



Full wwPDB EM Validation Report ⓘ

Feb 23, 2025 – 12:44 AM JST

PDB ID : 8IXN
EMDB ID : EMD-35799
Title : Curved structure of mPIEZO1-S2472E
Authors : Liu, S.; Yang, X.; Chen, X.; Li, X.; Xiao, B.
Deposited on : 2023-04-01
Resolution : 4.07 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

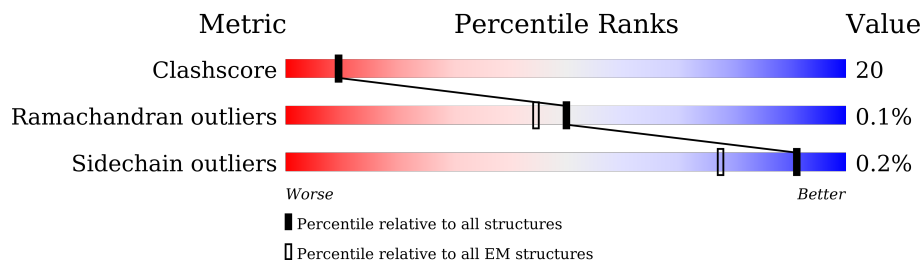
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.07 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	2547	
1	C	2547	
1	D	2547	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEE	A	2603	-	-	X	-
3	PEE	C	2603	-	-	X	-
3	PEE	D	2603	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	P5S	A	2604	-	-	X	-
4	P5S	C	2604	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 30043 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.

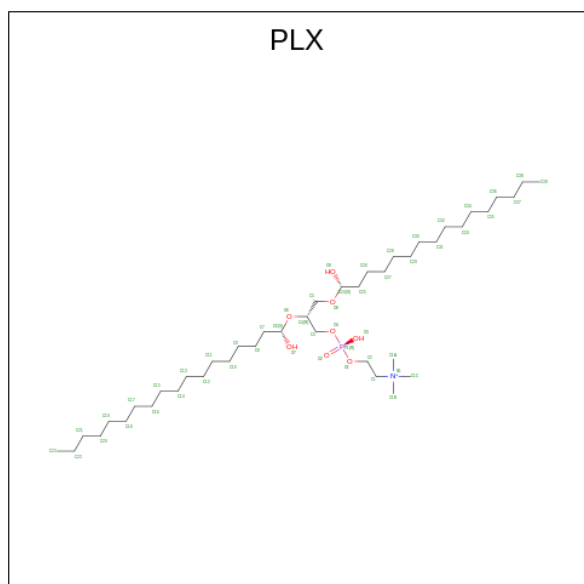
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1350	Total	C	N	O	S	0	0
			9804	6364	1661	1736	43		
1	A	1350	Total	C	N	O	S	0	0
			9802	6363	1660	1736	43		
1	D	1350	Total	C	N	O	S	0	0
			9810	6369	1661	1736	44		

There are 3 discrepancies between the modelled and reference sequences:

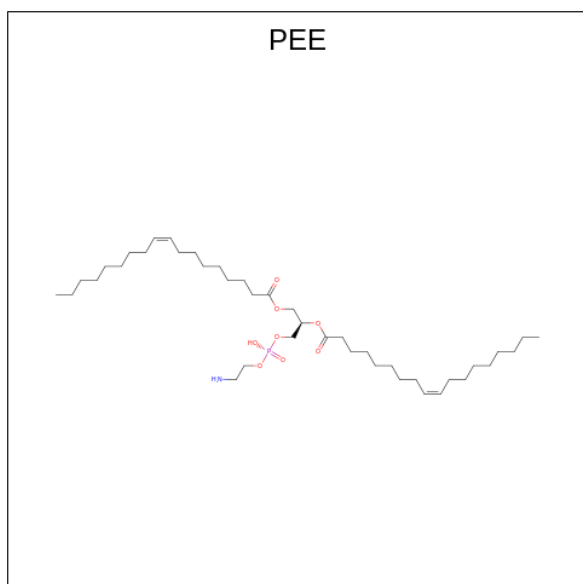
Chain	Residue	Modelled	Actual	Comment	Reference
C	2472	GLU	SER	engineered mutation	UNP E2JF22
A	2472	GLU	SER	engineered mutation	UNP E2JF22
D	2472	GLU	SER	engineered mutation	UNP E2JF22

