LYS:HZ3	1.81	0.45
1:C:110:LEU:HD13	1:C:110:LEU:O	2.16	0.45
1:C:498:ILE:HD11	1:C:501:PRO:HA	1.98	0.45
1:C:1216:VAL:HG21	1:C:1241:PHE:CE2	2.52	0.45
1:C:1795:GLN:O	1:C:1796:GLN:C	2.60	0.45
1:D:110:LEU:HD13	1:D:110:LEU:O	2.16	0.45
1:D:961:GLN:H	1:D:961:GLN:HG2	1.57	0.45
1:D:2632:MET:HA	1:D:2635:VAL:HG12	1.98	0.45
1:A:603:ARG:O	1:A:607:GLU:HB2	2.17	0.44
1:A:671:VAL:HG21	1:A:694:TRP:HB2	1.98	0.44
1:A:1795:GLN:O	1:A:1796:GLN:C	2.60	0.44
1:A:2048:LEU:O	1:A:2051:ILE:HG22	2.17	0.44
1:A:2168:ILE:HD13	1:A:2211:LYS:HD3	1.99	0.44
1:A:2357:MET:HA	1:A:2362:VAL:HG21	1.99	0.44
1:B:383:ARG:HA	1:B:383:ARG:HD3	1.84	0.44
1:B:603:ARG:O	1:B:607:GLU:HB2	2.17	0.44
1:B:606:LEU:HA	1:B:609:HIS:HB2	1.98	0.44
1:B:967:MET:HA	1:B:970:LYS:HG2	1.99	0.44
1:B:1062:ILE:HA	1:B:1065:ILE:HG22	1.98	0.44
1:B:1216:VAL:HG21	1:B:1241:PHE:CE2	2.52	0.44
1:C:758:VAL:CG1	1:C:785:MET:HE3	2.47	0.44
1:C:1062:ILE:HA	1:C:1065:ILE:HG22	1.98	0.44
1:C:2376:TYR:HD1	1:C:2377:ARG:HD2	1.81	0.44
1:D:1073:LEU:HD23	1:D:1659:HIS:ND1	2.32	0.44
1:D:1303:HIS:HB3	1:D:1306:HIS:HE1	1.82	0.44
1:D:2528:VAL:O	1:D:2532:VAL:HG22	2.17	0.44
1:A:812:THR:HG22	1:A:815:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2621:LYS:HE3	1:A:2621:LYS:HA	1.98	0.44
1:B:2357:MET:HA	1:B:2362:VAL:HG21	1.99	0.44
1:B:2371:LEU:HD12	1:B:2371:LEU:HA	1.84	0.44
1:C:648:THR:O	1:C:651:LEU:HG	2.17	0.44
1:C:1985:VAL:HA	1:C:1988:THR:HG22	1.99	0.44
1:D:666:ILE:HD11	1:D:729:TYR:HD1	1.83	0.44
1:D:1216:VAL:HG21	1:D:1241:PHE:CE2	2.52	0.44
1:A:616:GLU:HA	1:A:619:VAL:HG12	1.99	0.44
1:A:799:ARG:HH21	1:A:801:ALA:HB3	1.81	0.44
1:B:758:VAL:CG1	1:B:785:MET:HE3	2.47	0.44
1:B:988:ARG:NH1	1:B:1043:GLU:HB3	2.31	0.44
1:B:2048:LEU:O	1:B:2051:ILE:HG22	2.17	0.44
1:C:788:ASP:O	1:C:791:PRO:HD3	2.16	0.44
1:C:812:THR:HG22	1:C:815:GLU:OE1	2.17	0.44
1:C:855:LYS:HB2	1:C:855:LYS:HE2	1.69	0.44
1:C:1178:ASN:O	1:C:1182:VAL:HG13	2.16	0.44
1:D:606:LEU:HA	1:D:609:HIS:HB2	1.98	0.44
1:D:1950:ASN:HB3	1:D:1953:CYS:SG	2.58	0.44
1:A:110:LEU:HD13	1:A:110:LEU:O	2.16	0.44
1:A:1913:PRO:C	1:A:1916:THR:HG22	2.39	0.44
1:B:1950:ASN:HB3	1:B:1953:CYS:SG	2.58	0.44
1:B:2338:ARG:HG3	1:B:2340:VAL:HB	2.00	0.44
1:B:2361:PHE:O	1:B:2361:PHE:HD1	2.01	0.44
1:C:2168:ILE:HD13	1:C:2211:LYS:HD3	1.99	0.44
1:C:2338:ARG:HG3	1:C:2340:VAL:HB	2.00	0.44
1:C:2372:PHE:HA	1:C:2375:VAL:HG12	1.98	0.44
1:D:758:VAL:CG1	1:D:785:MET:HE3	2.47	0.44
1:D:769:SER:HB2	1:D:775:ARG:HH11	1.82	0.44
1:D:967:MET:HA	1:D:970:LYS:HG2	1.99	0.44
1:D:970:LYS:O	1:D:973:VAL:HG12	2.18	0.44
1:D:1178:ASN:O	1:D:1182:VAL:HG13	2.16	0.44
1:D:1795:GLN:O	1:D:1796:GLN:C	2.60	0.44
1:A:666:ILE:HD11	1:A:729:TYR:HD1	1.83	0.44
1:A:758:VAL:CG1	1:A:785:MET:HE3	2.47	0.44
1:A:2361:PHE:HD1	1:A:2361:PHE:O	2.01	0.44
1:B:769:SER:HB2	1:B:775:ARG:HH11	1.82	0.44
1:B:2372:PHE:HA	1:B:2375:VAL:HG12	1.98	0.44
1:B:2653:LEU:HD12	1:C:2652:LYS:HB2	2.00	0.44
1:C:1950:ASN:HB3	1:C:1953:CYS:SG	2.58	0.44
1:D:124:LEU:HD12	1:D:131:TYR:CZ	2.53	0.44
1:D:1279:MET:HE3	1:D:1279:MET:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2357:MET:HA	1:D:2362:VAL:HG21	1.99	0.44
1:D:2361:PHE:O	1:D:2361:PHE:HD1	2.01	0.44
1:A:648:THR:O	1:A:651:LEU:HG	2.17	0.44
1:A:970:LYS:O	1:A:973:VAL:HG12	2.18	0.44
1:A:1065:ILE:HD12	1:A:1073:LEU:HD12	2.00	0.44
1:A:1073:LEU:HD23	1:A:1659:HIS:ND1	2.32	0.44
1:B:666:ILE:HD11	1:B:729:TYR:HD1	1.83	0.44
1:B:996:TYR:HE1	1:B:1606:LEU:HD23	1.83	0.44
1:B:2168:ILE:HD13	1:B:2211:LYS:HD3	1.99	0.44
1:B:2554:LYS:HB3	1:B:2554:LYS:HE2	1.79	0.44
1:C:91:LYS:HG2	1:C:92:LEU:HD23	2.00	0.44
1:C:970:LYS:O	1:C:973:VAL:HG12	2.18	0.44
1:C:1636:GLU:HG2	1:C:1649:CYS:HB3	2.00	0.44
1:A:2551:LYS:HB2	1:A:2551:LYS:HE2	1.84	0.44
1:B:79:LYS:HA	1:B:79:LYS:HD3	1.67	0.44
1:B:970:LYS:O	1:B:973:VAL:HG12	2.18	0.44
1:B:1000:PHE:CE2	1:B:1602:ILE:HA	2.53	0.44
1:C:2077:MET:HE2	1:C:2077:MET:HB3	1.70	0.44
1:C:2344:MET:HE2	1:C:2344:MET:HB3	1.81	0.44
1:C:2361:PHE:HD1	1:C:2361:PHE:O	2.01	0.44
1:D:2168:ILE:HD13	1:D:2211:LYS:HD3	1.99	0.44
1:D:2563:PHE:H	3:D:2802:ATP:HN62	1.66	0.44
1:A:124:LEU:HD12	1:A:131:TYR:CZ	2.53	0.44
1:A:967:MET:HA	1:A:970:LYS:HG2	1.99	0.44
1:A:1279:MET:HE3	1:A:1279:MET:O	2.17	0.44
1:A:1952:VAL:HG12	1:A:1995:TYR:HD2	1.80	0.44
1:B:124:LEU:HD12	1:B:131:TYR:CZ	2.53	0.44
1:B:1279:MET:HE3	1:B:1279:MET:O	2.17	0.44
1:C:124:LEU:HD12	1:C:131:TYR:CZ	2.53	0.44
1:C:880:SER:HB2	1:C:884:ARG:HH21	1.83	0.44
1:C:967:MET:HA	1:C:970:LYS:HG2	1.99	0.44
1:C:1065:ILE:HD12	1:C:1073:LEU:HD12	2.00	0.44
1:C:1073:LEU:HD23	1:C:1659:HIS:ND1	2.32	0.44
1:C:1651:ALA:O	1:C:1652:PHE:HB3	2.17	0.44
1:D:498:ILE:HG23	1:D:499:THR:H	1.83	0.44
1:D:603:ARG:O	1:D:607:GLU:HB2	2.17	0.44
1:D:880:SER:HB2	1:D:884:ARG:HH21	1.83	0.44
1:D:1101:VAL:CG1	1:D:1102:SER:H	2.26	0.44
1:D:2338:ARG:HG3	1:D:2340:VAL:HB	2.00	0.44
1:A:769:SER:HB2	1:A:775:ARG:HH11	1.82	0.44
1:A:993:LEU:HD21	1:A:1099:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:HIS:HB3	1:A:1306:HIS:HE1	1.82	0.44
1:A:1636:GLU:HG2	1:A:1649:CYS:HB3	2.00	0.44
1:C:308:LEU:HD12	1:C:308:LEU:HA	1.86	0.44
1:D:1065:ILE:HD12	1:D:1073:LEU:HD12	2.00	0.44
1:D:2048:LEU:O	1:D:2051:ILE:HG22	2.17	0.44
1:D:616:GLU:HA	1:D:619:VAL:HG12	1.98	0.43
1:D:1636:GLU:HG2	1:D:1649:CYS:HB3	2.00	0.43
1:D:2423:MET:HE3	1:D:2423:MET:HA	2.01	0.43
1:A:149:VAL:HG11	1:A:209:VAL:HG23	1.99	0.43
1:A:1216:VAL:HG21	1:A:1241:PHE:CE2	2.52	0.43
1:A:1953:CYS:HB3	1:A:2006:CYS:HB3	1.74	0.43
1:A:2027:ASN:HB2	1:A:2028:PRO:HD3	2.00	0.43
1:A:2482:LEU:HD12	1:D:2245:ALA:O	2.18	0.43
1:B:350:ILE:HD12	1:B:418:GLY:HA3	2.00	0.43
1:B:745:GLN:HA	1:B:745:GLN:OE1	2.18	0.43
1:C:616:GLU:HA	1:C:619:VAL:HG12	1.98	0.43
1:C:1000:PHE:CE2	1:C:1602:ILE:HA	2.53	0.43
1:C:2048:LEU:O	1:C:2051:ILE:HG22	2.17	0.43
1:D:812:THR:HG22	1:D:815:GLU:OE1	2.17	0.43
1:D:1229:GLU:HA	1:D:1232:ASN:HD21	1.83	0.43
1:A:91:LYS:HG2	1:A:92:LEU:HD23	2.00	0.43
1:A:880:SER:HB2	1:A:884:ARG:HH21	1.83	0.43
1:A:1101:VAL:CG1	1:A:1102:SER:H	2.26	0.43
1:A:1229:GLU:HA	1:A:1232:ASN:HD21	1.83	0.43
1:A:1234:VAL:HA	1:A:1237:LEU:HB2	2.01	0.43
1:B:498:ILE:HG23	1:B:499:THR:H	1.83	0.43
1:B:2423:MET:HE3	1:B:2423:MET:HA	2.01	0.43
1:C:1229:GLU:HA	1:C:1232:ASN:HD21	1.83	0.43
1:C:2551:LYS:HB2	1:C:2551:LYS:HE2	1.84	0.43
1:D:1312:PHE:O	1:D:1316:ILE:HG22	2.19	0.43
1:B:91:LYS:HG2	1:B:92:LEU:HD23	2.00	0.43
1:B:2261:PRO:O	1:B:2265:VAL:HG23	2.19	0.43
1:C:498:ILE:HG23	1:C:499:THR:H	1.83	0.43
1:C:2423:MET:HE3	1:C:2423:MET:HA	2.01	0.43
1:D:799:ARG:NH2	1:D:1106:VAL:HG23	2.34	0.43
1:D:996:TYR:HE1	1:D:1606:LEU:HD23	1.83	0.43
1:D:2027:ASN:HB2	1:D:2028:PRO:HD3	2.00	0.43
1:A:39:VAL:HG22	1:A:207:LYS:HB2	2.00	0.43
1:A:799:ARG:NH2	1:A:1106:VAL:HG23	2.34	0.43
1:A:1000:PHE:CE2	1:A:1602:ILE:HA	2.53	0.43
1:A:1334:GLU:O	1:A:1339:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2261:PRO:O	1:A:2265:VAL:HG23	2.19	0.43
1:B:1234:VAL:HA	1:B:1237:LEU:HB2	2.01	0.43
1:B:1636:GLU:HG2	1:B:1649:CYS:HB3	2.00	0.43
1:B:2563:PHE:H	3:B:2802:ATP:HN62	1.66	0.43
1:C:1234:VAL:HA	1:C:1237:LEU:HB2	2.01	0.43
1:D:350:ILE:HD12	1:D:418:GLY:HA3	2.00	0.43
1:D:745:GLN:OE1	1:D:745:GLN:HA	2.18	0.43
1:B:1312:PHE:O	1:B:1316:ILE:HG22	2.19	0.43
1:C:2179:ARG:O	1:C:2183:THR:HG23	2.19	0.43
1:C:2261:PRO:O	1:C:2265:VAL:HG23	2.19	0.43
1:D:1000:PHE:CE2	1:D:1602:ILE:HA	2.53	0.43
1:D:1234:VAL:HA	1:D:1237:LEU:HB2	2.01	0.43
1:A:498:ILE:HG23	1:A:499:THR:H	1.83	0.43
1:A:1950:ASN:HB3	1:A:1953:CYS:SG	2.58	0.43
1:A:2423:MET:HA	1:A:2423:MET:HE3	2.01	0.43
1:B:376:ARG:HE	1:B:376:ARG:HB3	1.60	0.43
1:B:812:THR:HG22	1:B:815:GLU:OE1	2.17	0.43
1:B:1065:ILE:HD12	1:B:1073:LEU:HD12	2.00	0.43
1:C:79:LYS:HD3	1:C:79:LYS:HA	1.67	0.43
1:C:265:ARG:HA	1:C:265:ARG:HD2	1.69	0.43
1:C:666:ILE:HD11	1:C:729:TYR:HD1	1.83	0.43
1:D:993:LEU:HD21	1:D:1099:LEU:HD11	2.00	0.43
1:D:2179:ARG:O	1:D:2183:THR:HG23	2.19	0.43
1:D:2385:ILE:HA	1:D:2388:VAL:HG12	2.01	0.43
1:A:1306:HIS:C	1:A:1308:GLU:H	2.27	0.43
1:A:2401:LEU:O	1:A:2404:ILE:HG12	2.19	0.43
1:B:880:SER:HB2	1:B:884:ARG:HH21	1.83	0.43
1:B:893:LEU:HD11	1:B:1064:LEU:HD11	2.01	0.43
1:B:1045:THR:HB	1:B:1046:PRO:HD3	2.01	0.43
1:C:799:ARG:NH2	1:C:1106:VAL:HG23	2.34	0.43
1:C:2027:ASN:HB2	1:C:2028:PRO:HD3	2.00	0.43
1:D:1913:PRO:C	1:D:1916:THR:HG22	2.39	0.43
1:A:79:LYS:HA	1:A:79:LYS:HD3	1.67	0.43
1:A:2563:PHE:H	3:A:2802:ATP:HN62	1.66	0.43
1:B:613:LYS:O	1:B:616:GLU:HG2	2.19	0.43
1:B:721:LYS:HE3	1:B:721:LYS:HB2	1.67	0.43
1:B:984:ARG:HD3	1:B:988:ARG:NH2	2.34	0.43
1:B:1229:GLU:HA	1:B:1232:ASN:HD21	1.83	0.43
1:B:2385:ILE:HA	1:B:2388:VAL:HG12	2.01	0.43
1:C:2070:PRO:HG3	1:C:2121:LEU:HD23	2.01	0.43
1:C:2671:LYS:HA	1:C:2671:LYS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:984:ARG:HD3	1:D:988:ARG:NH2	2.34	0.43
1:D:1306:HIS:C	1:D:1308:GLU:H	2.27	0.43
1:D:1334:GLU:O	1:D:1339:GLY:HA3	2.19	0.43
1:D:2070:PRO:HG3	1:D:2121:LEU:HD23	2.01	0.43
1:D:2213:ILE:HD12	1:D:2216:ASN:HB3	2.01	0.43
1:A:731:ARG:HD2	1:A:773:ASP:HB3	2.01	0.43
1:A:745:GLN:OE1	1:A:745:GLN:HA	2.18	0.43
1:A:984:ARG:HD3	1:A:988:ARG:NH2	2.34	0.43
1:A:2049:LEU:HD23	1:A:2049:LEU:HA	1.91	0.43
1:A:2338:ARG:HG3	1:A:2340:VAL:HB	2.00	0.43
1:A:2671:LYS:HA	1:A:2671:LYS:HD2	1.83	0.43
1:C:39:VAL:HG22	1:C:207:LYS:HB2	2.01	0.43
1:C:149:VAL:HG11	1:C:209:VAL:HG23	1.99	0.43
1:C:450:LYS:HA	1:C:450:LYS:HD3	1.79	0.43
1:C:564:GLN:OE1	1:C:574:ILE:HD13	2.19	0.43
1:C:745:GLN:OE1	1:C:745:GLN:HA	2.18	0.43
1:C:996:TYR:HE1	1:C:1606:LEU:HD23	1.83	0.43
1:C:1045:THR:HB	1:C:1046:PRO:HD3	2.01	0.43
1:D:1628:LEU:HD21	1:D:1699:LEU:HB3	2.01	0.43
1:D:2031:LYS:HB3	1:D:2031:LYS:HE2	1.78	0.43
1:A:350:ILE:HD12	1:A:418:GLY:HA3	2.00	0.42
1:A:564:GLN:OE1	1:A:574:ILE:HD13	2.19	0.42
1:A:1045:THR:HB	1:A:1046:PRO:HD3	2.01	0.42
1:A:1312:PHE:O	1:A:1316:ILE:HG22	2.19	0.42
1:A:2070:PRO:HG3	1:A:2121:LEU:HD23	2.01	0.42
1:B:1334:GLU:O	1:B:1339:GLY:HA3	2.19	0.42
1:B:2003:ASN:O	1:B:2007:ILE:HG13	2.19	0.42
1:B:2260:SER:C	1:B:2262:MET:N	2.77	0.42
1:C:893:LEU:HD11	1:C:1064:LEU:HD11	2.01	0.42
1:C:993:LEU:HD21	1:C:1099:LEU:HD11	2.00	0.42
1:C:1042:LYS:HB3	1:C:1042:LYS:HE3	1.77	0.42
1:C:1334:GLU:O	1:C:1339:GLY:HA3	2.19	0.42
1:D:2003:ASN:O	1:D:2007:ILE:HG13	2.19	0.42
1:A:1247:ARG:NE	1:A:1247:ARG:HA	2.34	0.42
1:A:2484:MET:HE2	1:A:2484:MET:HB2	1.75	0.42
1:B:1039:ALA:HA	1:B:1042:LYS:HB2	2.02	0.42
1:C:140:ALA:HB2	1:C:148:ARG:N	2.34	0.42
1:C:1247:ARG:HA	1:C:1247:ARG:NE	2.34	0.42
1:C:1689:MET:HE3	1:C:1689:MET:N	2.34	0.42
1:C:2554:LYS:HE2	1:C:2554:LYS:HB3	1.79	0.42
1:D:515:LEU:HD23	1:D:515:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:613:LYS:O	1:D:616:GLU:HG2	2.19	0.42
1:D:2260:SER:C	1:D:2262:MET:N	2.77	0.42
1:A:146:ALA:HB2	1:A:212:VAL:HB	2.01	0.42
1:A:1100:LEU:HD12	1:A:1100:LEU:HA	1.84	0.42
1:A:2411:ILE:HG23	1:D:2364:GLU:HG2	2.01	0.42
1:B:39:VAL:HG22	1:B:207:LYS:HB2	2.00	0.42
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.92	0.42
1:B:2213:ILE:HD12	1:B:2216:ASN:HB3	2.01	0.42
1:B:2322:PHE:CD2	1:B:2347:LEU:HD11	2.55	0.42
1:C:1306:HIS:C	1:C:1308:GLU:H	2.27	0.42
1:C:2322:PHE:CD2	1:C:2347:LEU:HD11	2.55	0.42
1:D:91:LYS:HG2	1:D:92:LEU:HD23	2.00	0.42
1:D:1039:ALA:HA	1:D:1042:LYS:HB2	2.02	0.42
1:A:613:LYS:O	1:A:616:GLU:HG2	2.19	0.42
1:A:721:LYS:HB2	1:A:721:LYS:HE3	1.67	0.42
1:A:996:TYR:HE1	1:A:1606:LEU:HD23	1.83	0.42
1:A:1058:LEU:HD12	1:A:1058:LEU:HA	1.87	0.42
1:A:1689:MET:HE3	1:A:1689:MET:N	2.35	0.42
1:B:704:PRO:O	1:B:705:HIS:HB3	2.19	0.42
1:B:1628:LEU:HD21	1:B:1699:LEU:HB3	2.01	0.42
1:C:350:ILE:HD12	1:C:418:GLY:HA3	2.00	0.42
1:C:984:ARG:HD3	1:C:988:ARG:NH2	2.34	0.42
1:C:1919:ARG:O	1:C:1920:PRO:C	2.63	0.42
1:C:2003:ASN:O	1:C:2007:ILE:HG13	2.19	0.42
1:C:2553:LYS:O	1:C:2553:LYS:HD3	2.20	0.42
1:C:2563:PHE:H	3:C:2802:ATP:HN62	1.66	0.42
1:D:1058:LEU:HD12	1:D:1058:LEU:HA	1.87	0.42
1:D:1919:ARG:O	1:D:1920:PRO:C	2.63	0.42
1:D:2344:MET:HE2	1:D:2344:MET:HB3	1.81	0.42
1:D:2401:LEU:O	1:D:2404:ILE:HG12	2.19	0.42
1:A:1628:LEU:HD21	1:A:1699:LEU:HB3	2.01	0.42
1:A:2322:PHE:CD2	1:A:2347:LEU:HD11	2.55	0.42
1:B:2070:PRO:HG3	1:B:2121:LEU:HD23	2.01	0.42
1:B:2411:ILE:HD13	1:C:2364:GLU:CG	2.49	0.42
1:C:613:LYS:O	1:C:616:GLU:HG2	2.18	0.42
1:C:731:ARG:HD2	1:C:773:ASP:HB3	2.01	0.42
1:D:146:ALA:HB2	1:D:212:VAL:HB	2.01	0.42
1:D:704:PRO:O	1:D:705:HIS:HB3	2.19	0.42
1:D:893:LEU:HD11	1:D:1064:LEU:HD11	2.01	0.42
1:A:140:ALA:HB2	1:A:148:ARG:N	2.34	0.42
1:A:2553:LYS:O	1:A:2553:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2554:LYS:HB3	1:A:2554:LYS:HE2	1.79	0.42
1:B:2267:LEU:C	1:B:2269:VAL:N	2.77	0.42
1:C:137:ARG:H	1:C:137:ARG:HG2	1.64	0.42
1:C:704:PRO:O	1:C:705:HIS:HB3	2.19	0.42
1:C:1628:LEU:HD21	1:C:1699:LEU:HB3	2.01	0.42
1:D:2261:PRO:O	1:D:2265:VAL:HG23	2.19	0.42
1:D:2322:PHE:CD2	1:D:2347:LEU:HD11	2.55	0.42
1:A:704:PRO:O	1:A:705:HIS:HB3	2.19	0.42
1:A:2179:ARG:O	1:A:2183:THR:HG23	2.19	0.42
1:C:2385:ILE:O	1:C:2389:THR:HG23	2.20	0.42
1:C:2401:LEU:O	1:C:2404:ILE:HG12	2.19	0.42
1:D:79:LYS:HD3	1:D:79:LYS:HA	1.66	0.42
1:D:855:LYS:HA	1:D:858:ASN:ND2	2.35	0.42
1:A:855:LYS:HA	1:A:858:ASN:ND2	2.35	0.42
1:B:1222:ILE:HD13	1:B:1222:ILE:HA	1.94	0.42
1:B:2027:ASN:HB2	1:B:2028:PRO:HD3	2.00	0.42
1:C:1039:ALA:HA	1:C:1042:LYS:HB2	2.01	0.42
1:C:1312:PHE:O	1:C:1316:ILE:HG22	2.19	0.42
1:C:2267:LEU:C	1:C:2269:VAL:N	2.77	0.42
1:D:169:LEU:HD12	1:D:169:LEU:O	2.20	0.42
1:D:1045:THR:HB	1:D:1046:PRO:HD3	2.01	0.42
1:D:1100:LEU:HD12	1:D:1100:LEU:HA	1.84	0.42
1:A:91:LYS:HA	1:A:94:HIS:ND1	2.35	0.42
1:A:1117:ASP:HA	1:A:1120:ARG:HG2	2.02	0.42
1:A:2367:TYR:CE2	1:C:2411:ILE:HD12	2.54	0.42
1:B:140:ALA:HB2	1:B:148:ARG:N	2.34	0.42
1:B:564:GLN:OE1	1:B:574:ILE:HD13	2.19	0.42
1:B:799:ARG:NH2	1:B:1106:VAL:HG23	2.34	0.42
1:B:993:LEU:HD21	1:B:1099:LEU:HD11	2.00	0.42
1:D:39:VAL:HG22	1:D:207:LYS:HB2	2.00	0.42
1:D:1117:ASP:HA	1:D:1120:ARG:HG2	2.02	0.42
1:D:1689:MET:HE3	1:D:1689:MET:N	2.35	0.42
1:A:1108:ASN:O	1:A:1112:ILE:HG12	2.20	0.42
1:A:2415:LEU:HD12	1:A:2415:LEU:HA	1.88	0.42
1:B:169:LEU:HD12	1:B:169:LEU:O	2.20	0.42
1:B:1217:LEU:HD13	1:B:1220:LEU:HD12	2.02	0.42
1:B:1247:ARG:HA	1:B:1247:ARG:NE	2.34	0.42
1:B:1801:LYS:HA	1:B:1801:LYS:HD3	1.89	0.42
1:B:2179:ARG:O	1:B:2183:THR:HG23	2.19	0.42
1:B:2401:LEU:HD12	1:B:2404:ILE:HD11	2.02	0.42
1:C:91:LYS:HA	1:C:94:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ALA:HB2	1:D:148:ARG:N	2.34	0.42
1:D:731:ARG:HD2	1:D:773:ASP:HB3	2.01	0.42
1:D:1247:ARG:HA	1:D:1247:ARG:NE	2.34	0.42
1:D:1952:VAL:HG12	1:D:1995:TYR:HD2	1.80	0.42
1:D:2371:LEU:HD12	1:D:2371:LEU:HA	1.84	0.42
1:A:893:LEU:HD11	1:A:1064:LEU:HD11	2.01	0.41
1:A:1055:ARG:HD3	1:A:1703:TYR:HA	2.02	0.41
1:A:1217:LEU:HD13	1:A:1220:LEU:HD12	2.02	0.41
1:A:2086:GLU:HA	1:A:2089:HIS:NE2	2.35	0.41
1:A:2152:VAL:HG23	1:A:2158:MET:HE3	2.02	0.41
1:A:2213:ILE:HD12	1:A:2216:ASN:HB3	2.01	0.41
1:A:2397:LEU:O	1:A:2400:VAL:HG12	2.20	0.41
1:B:1306:HIS:C	1:B:1308:GLU:H	2.27	0.41
1:B:2385:ILE:O	1:B:2389:THR:HG23	2.20	0.41
1:C:2385:ILE:HA	1:C:2388:VAL:HG12	2.01	0.41
1:C:2401:LEU:HD12	1:C:2404:ILE:HD11	2.02	0.41
1:D:1038:PHE:CD1	1:D:1041:ARG:HD2	2.55	0.41
1:D:1108:ASN:O	1:D:1112:ILE:HG12	2.20	0.41
1:D:2086:GLU:HA	1:D:2089:HIS:NE2	2.35	0.41
1:D:2152:VAL:HG23	1:D:2158:MET:HE3	2.02	0.41
1:B:804:TRP:CH2	1:B:997:LYS:HG2	2.56	0.41
1:B:855:LYS:HA	1:B:858:ASN:ND2	2.35	0.41
1:B:1038:PHE:CD1	1:B:1041:ARG:HD2	2.56	0.41
1:B:1055:ARG:HD3	1:B:1703:TYR:HA	2.02	0.41
1:B:2553:LYS:O	1:B:2553:LYS:HD3	2.20	0.41
1:C:46:LEU:HD23	1:C:46:LEU:HA	1.92	0.41
1:C:1910:THR:HA	1:C:1913:PRO:HB2	2.02	0.41
1:C:1998:GLY:HA2	1:C:1999:PRO:HD3	1.88	0.41
1:C:2086:GLU:HA	1:C:2089:HIS:NE2	2.35	0.41
1:C:2213:ILE:HD12	1:C:2216:ASN:HB3	2.01	0.41
1:C:2484:MET:HE2	1:C:2484:MET:HB2	1.75	0.41
1:D:564:GLN:OE1	1:D:574:ILE:HD13	2.19	0.41
1:D:2385:ILE:O	1:D:2389:THR:HG23	2.20	0.41
1:A:1038:PHE:CD1	1:A:1041:ARG:HD2	2.56	0.41
1:A:2003:ASN:O	1:A:2007:ILE:HG13	2.19	0.41
1:A:2385:ILE:HA	1:A:2388:VAL:HG12	2.01	0.41
1:A:2385:ILE:O	1:A:2389:THR:HG23	2.20	0.41
1:B:146:ALA:HB2	1:B:212:VAL:HB	2.01	0.41
1:B:961:GLN:O	1:B:964:VAL:HG12	2.21	0.41
1:C:2260:SER:C	1:C:2262:MET:N	2.77	0.41
1:D:283:GLU:HB2	1:D:306:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:LYS:HD3	1:D:450:LYS:HA	1.79	0.41
1:D:961:GLN:O	1:D:964:VAL:HG12	2.21	0.41
1:D:2397:LEU:O	1:D:2400:VAL:HG12	2.20	0.41
1:A:351:MET:N	1:A:351:MET:HE2	2.36	0.41
1:A:406:ASP:HB3	1:A:414:MET:HG2	2.03	0.41
1:A:804:TRP:CH2	1:A:997:LYS:HG2	2.56	0.41
1:A:1039:ALA:HA	1:A:1042:LYS:HB2	2.02	0.41
1:A:2381:LEU:HD12	1:A:2381:LEU:HA	1.89	0.41
1:B:283:GLU:HB2	1:B:306:LYS:HB2	2.02	0.41
1:C:799:ARG:HD2	1:C:800:TYR:N	2.33	0.41
1:D:140:ALA:HB2	1:D:147:MET:C	2.46	0.41
1:D:1217:LEU:HD13	1:D:1220:LEU:HD12	2.02	0.41
1:A:140:ALA:HB2	1:A:147:MET:C	2.45	0.41
1:A:169:LEU:HD12	1:A:169:LEU:O	2.20	0.41
1:A:961:GLN:O	1:A:964:VAL:HG12	2.21	0.41
1:B:731:ARG:HD2	1:B:773:ASP:HB3	2.01	0.41
1:B:2401:LEU:O	1:B:2404:ILE:HG12	2.19	0.41
1:C:146:ALA:HB2	1:C:212:VAL:HB	2.01	0.41
1:C:169:LEU:HD12	1:C:169:LEU:O	2.20	0.41
1:C:527:LYS:HD3	1:C:527:LYS:HA	1.91	0.41
1:C:2152:VAL:HG23	1:C:2158:MET:HE3	2.02	0.41
1:D:2192:LYS:HD2	1:D:2563:PHE:CZ	2.56	0.41
1:D:2671:LYS:HA	1:D:2671:LYS:HD2	1.83	0.41
1:A:1910:THR:HA	1:A:1913:PRO:HB2	2.02	0.41
1:A:1993:THR:HA	1:A:2047:LEU:HD23	2.03	0.41
1:A:2192:LYS:HD2	1:A:2563:PHE:CZ	2.56	0.41
1:B:1689:MET:HE3	1:B:1689:MET:N	2.34	0.41
1:B:2397:LEU:O	1:B:2400:VAL:HG12	2.20	0.41
1:B:2567:LEU:HD23	1:B:2567:LEU:HA	1.91	0.41
1:C:1101:VAL:CG1	1:C:1102:SER:H	2.26	0.41
1:C:1217:LEU:HD13	1:C:1220:LEU:HD12	2.02	0.41
1:D:406:ASP:HB3	1:D:414:MET:HG2	2.03	0.41
1:D:802:ARG:H	1:D:802:ARG:HG2	1.65	0.41
1:D:1993:THR:HA	1:D:2047:LEU:HD23	2.03	0.41
1:D:2401:LEU:HD12	1:D:2404:ILE:HD11	2.02	0.41
1:A:2354:LEU:HA	1:A:2354:LEU:HD12	1.86	0.41
1:B:48:ASN:HA	1:B:49:PRO:HD3	1.94	0.41
1:B:799:ARG:HD2	1:B:800:TYR:N	2.33	0.41
1:B:1300:ILE:HD12	1:B:1304:GLY:HA2	2.03	0.41
1:B:2551:LYS:HE2	1:B:2551:LYS:HB2	1.84	0.41
1:C:1055:ARG:HD3	1:C:1703:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1222:ILE:HD13	1:C:1222:ILE:HA	1.94	0.41
1:D:436:LEU:HD23	1:D:436:LEU:HA	1.90	0.41
1:D:2415:LEU:HD12	1:D:2415:LEU:HA	1.88	0.41
1:A:9:LEU:HD23	1:A:115:VAL:HG11	2.03	0.41
1:A:494:LEU:HD12	1:A:494:LEU:HA	1.90	0.41
1:A:655:PHE:O	1:A:659:PRO:HD2	2.21	0.41
1:A:2267:LEU:C	1:A:2269:VAL:N	2.77	0.41
1:B:1042:LYS:HB3	1:B:1042:LYS:HE3	1.77	0.41
1:B:1059:ARG:HH11	1:B:1059:ARG:HB2	1.86	0.41
1:B:1108:ASN:O	1:B:1112:ILE:HG12	2.20	0.41
1:B:1269:LEU:HB3	1:B:1270:GLU:H	1.76	0.41
1:B:2086:GLU:HA	1:B:2089:HIS:NE2	2.35	0.41
1:C:804:TRP:CH2	1:C:997:LYS:HG2	2.56	0.41
1:C:1700:LEU:HD13	1:C:1700:LEU:HA	1.88	0.41
1:C:1933:ASN:HB3	1:C:1936:LEU:HB2	2.03	0.41
1:C:2681:LYS:HD2	1:C:2681:LYS:HA	1.91	0.41
1:D:1912:SER:O	1:D:1913:PRO:C	2.64	0.41
1:A:279:LYS:HD3	1:A:279:LYS:HA	1.90	0.41
1:A:1190:SER:O	1:A:1194:VAL:HG22	2.21	0.41
1:A:1300:ILE:HD12	1:A:1304:GLY:HA2	2.03	0.41
1:A:1919:ARG:O	1:A:1920:PRO:C	2.63	0.41
1:A:2401:LEU:HD12	1:A:2404:ILE:HD11	2.02	0.41
1:B:1117:ASP:HA	1:B:1120:ARG:HG2	2.02	0.41
1:B:1190:SER:O	1:B:1194:VAL:HG22	2.21	0.41
1:B:1919:ARG:O	1:B:1920:PRO:C	2.63	0.41
1:B:2192:LYS:HD2	1:B:2563:PHE:CZ	2.56	0.41
1:C:406:ASP:HB3	1:C:414:MET:HG2	2.03	0.41
1:C:655:PHE:O	1:C:659:PRO:HD2	2.21	0.41
1:C:855:LYS:HA	1:C:858:ASN:ND2	2.35	0.41
1:C:1108:ASN:O	1:C:1112:ILE:HG12	2.20	0.41
1:C:2192:LYS:HD2	1:C:2563:PHE:CZ	2.55	0.41
1:C:2397:LEU:O	1:C:2400:VAL:HG12	2.20	0.41
1:D:57:LEU:HD13	1:D:57:LEU:HA	1.94	0.41
1:D:91:LYS:HA	1:D:94:HIS:ND1	2.35	0.41
1:D:200:LEU:HD12	1:D:200:LEU:HA	1.90	0.41
1:D:1183:LYS:HE3	1:D:1183:LYS:HB3	1.92	0.41
1:D:1951:LEU:O	1:D:1955:THR:HG22	2.21	0.41
1:D:2553:LYS:O	1:D:2553:LYS:HD3	2.20	0.41
1:D:2648:ASN:HA	1:D:2651:GLU:HB3	2.03	0.41
1:A:91:LYS:HZ2	1:D:1972:LEU:H	1.69	0.41
1:A:756:LEU:HD23	1:A:756:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2262:MET:HE3	1:A:2262:MET:HB2	1.98	0.41
1:B:406:ASP:HB3	1:B:414:MET:HG2	2.03	0.41
1:B:889:LEU:HD23	1:B:972:LYS:HG2	2.03	0.41
1:B:995:ILE:HD13	1:B:995:ILE:HA	1.93	0.41
1:B:1668:GLU:HA	1:B:1671:CYS:HB2	2.03	0.41
1:B:1998:GLY:HA2	1:B:1999:PRO:HD3	1.88	0.41
1:B:2239:PHE:HD2	1:B:2239:PHE:HA	1.76	0.41
1:C:351:MET:HE2	1:C:351:MET:N	2.36	0.41
1:C:531:GLY:C	1:C:533:GLY:H	2.29	0.41
1:C:781:LEU:HD12	1:C:781:LEU:HA	1.98	0.41
1:C:961:GLN:O	1:C:964:VAL:HG12	2.21	0.41
1:C:1190:SER:O	1:C:1194:VAL:HG22	2.21	0.41
1:C:1268:LEU:O	1:C:1269:LEU:HB2	2.21	0.41
1:C:1993:THR:HA	1:C:2047:LEU:HD23	2.03	0.41
1:C:2371:LEU:HD12	1:C:2371:LEU:HA	1.84	0.41
1:D:494:LEU:HD12	1:D:494:LEU:HA	1.90	0.41
1:A:1222:ILE:HD13	1:A:1222:ILE:HA	1.94	0.40
1:A:1912:SER:O	1:A:1913:PRO:C	2.64	0.40
1:A:2648:ASN:HA	1:A:2651:GLU:HB3	2.03	0.40
1:B:351:MET:N	1:B:351:MET:HE2	2.36	0.40
1:B:1933:ASN:HB3	1:B:1936:LEU:HB2	2.03	0.40
1:B:2667:LEU:HD22	1:C:2662:GLN:HB3	2.02	0.40
1:C:721:LYS:HE3	1:C:721:LYS:HB2	1.67	0.40
1:C:1068:ASP:OD1	1:C:1068:ASP:C	2.64	0.40
1:C:1668:GLU:HA	1:C:1671:CYS:HB2	2.03	0.40
1:C:1951:LEU:O	1:C:1955:THR:HG22	2.21	0.40
1:C:2031:LYS:HE2	1:C:2031:LYS:HB3	1.78	0.40
1:C:2381:LEU:HD12	1:C:2381:LEU:HA	1.89	0.40
1:D:2267:LEU:C	1:D:2269:VAL:N	2.77	0.40
1:A:531:GLY:C	1:A:533:GLY:H	2.29	0.40
1:A:889:LEU:HD23	1:A:972:LYS:HG2	2.03	0.40
1:A:1066:MET:HE2	1:A:1066:MET:HA	2.04	0.40
1:A:1268:LEU:O	1:A:1269:LEU:HB2	2.21	0.40
1:A:2038:LEU:HD23	1:A:2038:LEU:HA	1.92	0.40
1:B:531:GLY:C	1:B:533:GLY:H	2.29	0.40
1:B:655:PHE:O	1:B:659:PRO:HD2	2.21	0.40
1:B:1068:ASP:OD1	1:B:1068:ASP:C	2.64	0.40
1:B:1268:LEU:O	1:B:1269:LEU:HB2	2.21	0.40
1:B:2574:ASN:HA	1:D:2628:ARG:NH2	2.33	0.40
1:B:2671:LYS:HA	1:B:2671:LYS:HD2	1.83	0.40
1:C:1059:ARG:HH11	1:C:1059:ARG:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1066:MET:HA	1:C:1066:MET:HE2	2.04	0.40
1:C:1117:ASP:HA	1:C:1120:ARG:HG2	2.02	0.40
1:C:1912:SER:O	1:C:1913:PRO:C	2.64	0.40
1:C:2126:LEU:HD12	1:C:2126:LEU:HA	1.88	0.40
1:D:804:TRP:CH2	1:D:997:LYS:HG2	2.56	0.40
1:D:889:LEU:HD23	1:D:972:LYS:HG2	2.03	0.40
1:D:1190:SER:O	1:D:1194:VAL:HG22	2.21	0.40
1:D:2681:LYS:HA	1:D:2681:LYS:HD2	1.91	0.40
1:A:283:GLU:HB2	1:A:306:LYS:HB2	2.02	0.40
1:A:515:LEU:HD23	1:A:515:LEU:HA	1.84	0.40
1:A:738:ALA:HB1	1:A:780:ARG:HG2	2.04	0.40
1:A:2126:LEU:HD12	1:A:2126:LEU:HA	1.88	0.40
1:B:91:LYS:HA	1:B:94:HIS:ND1	2.35	0.40
1:B:1951:LEU:O	1:B:1955:THR:HG22	2.21	0.40
1:C:140:ALA:HB2	1:C:147:MET:C	2.45	0.40
1:C:738:ALA:HB1	1:C:780:ARG:HG2	2.04	0.40
1:C:1749:LEU:HD23	1:C:1749:LEU:HA	1.90	0.40
1:D:1231:MET:SD	1:D:1231:MET:N	2.95	0.40
1:A:257:GLU:C	1:A:258:LYS:HE2	2.47	0.40
1:A:1956:LEU:HD23	1:A:2010:HIS:CD2	2.57	0.40
1:B:9:LEU:HD23	1:B:115:VAL:HG11	2.03	0.40
1:B:255:ASP:N	1:B:255:ASP:OD1	2.55	0.40
1:B:1664:MET:HE2	1:B:1664:MET:O	2.22	0.40
1:B:1910:THR:HA	1:B:1913:PRO:HB2	2.02	0.40
1:B:1993:THR:HA	1:B:2047:LEU:HD23	2.03	0.40
1:B:2048:LEU:HD13	1:B:2048:LEU:HA	1.92	0.40
1:C:734:LEU:HD23	1:C:734:LEU:HA	1.91	0.40
1:C:2262:MET:HE3	1:C:2262:MET:HB2	1.98	0.40
1:D:9:LEU:HD23	1:D:115:VAL:HG11	2.03	0.40
1:D:257:GLU:C	1:D:258:LYS:HE2	2.47	0.40
1:D:306:LYS:HB3	1:D:306:LYS:HE3	1.79	0.40
1:D:1910:THR:HA	1:D:1913:PRO:HB2	2.02	0.40
1:A:353:THR:O	1:A:354:LEU:HD23	2.22	0.40
1:A:1664:MET:O	1:A:1664:MET:HE2	2.22	0.40
1:A:1916:THR:HG23	1:A:1917:ILE:N	2.37	0.40
1:B:140:ALA:HB2	1:B:147:MET:C	2.46	0.40
1:B:450:LYS:HA	1:B:450:LYS:HD3	1.79	0.40
1:B:1231:MET:SD	1:B:1231:MET:N	2.95	0.40
1:B:1912:SER:O	1:B:1913:PRO:C	2.64	0.40
1:B:1956:LEU:HD23	1:B:2010:HIS:CD2	2.57	0.40
1:B:2152:VAL:HG23	1:B:2158:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1038:PHE:CD1	1:C:1041:ARG:HD2	2.55	0.40
1:C:2060:ASN:O	1:C:2064:ILE:HG12	2.22	0.40
1:D:1652:PHE:CE1	1:D:1656:LEU:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2282/2701 (84%)	2060 (90%)	212 (9%)	10 (0%)	30	59
1	B	2282/2701 (84%)	2061 (90%)	211 (9%)	10 (0%)	30	59
1	C	2282/2701 (84%)	2060 (90%)	212 (9%)	10 (0%)	30	59
1	D	2282/2701 (84%)	2060 (90%)	212 (9%)	10 (0%)	30	59
All	All	9128/10804 (84%)	8241 (90%)	847 (9%)	40 (0%)	31	59