- Molecule 2 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 (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



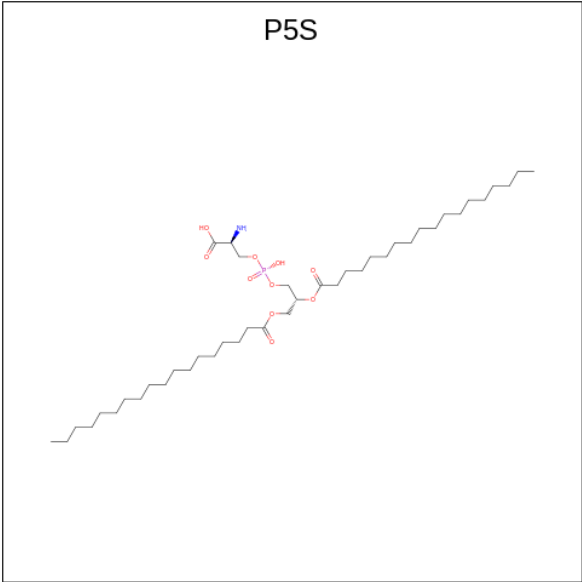
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	D	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).

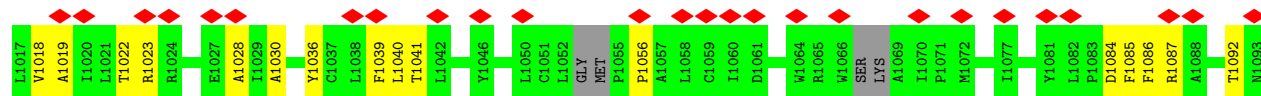


Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			54	42	1	10	1	
4	A	1	Total	C	N	O	P	0
			54	42	1	10	1	
4	D	1	Total	C	N	O	P	0
			54	42	1	10	1	