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	499	THR
1	A	1070	ALA
1	A	1307	VAL
1	A	1336	ILE
1	A	1506	GLN
1	A	1801	LYS
1	B	499	THR
1	B	1070	ALA
1	B	1307	VAL
1	B	1336	ILE
1	B	1506	GLN
1	B	1801	LYS

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Mol	Chain	Res	Type
1	C	499	THR
1	C	1070	ALA
1	C	1307	VAL
1	C	1336	ILE
1	C	1506	GLN
1	C	1801	LYS
1	D	499	THR
1	D	1070	ALA
1	D	1307	VAL
1	D	1336	ILE
1	D	1506	GLN
1	D	1801	LYS
1	A	1919	ARG
1	B	1919	ARG
1	C	1919	ARG
1	D	1919	ARG
1	A	705	HIS
1	B	705	HIS
1	C	705	HIS
1	D	705	HIS
1	A	1690	GLU
1	B	1690	GLU
1	C	1690	GLU
1	D	1690	GLU
1	A	1913	PRO
1	B	1913	PRO
1	C	1913	PRO
1	D	1913	PRO

5.3.2 Protein sidechains (i)

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	1854/2411 (77%)	1803 (97%)	51 (3%)	38 57
1	B	1854/2411 (77%)	1803 (97%)	51 (3%)	38 57
1	C	1854/2411 (77%)	1803 (97%)	51 (3%)	38 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	1854/2411 (77%)	1801 (97%)	53 (3%)	37 56
All	All	7416/9644 (77%)	7210 (97%)	206 (3%)	38 57

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	117	TYR
1	A	162	TYR
1	A	212	VAL
1	A	288	HIS
1	A	413	VAL
1	A	432	VAL
1	A	434	VAL
1	A	498	ILE
1	A	602	ASN
1	A	604	LYS
1	A	647	VAL
1	A	786	HIS
1	A	864	VAL
1	A	873	TYR
1	A	885	LEU
1	A	973	VAL
1	A	1000	PHE
1	A	1106	VAL
1	A	1186	LEU
1	A	1210	MET
1	A	1224	TYR
1	A	1256	LEU
1	A	1259	HIS
1	A	1293	VAL
1	A	1628	LEU
1	A	1629	VAL
1	A	1634	SER
1	A	1638	LEU
1	A	1682	LEU
1	A	1700	LEU
1	A	1788	GLN
1	A	1913	PRO
1	A	1917	ILE
1	A	1953	CYS
1	A	2011	GLU

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Mol	Chain	Res	Type
1	A	2034	MET
1	A	2048	LEU
1	A	2106	HIS
1	A	2182	ASN
1	A	2219	LEU
1	A	2344	MET
1	A	2348	TYR
1	A	2354	LEU
1	A	2360	LEU
1	A	2367	TYR
1	A	2387	SER
1	A	2425	VAL
1	A	2532	VAL
1	A	2582	HIS
1	A	2622	ASN
1	B	35	ASP
1	B	117	TYR
1	B	162	TYR
1	B	212	VAL
1	B	288	HIS
1	B	413	VAL
1	B	432	VAL
1	B	434	VAL
1	B	498	ILE
1	B	602	ASN
1	B	604	LYS
1	B	647	VAL
1	B	761	ILE
1	B	786	HIS
1	B	864	VAL
1	B	873	TYR
1	B	885	LEU
1	B	973	VAL
1	B	1000	PHE
1	B	1106	VAL
1	B	1186	LEU
1	B	1210	MET
1	B	1224	TYR
1	B	1256	LEU
1	B	1259	HIS
1	B	1293	VAL
1	B	1628	LEU

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Mol	Chain	Res	Type
1	B	1629	VAL
1	B	1634	SER
1	B	1638	LEU
1	B	1682	LEU
1	B	1700	LEU
1	B	1788	GLN
1	B	1913	PRO
1	B	1917	ILE
1	B	1953	CYS
1	B	2011	GLU
1	B	2048	LEU
1	B	2106	HIS
1	B	2182	ASN
1	B	2219	LEU
1	B	2344	MET
1	B	2348	TYR
1	B	2354	LEU
1	B	2360	LEU
1	B	2367	TYR
1	B	2387	SER
1	B	2425	VAL
1	B	2532	VAL
1	B	2582	HIS
1	B	2622	ASN
1	C	35	ASP
1	C	117	TYR
1	C	162	TYR
1	C	212	VAL
1	C	288	HIS
1	C	413	VAL
1	C	432	VAL
1	C	434	VAL
1	C	498	ILE
1	C	602	ASN
1	C	604	LYS
1	C	647	VAL
1	C	761	ILE
1	C	786	HIS
1	C	873	TYR
1	C	885	LEU
1	C	973	VAL
1	C	1000	PHE

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Mol	Chain	Res	Type
1	C	1106	VAL
1	C	1186	LEU
1	C	1210	MET
1	C	1224	TYR
1	C	1256	LEU
1	C	1259	HIS
1	C	1293	VAL
1	C	1628	LEU
1	C	1629	VAL
1	C	1634	SER
1	C	1637	LEU
1	C	1638	LEU
1	C	1675	LEU
1	C	1682	LEU
1	C	1700	LEU
1	C	1788	GLN
1	C	1913	PRO
1	C	1917	ILE
1	C	1953	CYS
1	C	2011	GLU
1	C	2034	MET
1	C	2048	LEU
1	C	2182	ASN
1	C	2344	MET
1	C	2348	TYR
1	C	2354	LEU
1	C	2360	LEU
1	C	2367	TYR
1	C	2387	SER
1	C	2425	VAL
1	C	2532	VAL
1	C	2582	HIS
1	C	2622	ASN
1	D	35	ASP
1	D	117	TYR
1	D	162	TYR
1	D	212	VAL
1	D	288	HIS
1	D	413	VAL
1	D	432	VAL
1	D	434	VAL
1	D	498	ILE

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Mol	Chain	Res	Type
1	D	602	ASN
1	D	604	LYS
1	D	647	VAL
1	D	761	ILE
1	D	786	HIS
1	D	873	TYR
1	D	885	LEU
1	D	973	VAL
1	D	1000	PHE
1	D	1106	VAL
1	D	1186	LEU
1	D	1210	MET
1	D	1224	TYR
1	D	1256	LEU
1	D	1259	HIS
1	D	1293	VAL
1	D	1628	LEU
1	D	1629	VAL
1	D	1634	SER
1	D	1638	LEU
1	D	1675	LEU
1	D	1682	LEU
1	D	1700	LEU
1	D	1788	GLN
1	D	1913	PRO
1	D	1917	ILE
1	D	1953	CYS
1	D	2011	GLU
1	D	2034	MET
1	D	2048	LEU
1	D	2068	MET
1	D	2125	MET
1	D	2126	LEU
1	D	2182	ASN
1	D	2344	MET
1	D	2348	TYR
1	D	2354	LEU
1	D	2360	LEU
1	D	2367	TYR
1	D	2387	SER
1	D	2425	VAL
1	D	2532	VAL

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Mol	Chain	Res	Type
1	D	2582	HIS
1	D	2622	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	ASN
1	A	491	GLN
1	A	745	GLN
1	A	848	GLN
1	A	1033	GLN
1	A	1078	GLN
1	A	1096	GLN
1	A	1118	GLN
1	A	1196	ASN
1	A	1276	HIS
1	A	1298	HIS
1	A	1306	HIS
1	A	1701	ASN
1	A	2241	ASN
1	A	2383	ASN
1	A	2574	ASN
1	A	2644	ASN
1	B	107	ASN
1	B	449	ASN
1	B	491	GLN
1	B	745	GLN
1	B	848	GLN
1	B	1033	GLN
1	B	1078	GLN
1	B	1092	GLN
1	B	1096	GLN
1	B	1118	GLN
1	B	1196	ASN
1	B	1202	GLN
1	B	1276	HIS
1	B	1298	HIS
1	B	1306	HIS
1	B	1701	ASN
1	B	2241	ASN
1	B	2349	HIS
1	B	2383	ASN

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Mol	Chain	Res	Type
1	B	2574	ASN
1	B	2644	ASN
1	B	2662	GLN
1	C	449	ASN
1	C	491	GLN
1	C	745	GLN
1	C	750	ASN
1	C	848	GLN
1	C	1033	GLN
1	C	1067	HIS
1	C	1078	GLN
1	C	1092	GLN
1	C	1096	GLN
1	C	1118	GLN
1	C	1196	ASN
1	C	1276	HIS
1	C	1298	HIS
1	C	1701	ASN
1	C	2241	ASN
1	C	2349	HIS
1	C	2383	ASN
1	C	2574	ASN
1	C	2582	HIS
1	C	2644	ASN
1	C	2662	GLN
1	D	449	ASN
1	D	491	GLN
1	D	745	GLN
1	D	848	GLN
1	D	1033	GLN
1	D	1078	GLN
1	D	1092	GLN
1	D	1096	GLN
1	D	1118	GLN
1	D	1196	ASN
1	D	1202	GLN
1	D	1276	HIS
1	D	1298	HIS
1	D	1701	ASN
1	D	2241	ASN
1	D	2349	HIS
1	D	2383	ASN

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Mol	Chain	Res	Type
1	D	2574	ASN
1	D	2644	ASN
1	D	2662	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	I3P	C	2803	-	24,24,24	2.18	3 (12%)	39,39,39	0.87	0
6	PLX	B	2805	-	39,39,51	0.40	0	41,47,59	0.38	0
6	PLX	A	2805	-	39,39,51	0.41	0	41,47,59	0.38	0
6	PLX	D	2805	-	39,39,51	0.40	0	41,47,59	0.38	0
3	ATP	C	2802	-	32,33,33	0.27	0	48,52,52	0.37	0
3	ATP	A	2802	-	32,33,33	0.27	0	48,52,52	0.37	0
4	I3P	B	2803	-	24,24,24	2.19	3 (12%)	39,39,39	0.87	0
3	ATP	B	2802	-	32,33,33	0.27	0	48,52,52	0.37	0
4	I3P	D	2803	-	24,24,24	2.18	3 (12%)	39,39,39	0.87	0
4	I3P	A	2803	-	24,24,24	2.19	3 (12%)	39,39,39	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ATP	D	2802	-	32,33,33	0.28	0	48,52,52	0.37	0
6	PLX	C	2805	-	39,39,51	0.41	0	41,47,59	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	I3P	C	2803	-	-	1/15/39/39	0/1/1/1
6	PLX	B	2805	-	-	9/43/43/55	-
6	PLX	A	2805	-	-	8/43/43/55	-
6	PLX	D	2805	-	-	8/43/43/55	-
3	ATP	C	2802	-	-	6/22/38/38	0/3/3/3
3	ATP	A	2802	-	-	6/22/38/38	0/3/3/3
4	I3P	B	2803	-	-	1/15/39/39	0/1/1/1
3	ATP	B	2802	-	-	6/22/38/38	0/3/3/3
4	I3P	D	2803	-	-	1/15/39/39	0/1/1/1
4	I3P	A	2803	-	-	1/15/39/39	0/1/1/1
3	ATP	D	2802	-	-	6/22/38/38	0/3/3/3
6	PLX	C	2805	-	-	8/43/43/55	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2803	I3P	P4-O4	6.06	1.70	1.59
4	A	2803	I3P	P4-O4	6.02	1.70	1.59
4	D	2803	I3P	P4-O4	6.01	1.70	1.59
4	C	2803	I3P	P4-O4	5.99	1.70	1.59
4	A	2803	I3P	P5-O5	5.97	1.70	1.59
4	D	2803	I3P	P5-O5	5.96	1.70	1.59
4	B	2803	I3P	P5-O5	5.93	1.69	1.59
4	C	2803	I3P	P5-O5	5.93	1.69	1.59
4	A	2803	I3P	P1-O1	5.70	1.69	1.59
4	D	2803	I3P	P1-O1	5.69	1.69	1.59
4	B	2803	I3P	P1-O1	5.68	1.69	1.59
4	C	2803	I3P	P1-O1	5.68	1.69	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2805	PLX	C3-C4-O6-C6
6	A	2805	PLX	C5-C4-O6-C6
6	A	2805	PLX	C2-O1-P1-O2
6	B	2805	PLX	C3-C4-O6-C6
6	B	2805	PLX	C5-C4-O6-C6
6	B	2805	PLX	C2-O1-P1-O2
6	C	2805	PLX	C3-C4-O6-C6
6	C	2805	PLX	C5-C4-O6-C6
6	C	2805	PLX	C2-O1-P1-O2
6	D	2805	PLX	C3-C4-O6-C6
6	D	2805	PLX	C5-C4-O6-C6
6	D	2805	PLX	C2-O1-P1-O2
3	A	2802	ATP	O4'-C4'-C5'-O5'
3	B	2802	ATP	O4'-C4'-C5'-O5'
3	C	2802	ATP	O4'-C4'-C5'-O5'
3	D	2802	ATP	O4'-C4'-C5'-O5'
6	A	2805	PLX	O9-C24-C25-C26
6	B	2805	PLX	O9-C24-C25-C26
6	C	2805	PLX	O9-C24-C25-C26
6	D	2805	PLX	O9-C24-C25-C26
3	A	2802	ATP	C3'-C4'-C5'-O5'
3	B	2802	ATP	C3'-C4'-C5'-O5'
3	C	2802	ATP	C3'-C4'-C5'-O5'
3	D	2802	ATP	C3'-C4'-C5'-O5'
3	A	2802	ATP	PB-O3A-PA-O5'
3	B	2802	ATP	PB-O3A-PA-O5'
3	C	2802	ATP	PB-O3A-PA-O5'
3	D	2802	ATP	PB-O3A-PA-O5'
6	A	2805	PLX	C1-C2-O1-P1
6	B	2805	PLX	C1-C2-O1-P1
6	C	2805	PLX	C1-C2-O1-P1
6	D	2805	PLX	C1-C2-O1-P1
6	A	2805	PLX	N1-C1-C2-O1
6	B	2805	PLX	N1-C1-C2-O1
6	C	2805	PLX	N1-C1-C2-O1
6	D	2805	PLX	N1-C1-C2-O1
4	A	2803	I3P	C5-O5-P5-O51
4	B	2803	I3P	C5-O5-P5-O51
4	C	2803	I3P	C5-O5-P5-O51
4	D	2803	I3P	C5-O5-P5-O51
6	A	2805	PLX	C3-C4-C5-O8
6	B	2805	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
6	C	2805	PLX	C3-C4-C5-O8
6	D	2805	PLX	C3-C4-C5-O8
3	A	2802	ATP	C5'-O5'-PA-O1A
3	B	2802	ATP	C5'-O5'-PA-O1A
3	C	2802	ATP	C5'-O5'-PA-O1A
3	D	2802	ATP	C5'-O5'-PA-O1A
6	A	2805	PLX	O6-C4-C5-O8
6	B	2805	PLX	O6-C4-C5-O8
6	C	2805	PLX	O6-C4-C5-O8
6	D	2805	PLX	O6-C4-C5-O8
3	B	2802	ATP	PB-O3A-PA-O1A
3	C	2802	ATP	PB-O3A-PA-O1A
3	D	2802	ATP	PB-O3A-PA-O1A
6	B	2805	PLX	O9-C24-O8-C5
3	A	2802	ATP	PB-O3A-PA-O1A
3	A	2802	ATP	PB-O3A-PA-O2A
3	B	2802	ATP	PB-O3A-PA-O2A
3	C	2802	ATP	PB-O3A-PA-O2A
3	D	2802	ATP	PB-O3A-PA-O2A

There are no ring outliers.

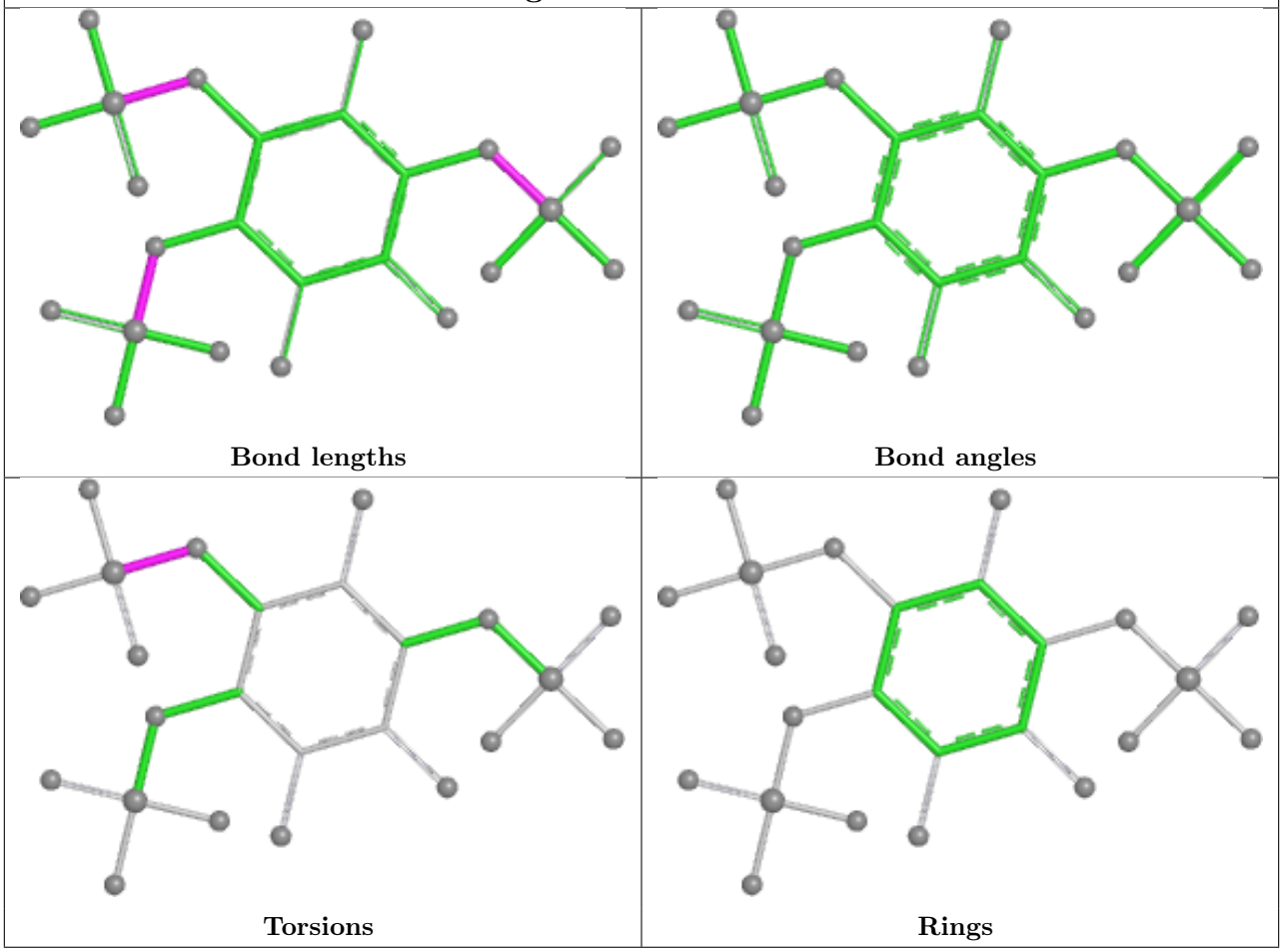
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2805	PLX	1	0
6	A	2805	PLX	1	0
6	D	2805	PLX	1	0
3	C	2802	ATP	2	0
3	A	2802	ATP	2	0
3	B	2802	ATP	2	0
3	D	2802	ATP	2	0
6	C	2805	PLX	1	0

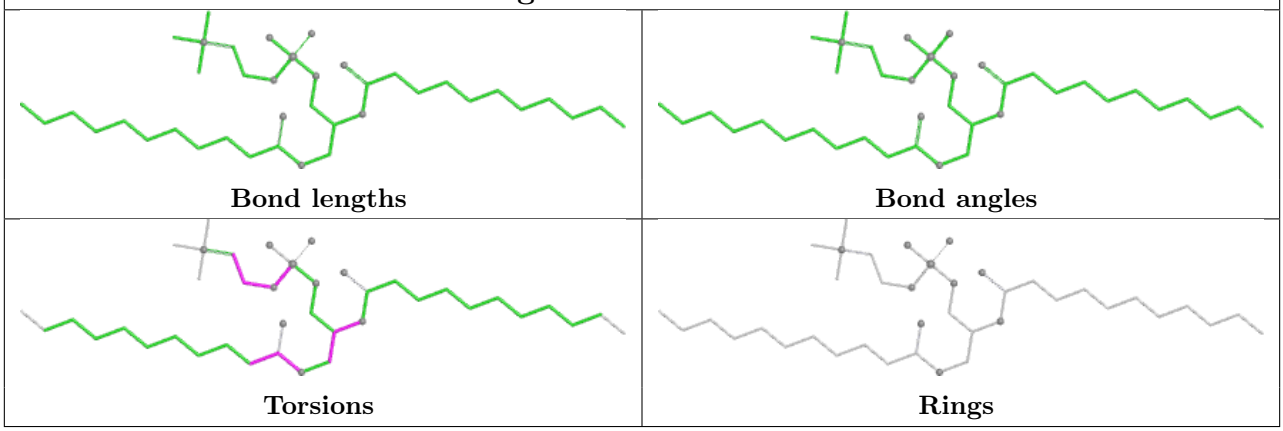
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