P2498	P2501	D2501	R2502	T2503	L2504	K2505	Q2508	D2509	T2510	F2511	L2512	E2515	T2516	R2517	E2522	E2523	E2524	L2525	Y2526	K2528	L2529	T2530	F2531	Y2532	R2533	T2534	S2535	T2538	W2542	T2543	R2544	E2545	R2546	E2547																						
W2430	V2431	L2434	Q2435	D2436	D2437	K2438	A2439	D2440	C2441	N2442	L2443	L2444	V2447	I2448	F2449	S2450	D2451	K2452	V2453	S2454	P2455	P2456	S2457	L2458	G2459	F2460	L2461	A2462	G2463	Y2464	G2465	I2466	V2467	G2468	L2469	Y2470	V2471	E2472	L2473	V2474	L2475	V2476	V2477	G2478	K2479	F2480	V2481	R2482	F2485	S2486	E2487	T2488	E2495	E2496	L2497	
Q2364	H2370	L2371	F2372	P2373	K2374	Y2375	I2376	R2377	A2378	P2379	N2380	G2381	E2383	A2384	N2385	P2386	V2387	K2388	Q2389	L2390	Q2391	P2392	D2393	E2394	E2395	E2396	D2397	Y2398	L2399	G2400	Q2404	L2405	R2406	R2407	E2408	Q2409	V2410	G2411	THR	GLY	ALA	SER	GLY	GLU	GLN	ALA	G2420	T2421	K2422	A2423	S2424	D2425	F2426	L2427	E2428	W2429
G2291	A2292	L2293	W2294	R2295	L2296	S2297	P2298	S2299	S2300	K2173	R2301	W2304	K2305	Q2306	V2309	N2310	G2311	T2312	A2313	D2314	T2315	T2316	L2317	R2318	F2319	T2320	W2321	Q2324	R2325	D2326	L2327	A2328	K2329	G2330	G2331	T2332	V2333	E2334	T2335	T2336	N2337	L2342	W2347	S2348	T2349	A2350	R2351	L2357	L2358	E2359	G2360	R2361	P2362	D2363		
T2227	V2228	K2231	L2232	G2233	G2234	Y2235	E2236	P2237	L2238	F2239	T2240	M2241	S2242	A2243	Q2244	P2246	I2248	V2249	P2250	F2251	T2252	P2253	Q2254	A2255	Y2256	E2257	E2258	Q2261	D2264	P2265	Y2266	P2267	L2268	A2269	M2270	Q2271	F2272	I2273	S2274	Q2275	Y2276	S2277	P2278	E2279	D2280	L2281	V2282	Q2285	L2286	E2287	G2288	S2289	S2290			
I2165	K2166	C2167	S2168	R2169	E2170	T2171	E2172	K2173	Q2174	Q2177	P2178	K2179	G2180	Q2181	K2182	K2183	K2184	K2185	K2188	Y2189	G2190	M2191	G2192	G2193	L2194	L2195	T2196	L2197	F2198	L2199	L2200	A2201	L2202	I2203	W2204	F2205	P2206	L2207	L2208	F2209	M2210	S2211	L2212	L2213	R2214	S2215	V2216	V2217	G2218	V2219	V2220	N2221	P2223	I2224	V2225	V2226
Y2083	F2084	V2085	K2086	C2087	L2088	Y2089	F2090	A2091	L2092	S2093	I2097	R2098	Y2101	P2102	F2109	K2112	N2117	L2118	L2119	F2120	Q2123	G2124	R2125	K2126	L2127	V2128	V2132	R2135	M2138	D2139	W2140	V2141	W2142	T2143	D2144	T2145	T2146	L2147	S2148	M2151	W2152	V2155	E2156	A2160	T2161	T2162										
Q2015	V2016	A2019	F2020	L2021	F2022	M2023	L2024	L2025	V2026	Q2027	T2030	L2033	D2034	R2035	A2036	L2037	K2041	T2042	V2043	L2044	G2045	K2046	L2047	Q2050	V2051	L2052	L2053	V2054	V2055	A2056	I2057	H2058	L2059	W2060	M2061	I2064	LEU	PRO	ALA	VAL	THR	GLU	R2071	M2072	F2073	Q2074	S2075	N2076	A2077	Q2080	L2081	W2082				
SER	LEU	ALA	GLN	SER	PHE	TYR	Q1966	Q1969	R1960	F1961	I1965	K1969	A1972	A1973	T1974	D1975	Y1976	Y1977	A1978	I1979	M1980	F1981	L1982	A1983	D1984	I1985	V1986	D1987	I1988	I1989	I1990	I1991	I1992	F1993	G1994	F1995	W1996	ALA	PHE	GLY	LYS	HIS	SER	ALA	ALA	THR	ASP	ILE	ALA	SER	SER	LEU	SER	ASP		
ARG	PHE	ARG	ARG	ARG	LYS	GLU	THR	PRO	GLY	GLN	LYS	THR	ALA	VAL	GLU	MET	GLY	THR	THR	LYS	GLU	HIS	GLU	VAL	GLY	ALA	GLY	THR	PRO	ARG	HIS	THR	GLN	ASP	PRO	GLU	MET	LYS	ALA	ALA	GLY	ARG	ARG	ARG	THR	GLN	SER	PHE	ILE	CYS	VAL					
ASN	LYS	PRO	TYR	PHE	PRO	ARG	ILE	SER	GLY	LEU	THR	THR	ASP	SER	Y1782	I1783	K1784	Y1785	D1786	L1787	V1788	Q1789	M1790	M1791	K1792	R1793	F1794	F1795	Q1798	Q1799	Y1803	GLY	LEU	TRP	ASP	HIS	ASP	VAL	ILE	GLN	ASP	PRO	GLU	PRO	LYS	ASP	ASP	TYR	SER	ARG	VAL	ALA	LYS			

- Molecule 1: Piezo-type mechanosensitive ion channel component 1

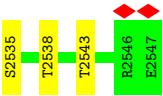




[illegible]







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	488709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	22.183	Depositor
Minimum map value	-9.040	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.021	Depositor
Recommended contour level	8.23	Depositor
Map size (\AA)	404.02722, 404.02722, 404.02722	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P5S, PLX, PEE

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	0.29	0/9986	0.54	0/13618
1	C	0.29	0/9990	0.55	0/13625
1	D	0.28	0/9995	0.53	0/13630
All	All	0.28	0/29971	0.54	0/40873

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9802	0	8926	372	0
1	C	9804	0	8928	401	0
1	D	9810	0	8942	334	0
2	A	104	0	176	14	0
2	C	104	0	176	14	0
2	D	104	0	176	14	0
3	A	51	0	82	60	0
3	C	51	0	82	70	0
3	D	51	0	82	64	0
4	A	54	0	80	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	54	0	80	25	0
4	D	54	0	80	17	0
All	All	30043	0	27810	1147	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 20.

All (1147) 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:2109:PHE:HB2	3:D:2603:PEE:C5	1.55	1.34
1:A:1981:PHE:CE2	3:A:2603:PEE:H17	1.66	1.30
1:D:1981:PHE:CE2	3:D:2603:PEE:H17	1.77	1.17
1:C:1981:PHE:CD2	3:C:2603:PEE:H17	1.78	1.17
1:A:1981:PHE:CD2	3:A:2603:PEE:H13	1.82	1.13
1:A:1981:PHE:CD2	3:A:2603:PEE:H17	1.83	1.13
1:A:1989:ILE:HD11	3:A:2603:PEE:H37	1.19	1.12
1:A:1981:PHE:CE2	3:A:2603:PEE:C13	2.33	1.12
1:A:1153:LEU:CD1	4:A:2604:P5S:H49	1.80	1.11
1:D:1981:PHE:CD2	3:D:2603:PEE:H17	1.85	1.11
1:C:1989:ILE:HD11	3:C:2603:PEE:H37	1.20	1.11
1:D:1989:ILE:HD11	3:D:2603:PEE:H37	1.17	1.10
1:D:1989:ILE:CD1	3:D:2603:PEE:H37	1.81	1.10
1:C:1153:LEU:CD1	4:C:2604:P5S:H49	1.81	1.09
1:C:1981:PHE:CE2	3:C:2603:PEE:H17	1.87	1.09
1:A:1989:ILE:HD11	3:A:2603:PEE:C23	1.82	1.09
1:C:1989:ILE:HD11	3:C:2603:PEE:C23	1.83	1.08
1:A:1989:ILE:CD1	3:A:2603:PEE:H37	1.85	1.07
1:A:1981:PHE:HZ	4:A:2604:P5S:H41A	1.18	1.06
1:D:1981:PHE:CD2	3:D:2603:PEE:H13	1.91	1.06
1:A:1153:LEU:HD12	4:A:2604:P5S:H46	1.33	1.05
1:A:1153:LEU:HD11	4:A:2604:P5S:H49	1.34	1.05
1:C:1989:ILE:CD1	3:C:2603:PEE:H37	1.85	1.05
1:D:2109:PHE:HB2	3:D:2603:PEE:H12	1.07	1.05
1:C:1981:PHE:HZ	4:C:2604:P5S:H41A	1.19	1.04
1:A:1981:PHE:HE2	3:A:2603:PEE:C13	1.66	1.04
1:D:1989:ILE:HD11	3:D:2603:PEE:C23	1.86	1.04
1:D:1981:PHE:HZ	4:D:2604:P5S:H41A	1.20	1.04
1:C:1153:LEU:HD12	4:C:2604:P5S:H46	1.43	1.00
1:C:2109:PHE:CB	3:C:2603:PEE:H12	1.92	1.00
1:C:1153:LEU:HD11	4:C:2604:P5S:H49	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2603:PEE:H40	3:C:2603:PEE:H81	1.44	0.99
1:A:1989:ILE:CD1	3:A:2603:PEE:C23	2.41	0.99
1:D:1981:PHE:CE2	3:D:2603:PEE:C13	2.44	0.99
1:D:2109:PHE:HB2	3:D:2603:PEE:H11	1.44	0.99
1:C:1989:ILE:CD1	3:C:2603:PEE:C23	2.40	0.99
1:D:1989:ILE:CD1	3:D:2603:PEE:C23	2.41	0.98
3:A:2603:PEE:H40	3:A:2603:PEE:H81	1.44	0.97
3:D:2603:PEE:H68	3:D:2603:PEE:C46	1.95	0.97
1:A:1981:PHE:HD2	3:A:2603:PEE:H13	1.27	0.97
1:D:2109:PHE:CB	3:D:2603:PEE:H12	1.95	0.96
3:C:2603:PEE:C46	3:C:2603:PEE:H68	1.95	0.96
3:D:2603:PEE:H40	3:D:2603:PEE:H81	1.44	0.96
3:A:2603:PEE:H68	3:A:2603:PEE:C46	1.95	0.95