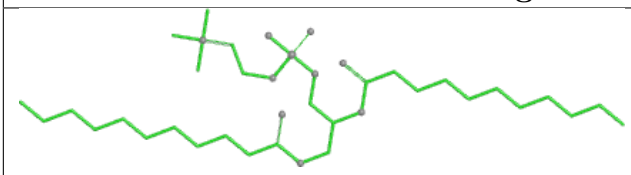
Ligand I3P C 2803



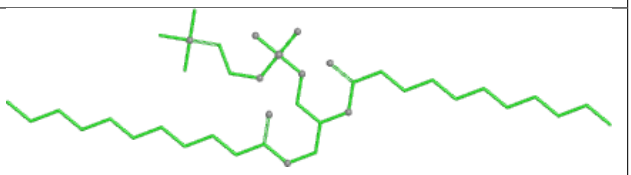
Ligand PLX B 2805



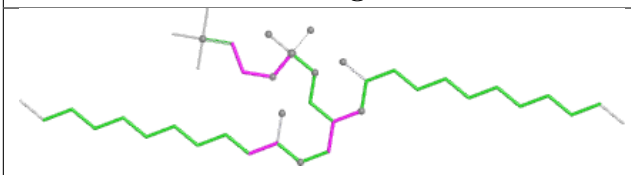
Ligand PLX A 2805



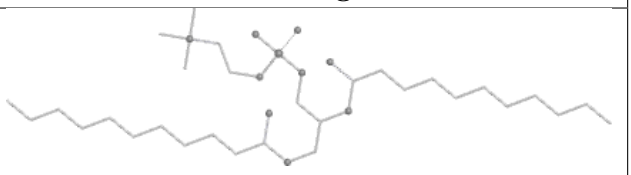
Bond lengths



Bond angles

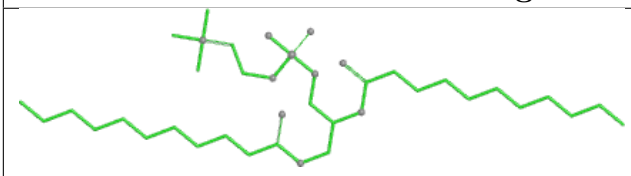


Torsions

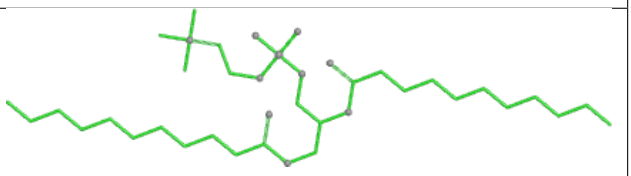


Rings

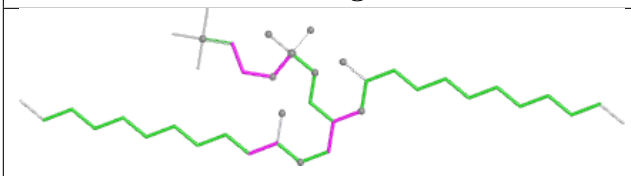
Ligand PLX D 2805



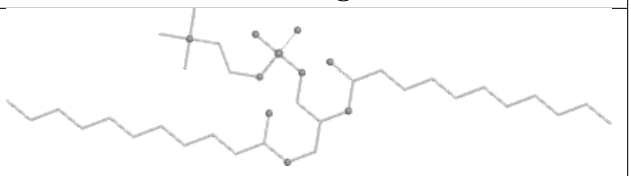
Bond lengths



Bond angles

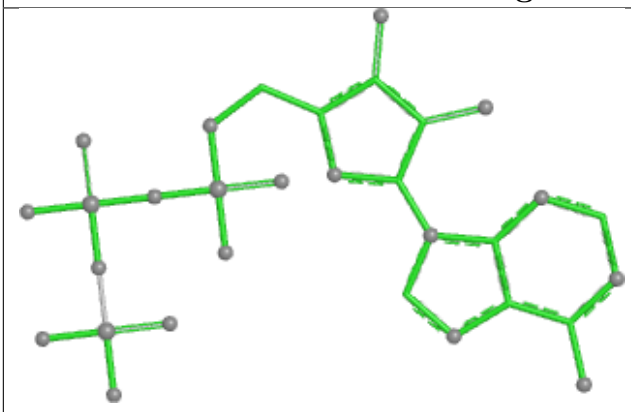


Torsions

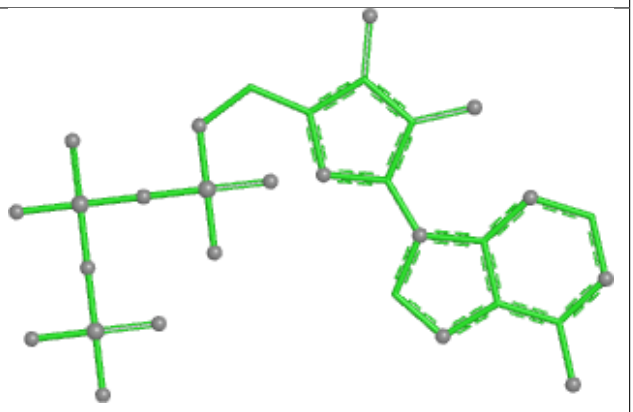


Rings

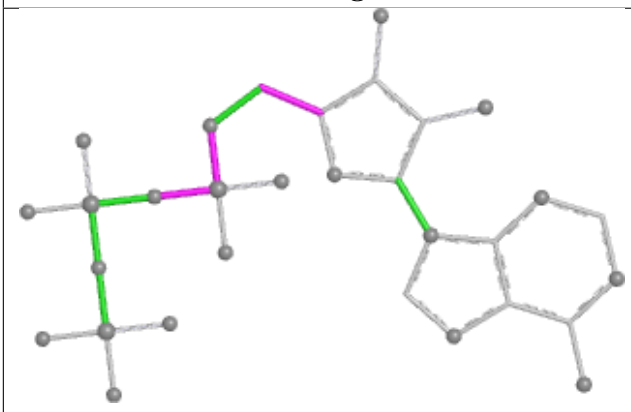
Ligand ATP C 2802



Bond lengths



Bond angles



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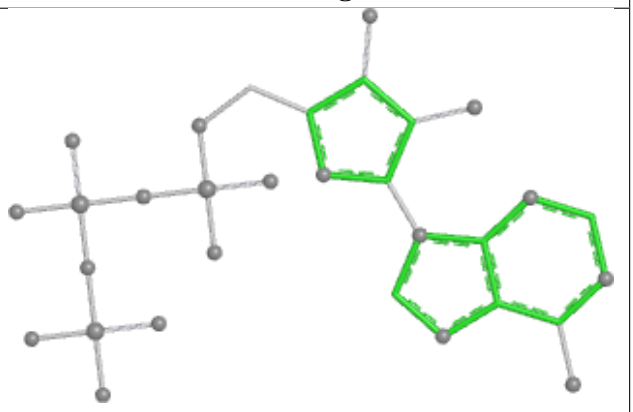
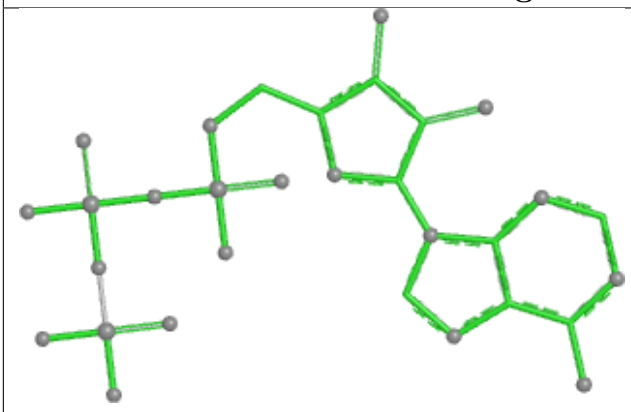
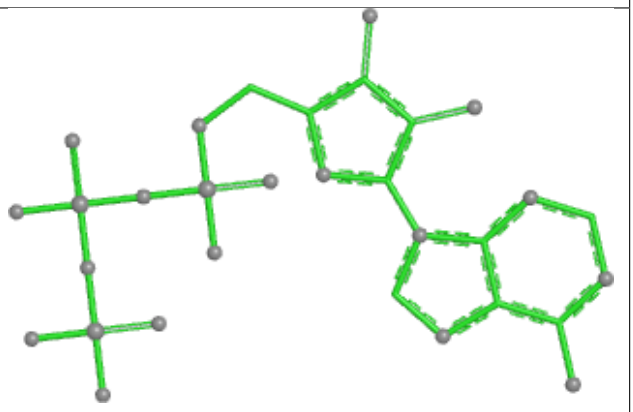


Rings

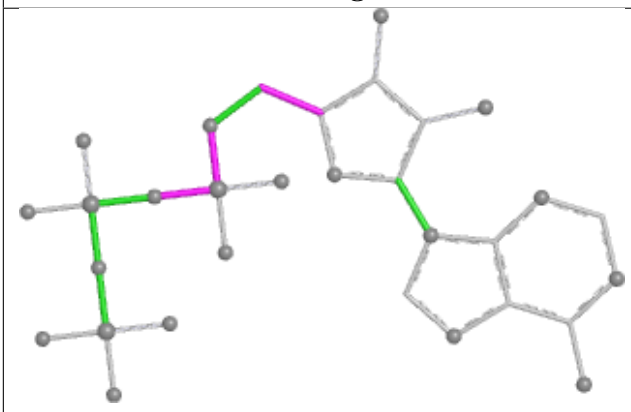
Ligand ATP A 2802



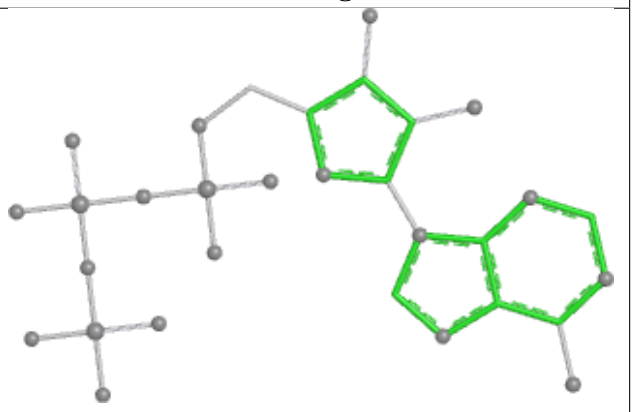
Bond lengths



Bond angles

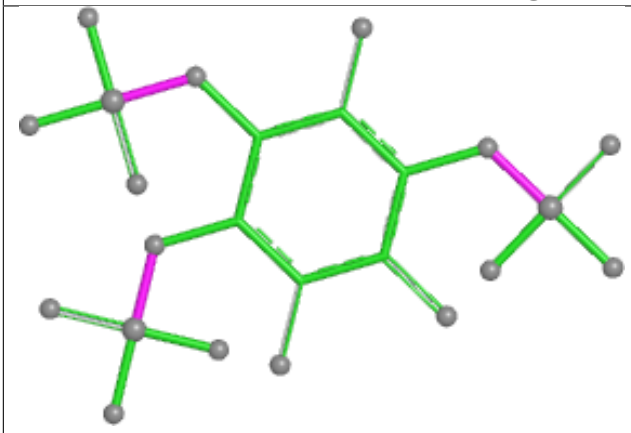


Torsions

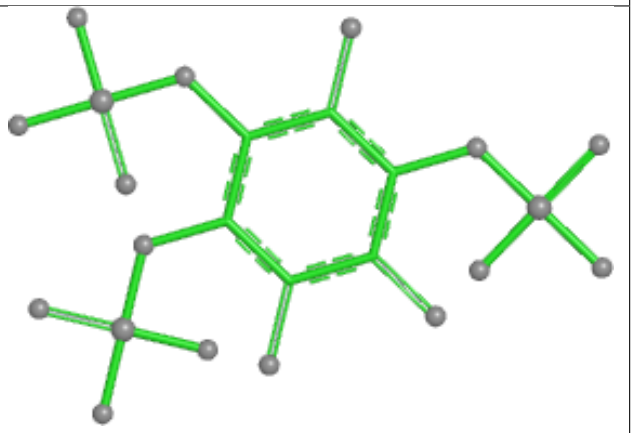


Rings

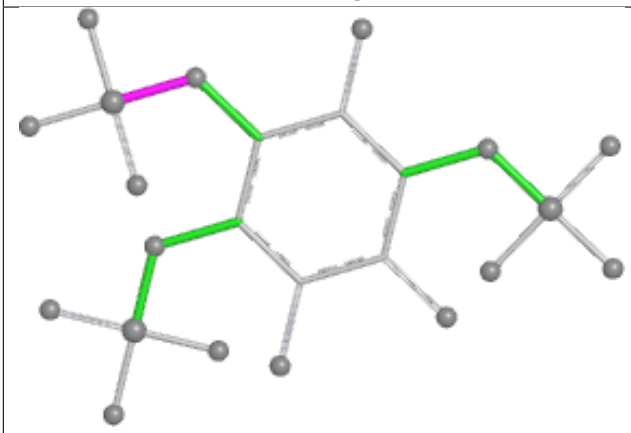
Ligand I3P B 2803



Bond lengths



Bond angles



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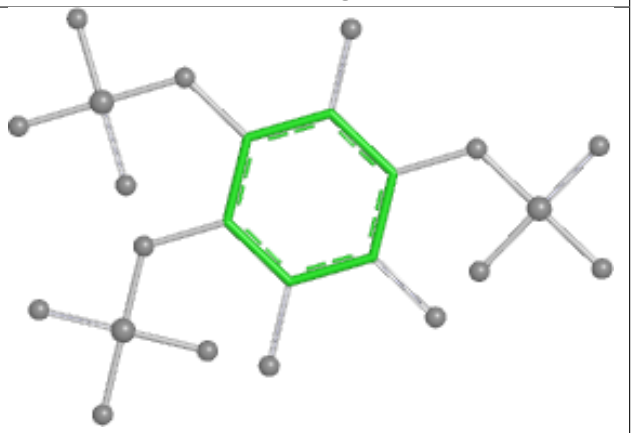
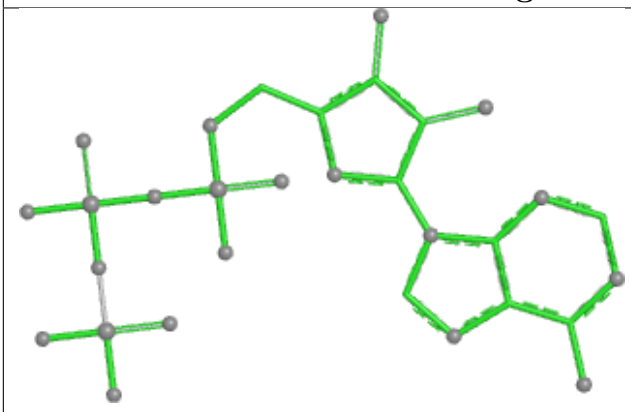
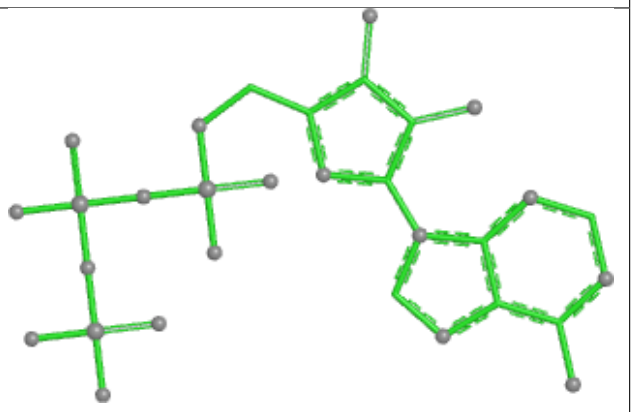


Rings

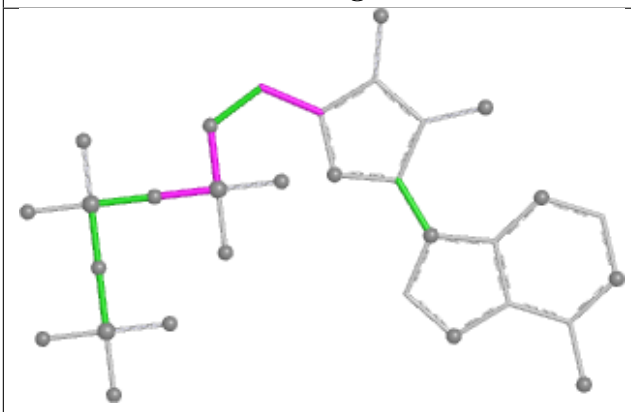
Ligand ATP B 2802



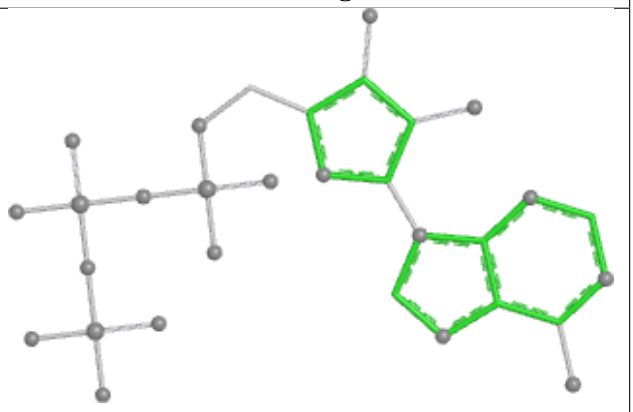
Bond lengths



Bond angles

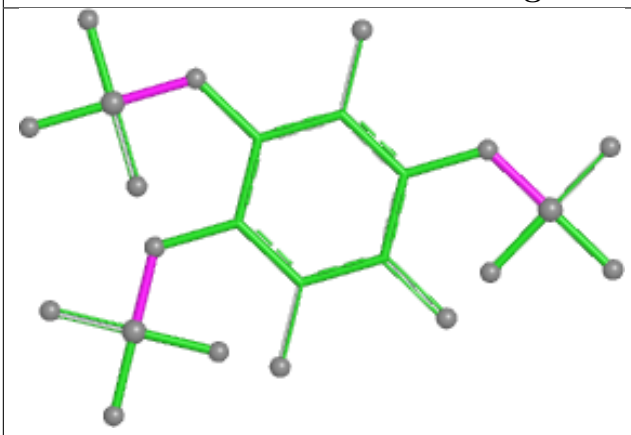


Torsions

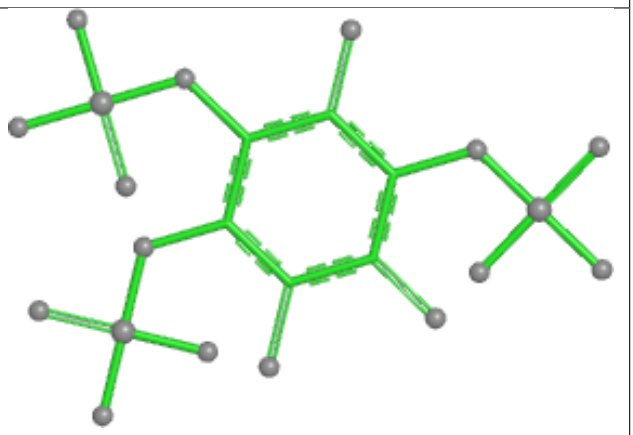


Rings

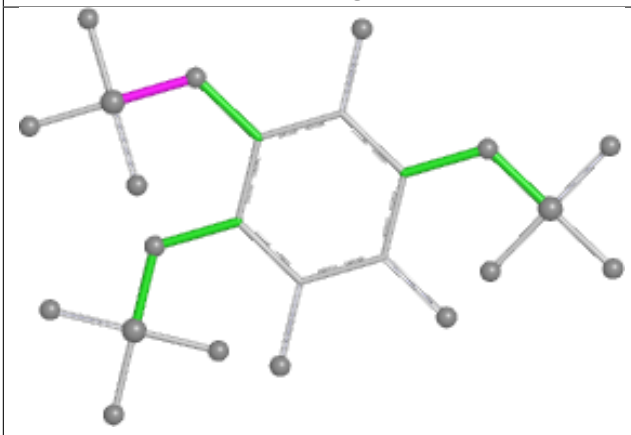
Ligand I3P D 2803



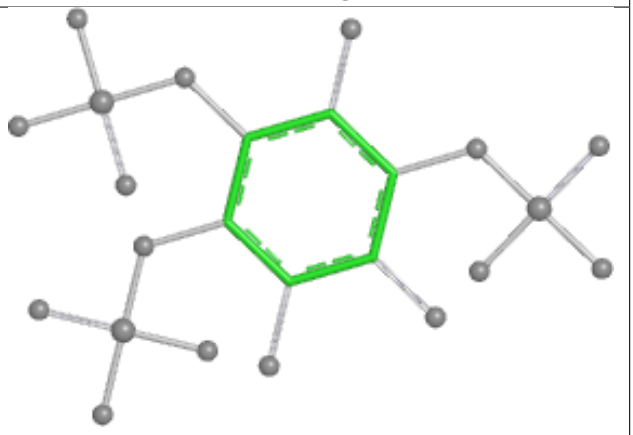
Bond lengths



Bond angles

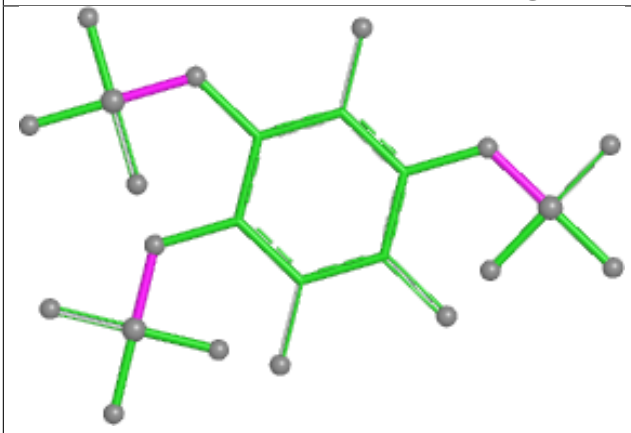


Torsions

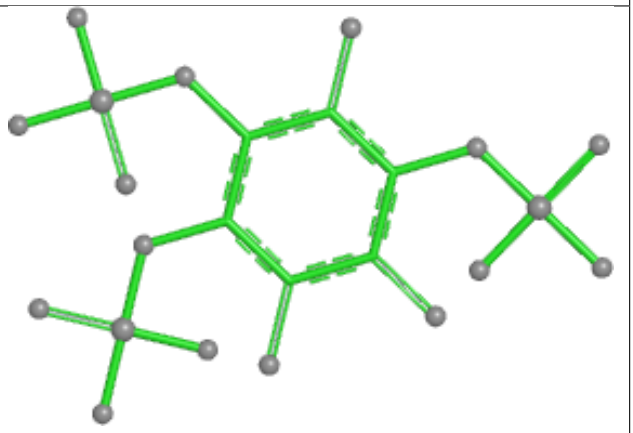


Rings

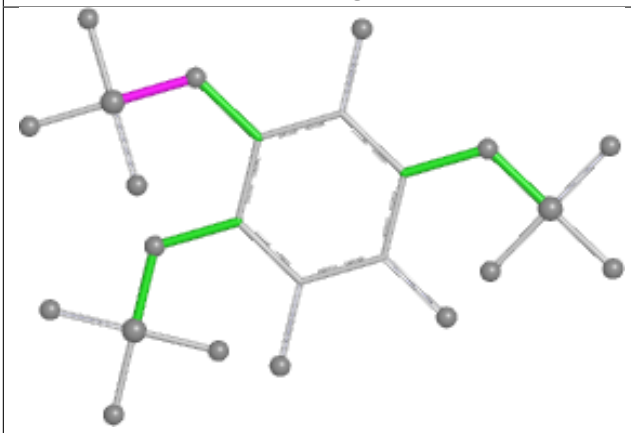
Ligand I3P A 2803



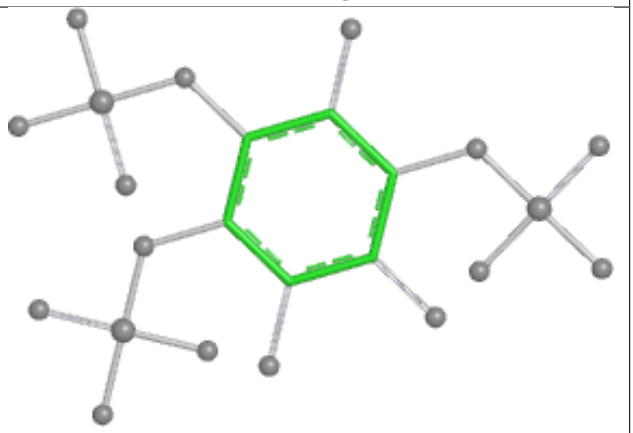
Bond lengths



Bond angles

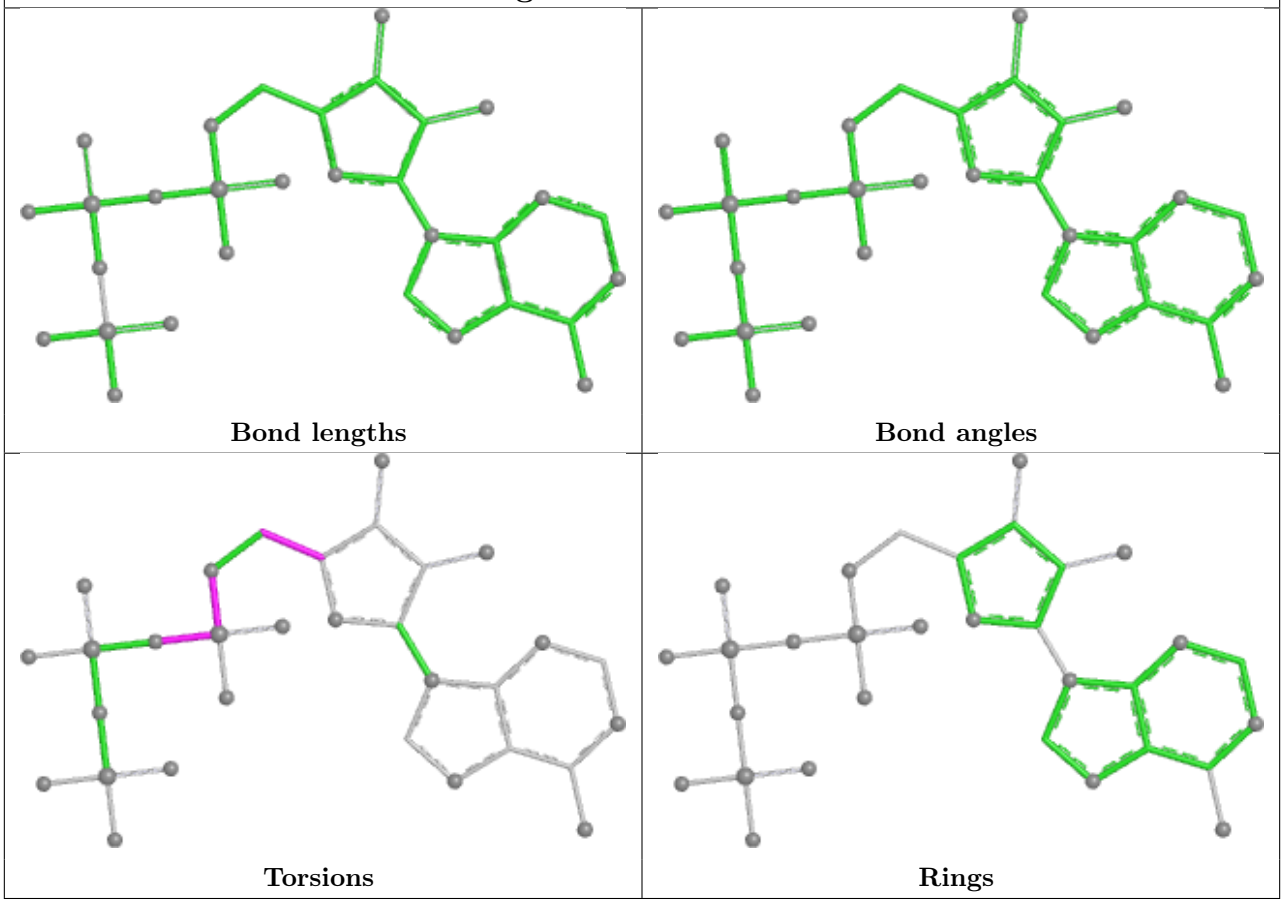


Torsions

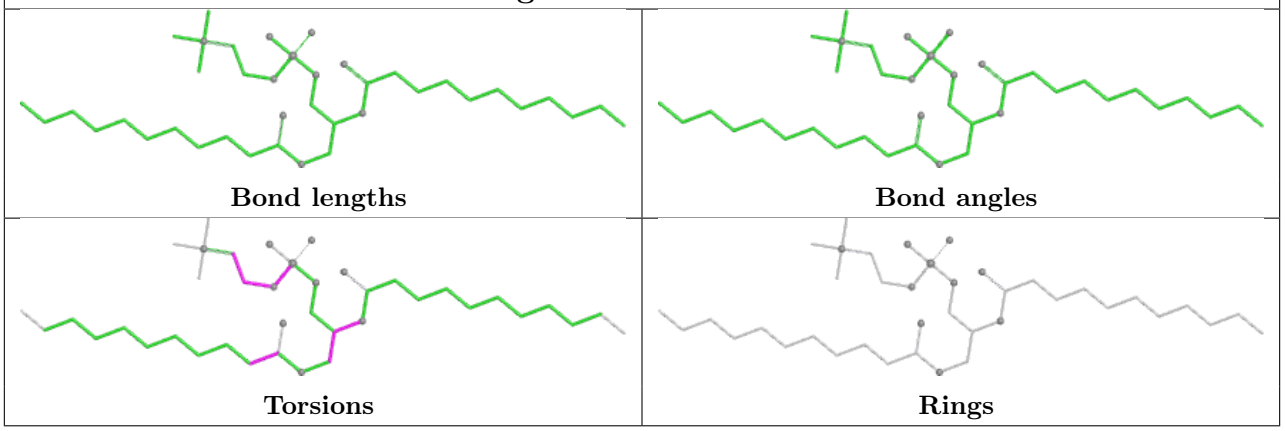


Rings

Ligand ATP D 2802



Ligand PLX C 2805



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.

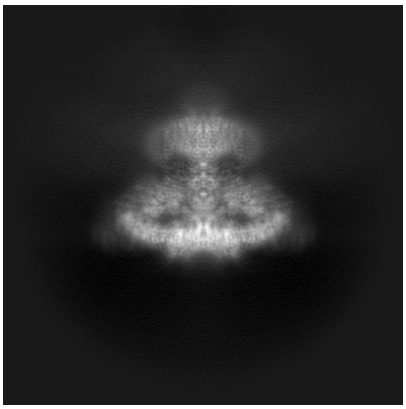
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76264. These allow visual inspection of the internal detail of the map and identification of artifacts.

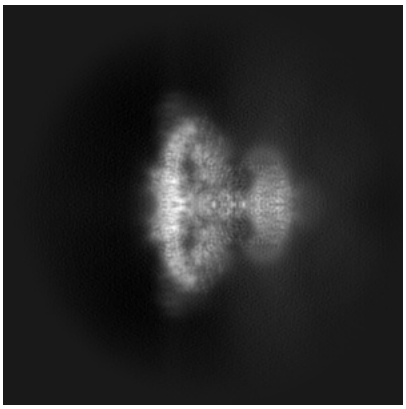
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

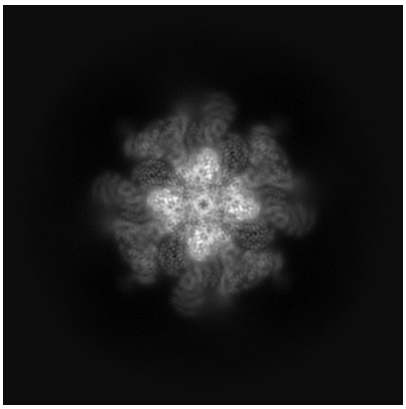
6.1.1 Primary map



X

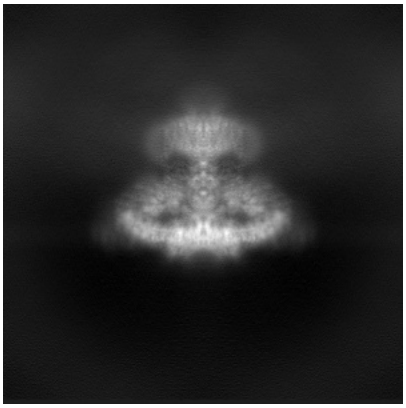


Y

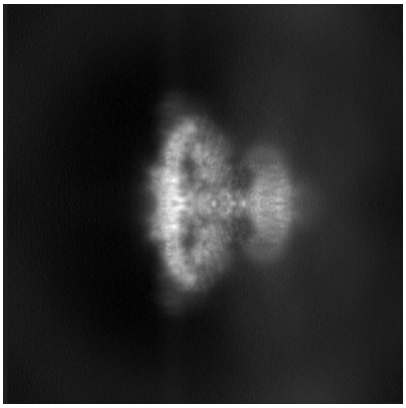


Z

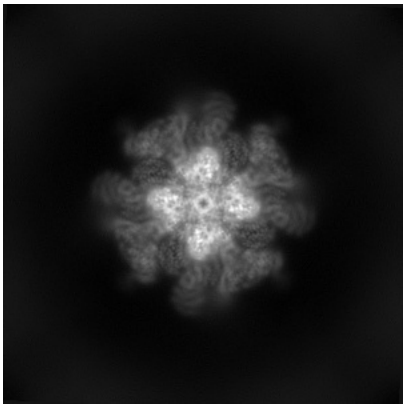
6.1.2 Raw map



X



Y

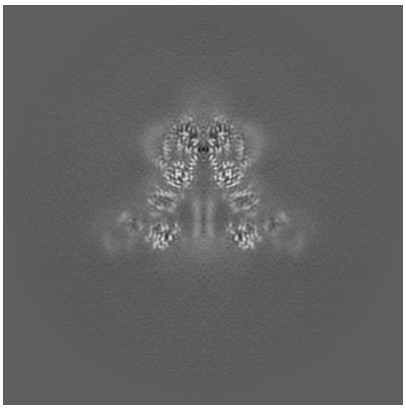


Z

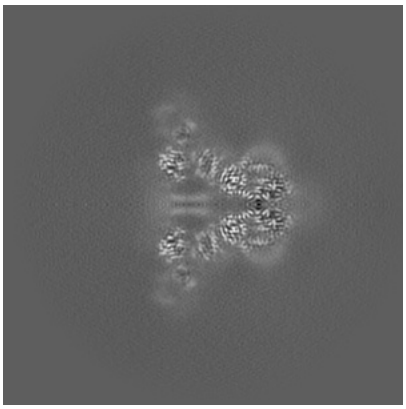
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