1:C:1981:PHE:CD2	3:C:2603:PEE:H13	2.01	0.95
1:C:1981:PHE:CE2	3:C:2603:PEE:C13	2.50	0.94
1:A:1230:LEU:HD22	1:A:1251:LEU:HD22	1.49	0.94
3:A:2603:PEE:H68	3:A:2603:PEE:H82	1.48	0.94
3:D:2603:PEE:H68	3:D:2603:PEE:H82	1.48	0.93
1:C:2109:PHE:CB	3:C:2603:PEE:C5	2.47	0.92
1:A:1163:TRP:HB3	2:A:2602:PLX:H282	1.50	0.92
3:D:2603:PEE:C46	3:D:2603:PEE:H40	2.00	0.92
1:C:1163:TRP:HB3	2:C:2602:PLX:H282	1.49	0.92
3:C:2603:PEE:H68	3:C:2603:PEE:H82	1.48	0.91
3:C:2603:PEE:H40	3:C:2603:PEE:C46	2.00	0.91
3:A:2603:PEE:H40	3:A:2603:PEE:C46	2.00	0.91
3:D:2603:PEE:H40	3:D:2603:PEE:C47	2.01	0.91
1:D:1981:PHE:HD2	3:D:2603:PEE:H13	1.31	0.91
3:C:2603:PEE:H40	3:C:2603:PEE:C47	2.01	0.90
3:C:2603:PEE:H68	3:C:2603:PEE:C47	2.02	0.90
3:A:2603:PEE:H40	3:A:2603:PEE:C47	2.01	0.90
1:D:2109:PHE:CB	3:D:2603:PEE:C5	2.49	0.90
3:A:2603:PEE:H68	3:A:2603:PEE:C47	2.02	0.90
3:D:2603:PEE:H68	3:D:2603:PEE:C47	2.02	0.90
1:C:981:PHE:CZ	4:C:2604:P5S:H41A	2.07	0.89
1:D:1981:PHE:HE2	3:D:2603:PEE:C13	1.81	0.89
1:A:1981:PHE:CD2	3:A:2603:PEE:C11	2.54	0.89
1:C:1981:PHE:HD2	3:C:2603:PEE:H17	1.36	0.88
1:A:981:PHE:CZ	4:A:2604:P5S:H41A	2.07	0.88
1:D:1163:TRP:HB3	2:D:2602:PLX:H282	1.54	0.88
1:C:1981:PHE:CD2	3:C:2603:PEE:C13	2.56	0.87
1:D:981:PHE:CZ	4:D:2604:P5S:H41A	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1157:VAL:HG11	4:D:2604:P5S:H21	1.57	0.87
1:A:1981:PHE:CE2	3:A:2603:PEE:C12	2.58	0.86
1:C:1981:PHE:HD2	3:C:2603:PEE:H13	1.40	0.86
1:A:1153:LEU:HD12	4:A:2604:P5S:C46	2.05	0.86
3:A:2603:PEE:H40	3:A:2603:PEE:C45	2.06	0.85
3:A:2603:PEE:H74	3:A:2603:PEE:H41	1.59	0.85
1:D:1157:VAL:HG21	4:D:2604:P5S:H44A	1.59	0.85
3:D:2603:PEE:H40	3:D:2603:PEE:C45	2.06	0.84
3:C:2603:PEE:H40	3:C:2603:PEE:C45	2.06	0.84
3:C:2603:PEE:H74	3:C:2603:PEE:H41	1.59	0.83
1:D:2321:TRP:HH2	1:D:2373:PRO:HG2	1.43	0.83
3:D:2603:PEE:H41	3:D:2603:PEE:H74	1.59	0.83
3:D:2603:PEE:H81	3:D:2603:PEE:C24	2.09	0.83
1:C:2321:TRP:HH2	1:C:2373:PRO:HG2	1.40	0.82
3:C:2603:PEE:H81	3:C:2603:PEE:C24	2.09	0.82
3:A:2603:PEE:H81	3:A:2603:PEE:C24	2.09	0.82
1:D:1981:PHE:CD2	3:D:2603:PEE:C11	2.62	0.82