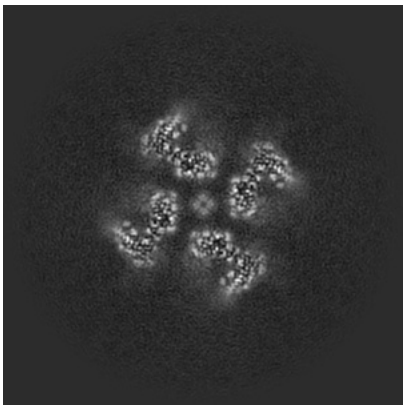
6.2.1 Primary map



X Index: 220

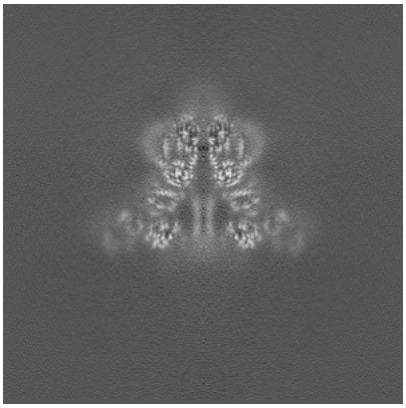


Y Index: 220

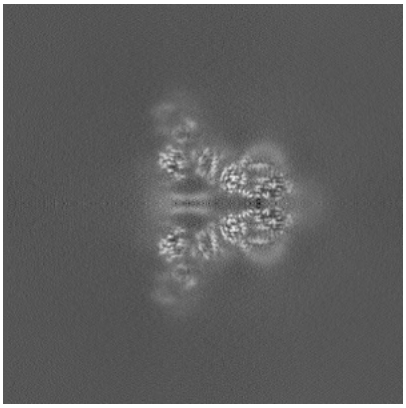


Z Index: 220

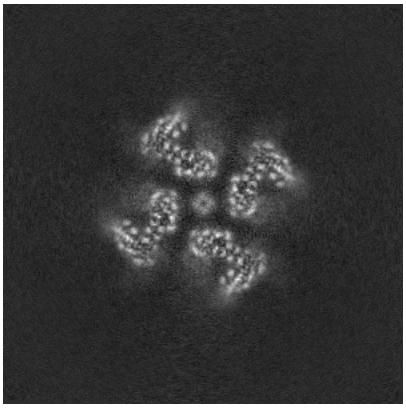
6.2.2 Raw map



X Index: 220



Y Index: 220

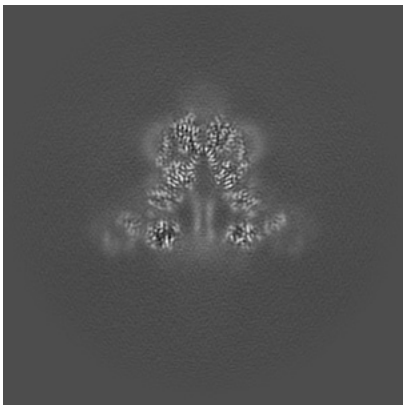


Z Index: 220

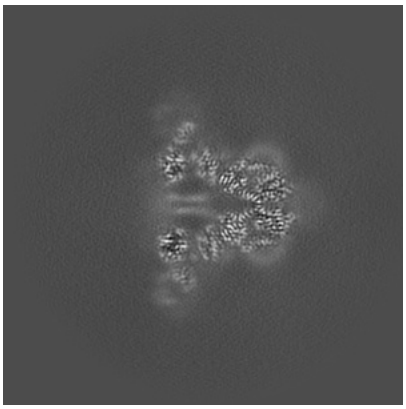
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

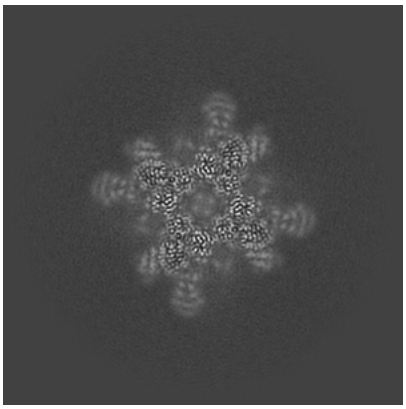
6.3.1 Primary map



X Index: 218

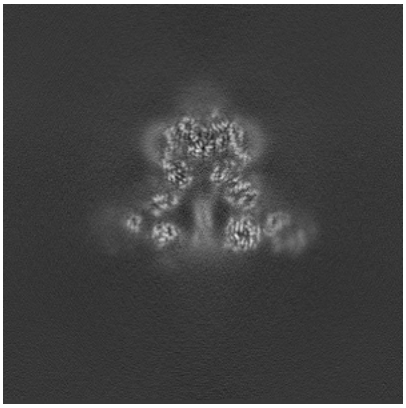


Y Index: 222

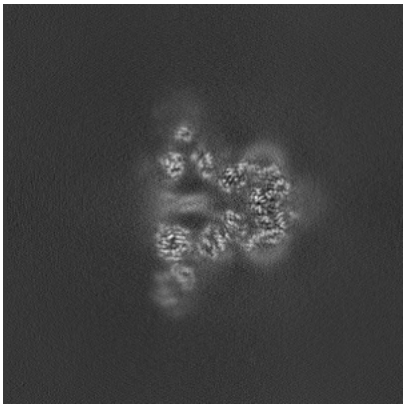


Z Index: 183

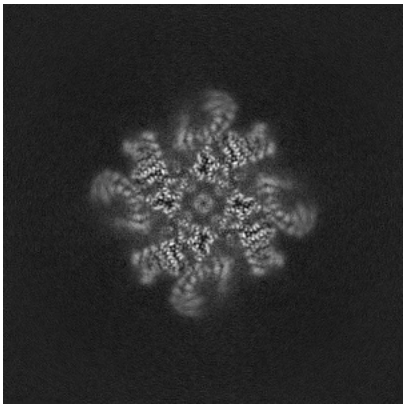
6.3.2 Raw map



X Index: 225



Y Index: 225

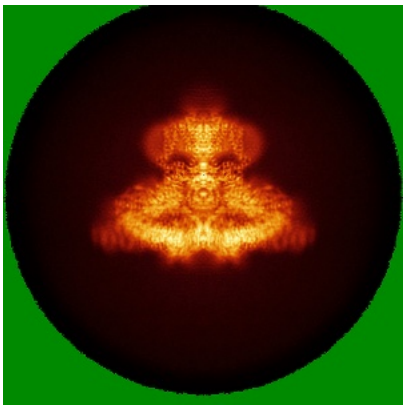


Z Index: 189

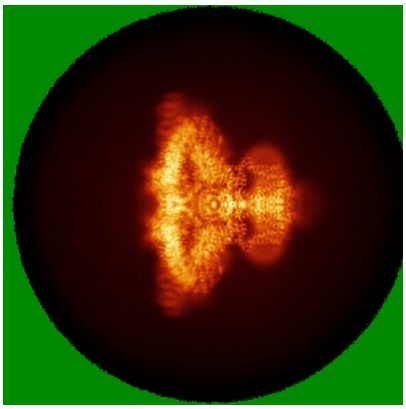
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

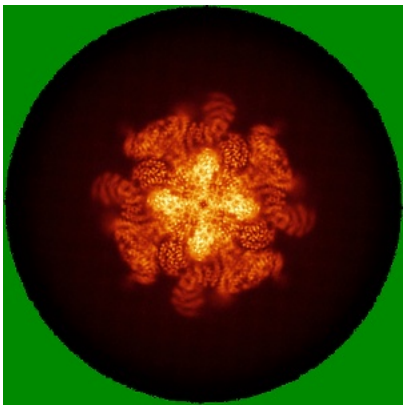
6.4.1 Primary map



X

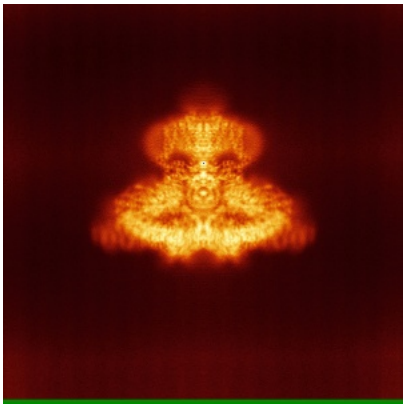


Y

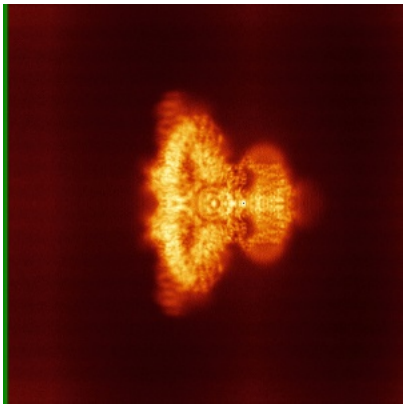


Z

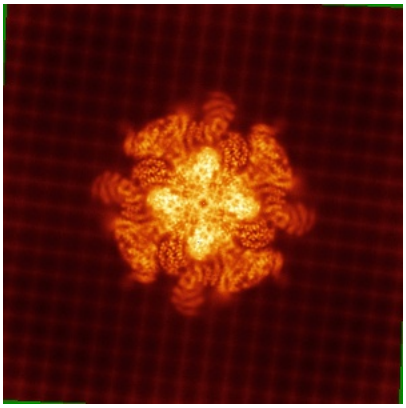
6.4.2 Raw map



X



Y

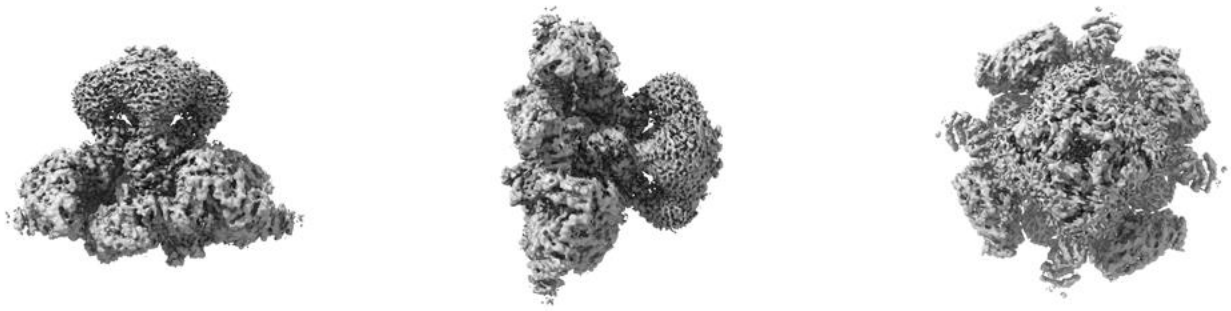


Z

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)

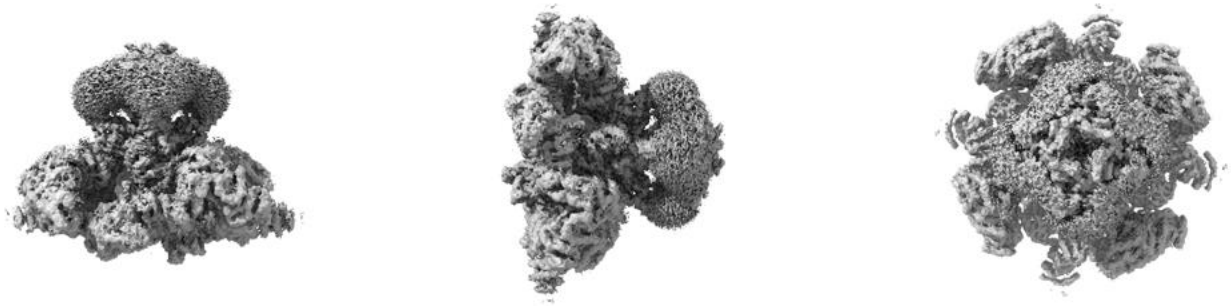
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.078. 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.

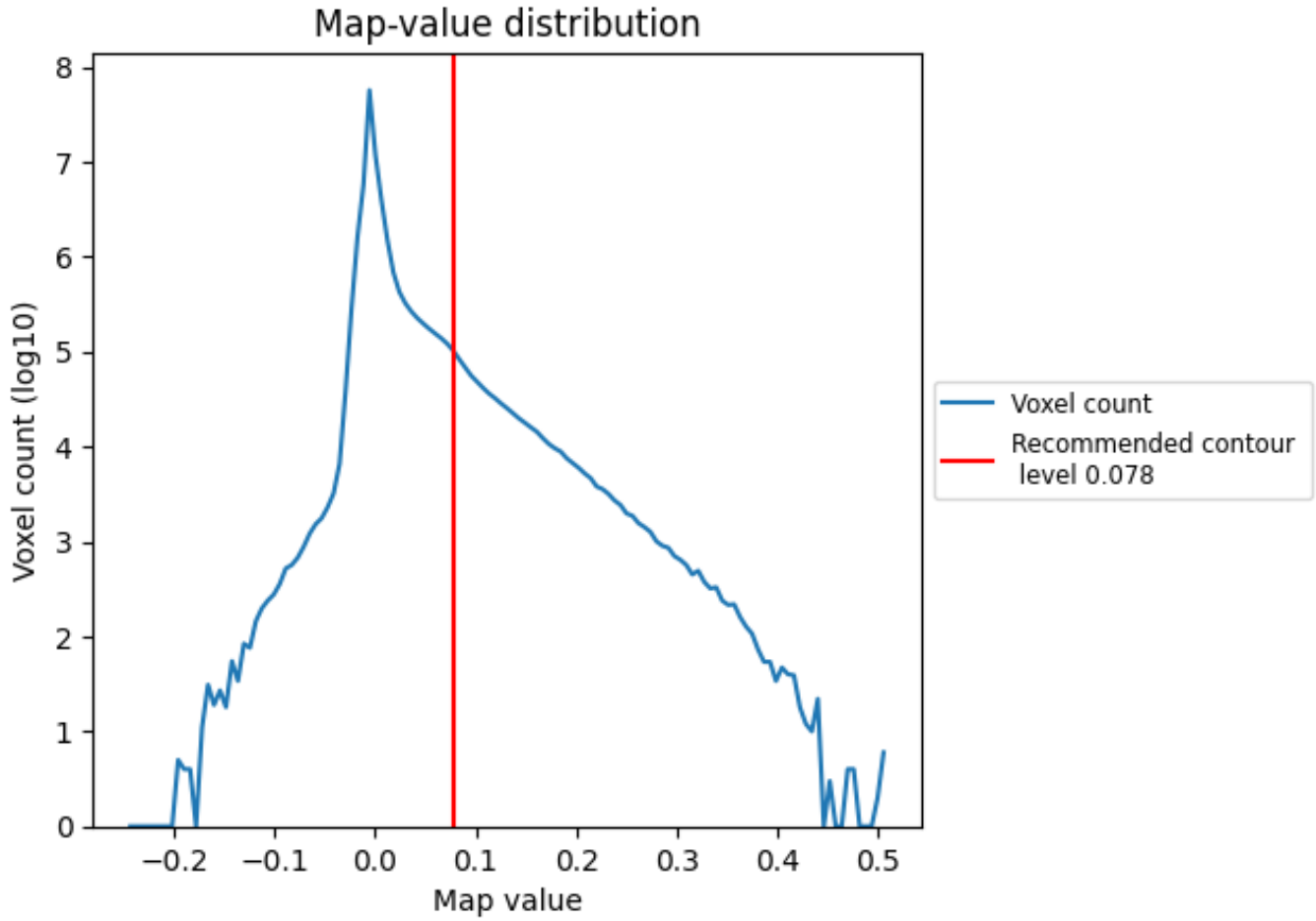
6.6 Mask visualisation (i)

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

7 Map analysis

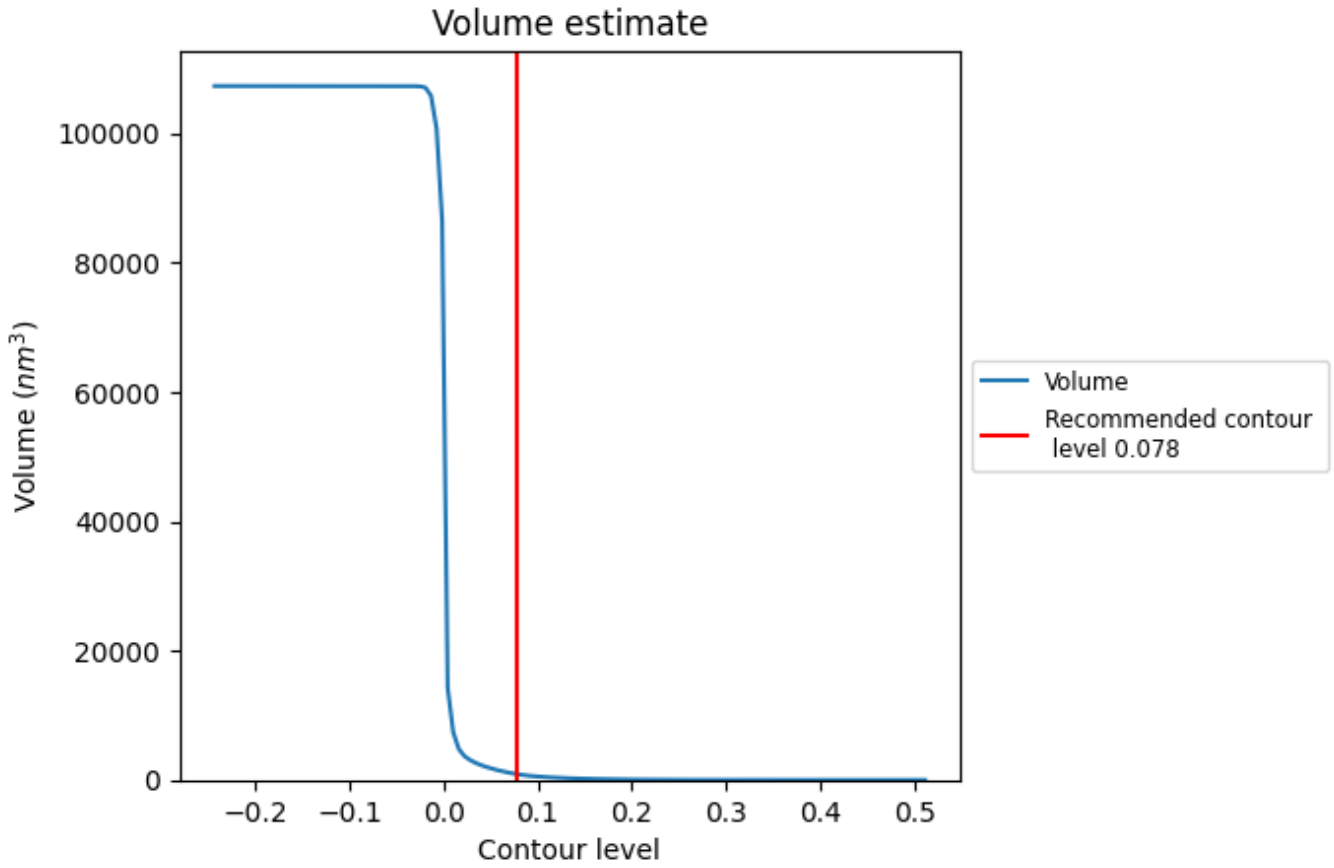
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

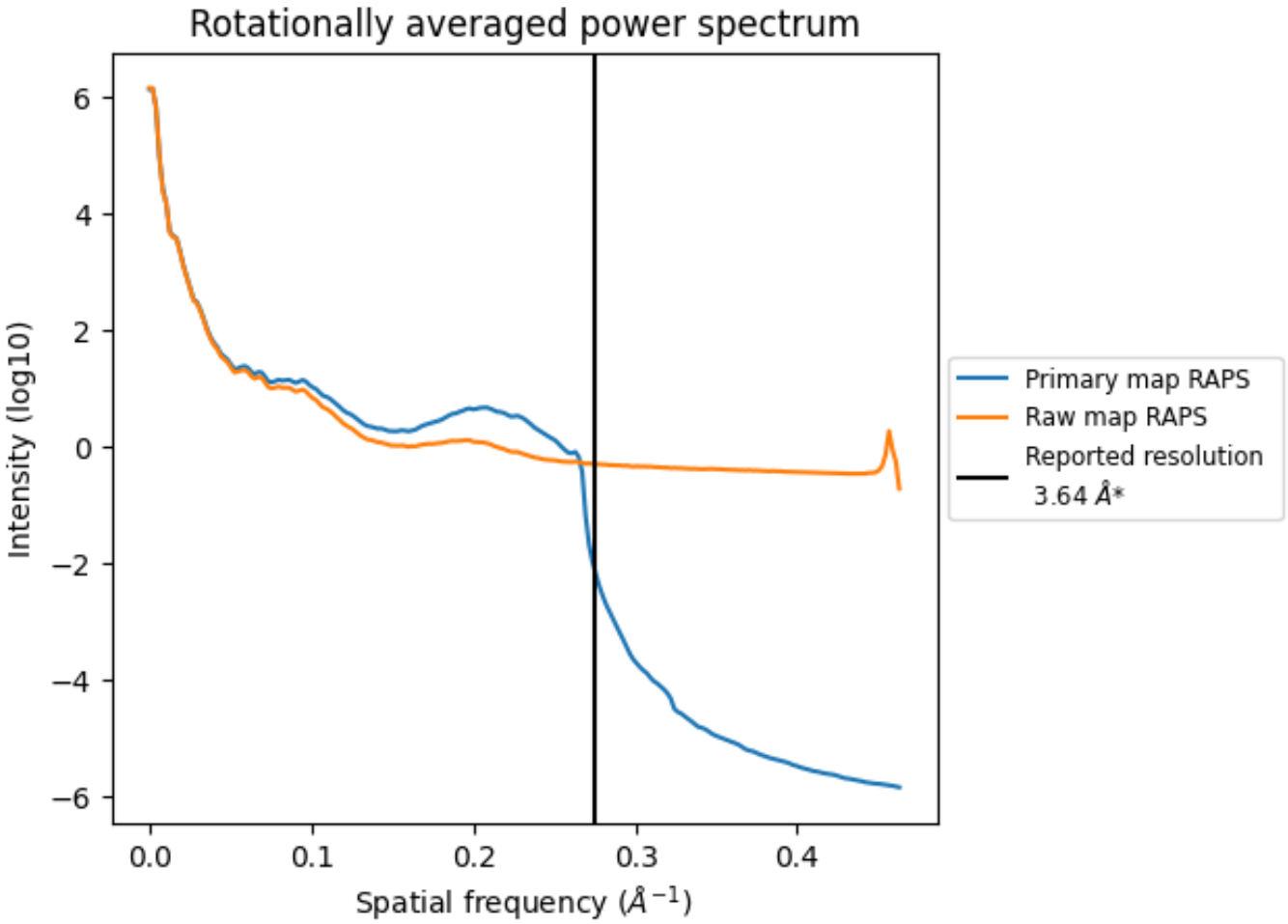
7.2 Volume estimate



The volume at the recommended contour level is 898 nm^3; this corresponds to an approximate mass of 811 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 (i)

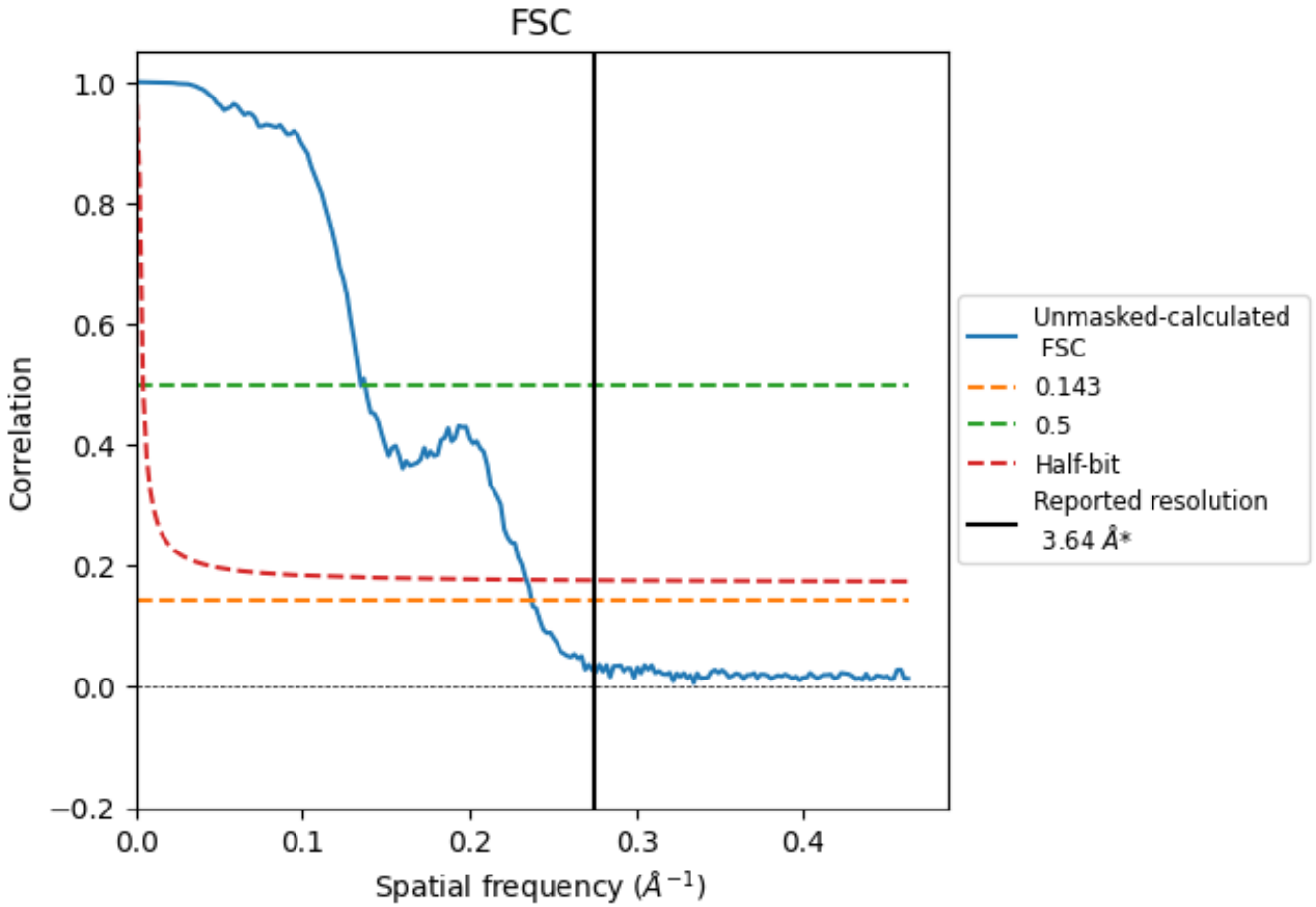


*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

8.2 Resolution estimates (i)

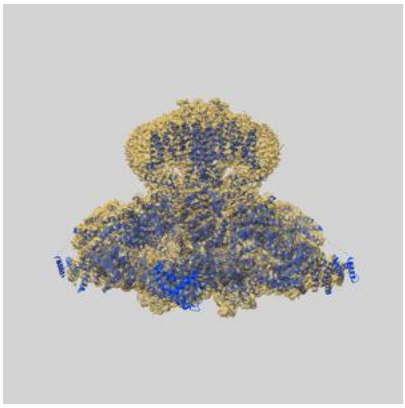
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.22	7.43	4.27

*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 4.22 differs from the reported value 3.64 by more than 10 %

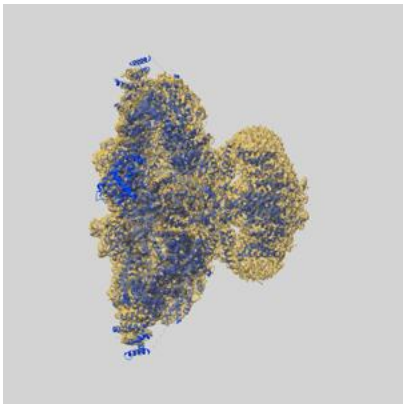
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76264 and PDB model 12AI. Per-residue inclusion information can be found in section 3 on page 7.

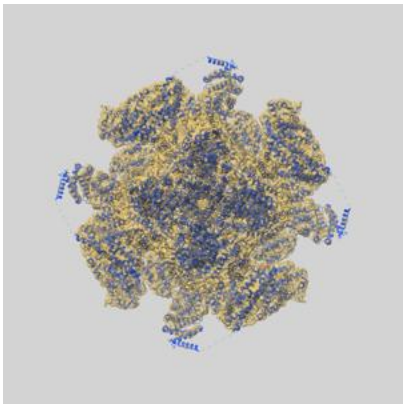
9.1 Map-model overlay



X



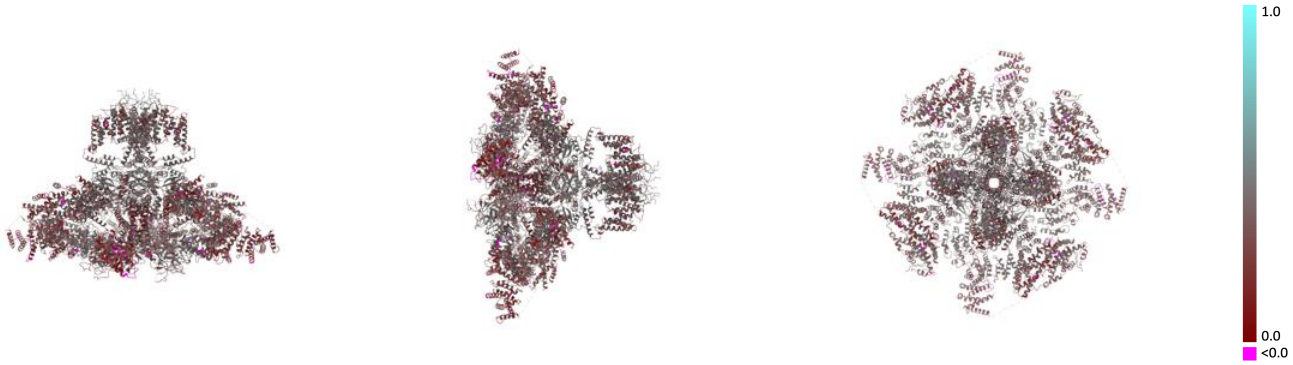
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.078 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.

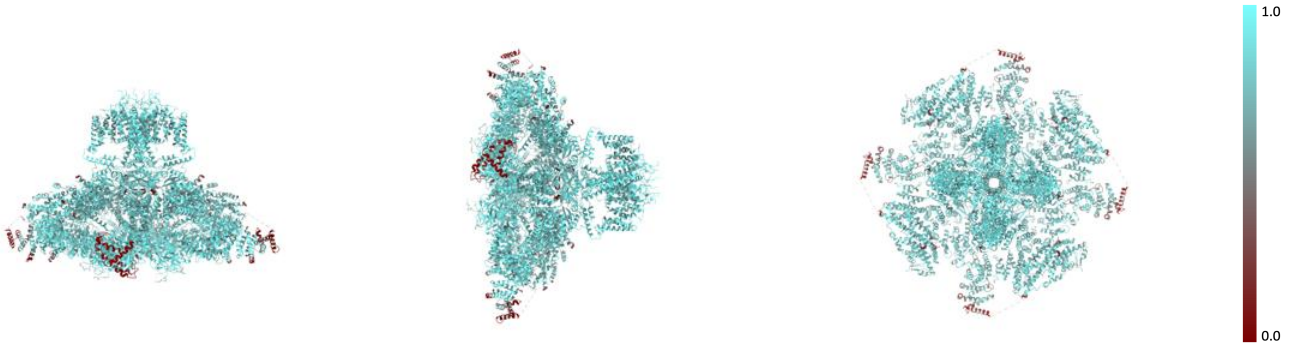
9.2 Q-score mapped to coordinate model



X Y Z

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.

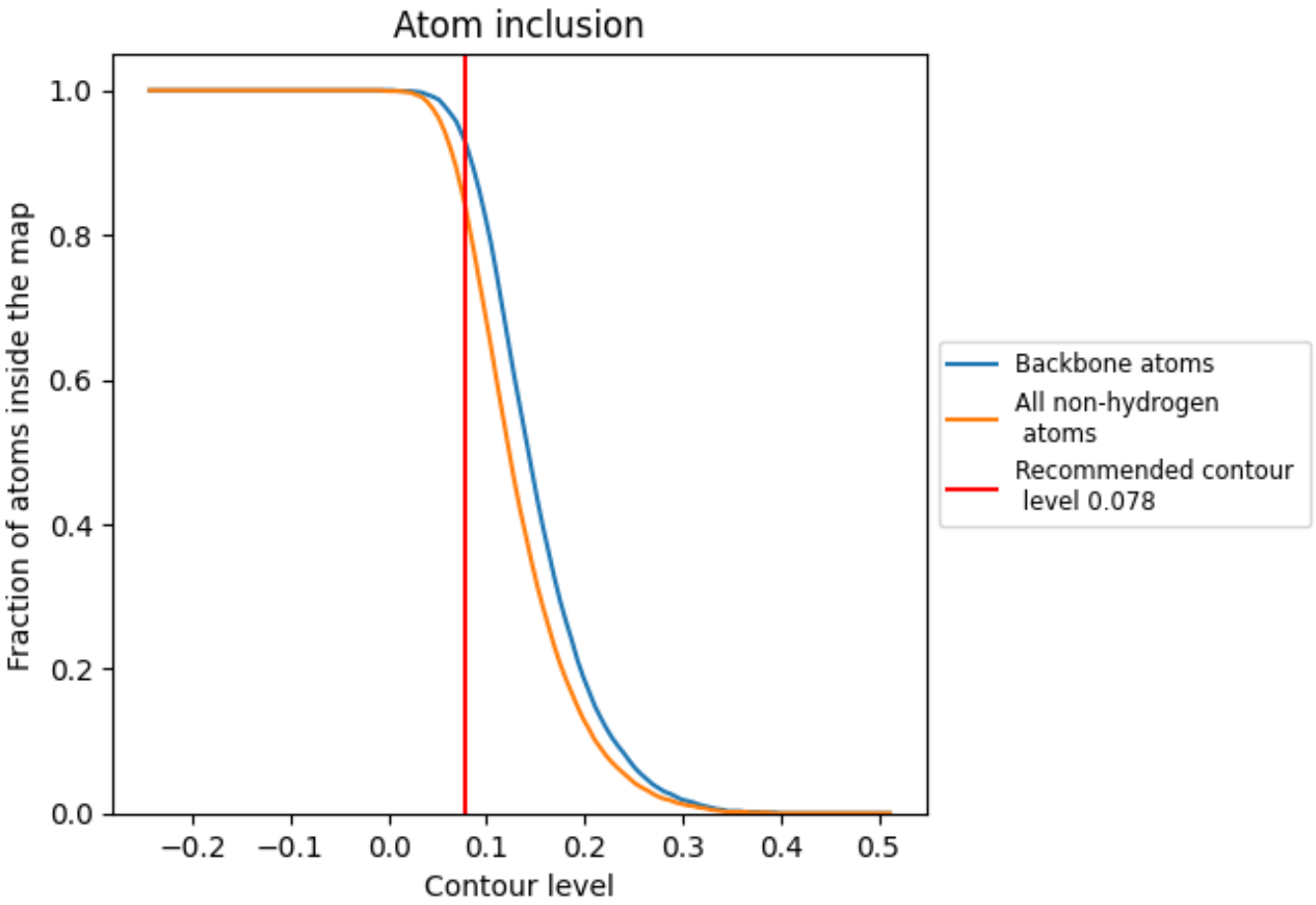
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.078).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 84% 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 (0.078) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.3510
A	0.8430	0.3510
B	0.8440	0.3520
C	0.8420	0.3500
D	0.8430	0.3510