1:C:1695:ILE:HD11	1:C:1710:LEU:HG	1.60	0.81
1:D:1981:PHE:CD2	3:D:2603:PEE:C13	2.64	0.81
1:C:1981:PHE:HE2	3:C:2603:PEE:C13	1.94	0.80
1:C:1153:LEU:HD12	4:C:2604:P5S:H49	1.64	0.79
1:A:2321:TRP:HH2	1:A:2373:PRO:HG2	1.47	0.79
3:C:2603:PEE:H68	3:C:2603:PEE:C45	2.12	0.78
3:D:2603:PEE:H68	3:D:2603:PEE:C45	2.12	0.78
1:C:1153:LEU:HD12	4:C:2604:P5S:C46	2.13	0.78
1:A:2109:PHE:CB	3:A:2603:PEE:H12	2.14	0.78
1:C:2138:MET:HE3	3:C:2603:PEE:H49	1.64	0.78
1:A:1981:PHE:CD2	3:A:2603:PEE:C13	2.61	0.78
1:A:2325:ARG:HD2	1:A:2334:GLU:HA	1.63	0.78
1:C:2185:LYS:O	1:C:2188:LYS:HB3	1.84	0.77
1:D:1981:PHE:HE2	3:D:2603:PEE:H17	1.38	0.77
1:C:1981:PHE:CD2	3:C:2603:PEE:C11	2.67	0.77
1:A:1157:VAL:HG11	4:A:2604:P5S:H44A	1.66	0.77
1:C:2410:VAL:HG23	1:D:2425:ASP:HA	1.67	0.77
1:A:1979:LEU:HB3	1:A:2092:LEU:HD13	1.67	0.77
1:D:2294:TRP:HB3	1:D:2429:TRP:HA	1.67	0.77
1:C:1989:ILE:CD1	3:C:2603:PEE:H38	2.13	0.76
1:A:1981:PHE:CE2	3:A:2603:PEE:H16	2.20	0.76
1:A:1989:ILE:CD1	3:A:2603:PEE:H38	2.14	0.76
1:C:1157:VAL:HG11	4:C:2604:P5S:H23	1.67	0.76
1:C:1981:PHE:CD2	3:C:2603:PEE:C12	2.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2425:ASP:HA	1:A:2410:VAL:HG23	1.67	0.76
1:A:1153:LEU:HD12	4:A:2604:P5S:H49	1.69	0.75
1:A:2294:TRP:HB3	1:A:2429:TRP:HA	1.67	0.75
1:C:1166:LEU:HD13	1:C:1192:LEU:HD12	1.69	0.74
1:C:2498:PRO:HD3	1:A:2534:ARG:HH22	1.49	0.74
1:A:2404:GLN:HB3	1:A:2431:VAL:HB	1.69	0.74
1:D:2380:ASN:HD21	1:D:2453:VAL:HA	1.52	0.74
1:C:2294:TRP:HB3	1:C:2429:TRP:HA	1.67	0.74
1:A:1695:ILE:HD11	1:A:1710:LEU:HG	1.70	0.74
1:C:1165:VAL:HG23	1:C:1289:PHE:HB3	1.69	0.74
1:D:1981:PHE:CE2	3:D:2603:PEE:C12	2.70	0.74
3:A:2603:PEE:H68	3:A:2603:PEE:C45	2.12	0.73
1:C:2380:ASN:HD21	1:C:2453:VAL:HA	1.52	0.73
1:C:2534:ARG:HH22	1:D:2498:PRO:HD3	1.54	0.73
1:A:2498:PRO:HD3	1:D:2534:ARG:HH22	1.52	0.73
1:A:2425:ASP:HA	1:D:2410:VAL:HG23	1.69	0.73
1:A:1981:PHE:CD2	3:A:2603:PEE:C12	2.72	0.73
1:C:1722:ILE:HG22	1:C:1724:ARG:H	1.54	0.72
1:D:1981:PHE:HD2	3:D:2603:PEE:H17	1.53	0.72
1:D:2404:GLN:HB3	1:D:2431:VAL:HB	1.70	0.72
1:A:2380:ASN:HD21	1:A:2453:VAL:HA	1.53	0.72
1:C:1157:VAL:CG1	4:C:2604:P5S:H23	2.19	0.72
1:D:2325:ARG:HD2	1:D:2334:GLU:HA	1.72	0.71
1:A:2434:LEU:HB2	1:A:2437:CYS:HB3	1.72	0.71
1:C:1734:ILE:HG12	1:C:1794:PHE:CE1	2.25	0.71
1:D:2185:LYS:O	1:D:2188:LYS:HB3	1.90	0.71
1:C:966:THR:HG21	1:C:969:ARG:HH21	1.54	0.71
1:D:1989:ILE:CD1	3:D:2603:PEE:H38	2.19	0.71
1:A:2147:LEU:HB3	1:A:2151:ASN:HB2	1.71	0.71
1:C:1982:LEU:HD11	3:C:2603:PEE:H24	1.72	0.71
1:C:1716:LEU:HD21	1:C:2054:VAL:HG11	1.73	0.70
1:D:2393:ASP:HB3	1:D:2396:GLU:HB2	1.73	0.70
1:D:1722:ILE:HG22	1:D:1724:ARG:H	1.56	0.70
1:A:1981:PHE:CE1	3:A:2603:PEE:H8	2.26	0.70
1:A:2393:ASP:HB3	1:A:2396:GLU:HB2	1.73	0.70
1:A:1981:PHE:HE2	3:A:2603:PEE:C14	2.05	0.70
1:D:2147:LEU:HB3	1:D:2151:ASN:HB2	1.74	0.70
1:C:2138:MET:CE	3:C:2603:PEE:H49	2.23	0.69
1:C:2325:ARG:HD2	1:C:2334:GLU:HA	1.74	0.69
3:D:2603:PEE:H82	3:D:2603:PEE:C41	2.23	0.69
1:C:2109:PHE:CB	3:C:2603:PEE:H11	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2461:LEU:HG	1:D:2462:ALA:H	1.57	0.69
1:C:2223:PRO:HA	1:C:2325:ARG:HA	1.73	0.69
1:A:1722:ILE:HG22	1:A:1724:ARG:H	1.56	0.69
1:C:1981:PHE:CE2	3:C:2603:PEE:C12	2.76	0.69
1:C:2393:ASP:HB3	1:C:2396:GLU:HB2	1.73	0.69
1:D:1981:PHE:CD2	3:D:2603:PEE:C12	2.75	0.69
1:D:2228:VAL:HG23	1:D:2321:TRP:CD1	2.28	0.68
1:A:1166:LEU:HD13	1:A:1192:LEU:HG	1.75	0.68
4:D:2604:P5S:H56A	4:D:2604:P5S:H34A	1.75	0.68
1:C:1217:ASN:O	1:C:1221:ILE:HG12	1.93	0.68
4:C:2604:P5S:H56A	4:C:2604:P5S:H34A	1.75	0.68
1:A:1734:ILE:HG12	1:A:1794:PHE:CE1	2.29	0.68
1:C:2256:TYR:HB2	1:C:2278:PRO:HB3	1.74	0.68
1:A:2206:PRO:HG2	1:A:2470:TYR:HE1	1.59	0.68
1:D:2375:TYR:H	1:D:2391:GLN:HE22	1.41	0.68
1:A:2031:MET:HE2	3:A:2603:PEE:H56	1.75	0.68
1:D:2223:PRO:HA	1:D:2325:ARG:HA	1.76	0.68
3:A:2603:PEE:H82	3:A:2603:PEE:C41	2.23	0.67
1:D:2228:VAL:HG23	1:D:2321:TRP:HD1	1.59	0.67
1:D:1981:PHE:CE2	3:D:2603:PEE:H16	2.30	0.67
1:D:2256:TYR:HB2	1:D:2278:PRO:HB3	1.76	0.67
1:D:2434:LEU:HB2	1:D:2437:CYS:HB3	1.75	0.67
1:A:2256:TYR:HB2	1:A:2278:PRO:HB3	1.75	0.67
4:A:2604:P5S:H34A	4:A:2604:P5S:H56A	1.75	0.67
1:C:2188:LYS:HG3	1:A:2140:TRP:CH2	2.30	0.67
1:A:2374:LYS:NZ	1:A:2445:PRO:O	2.23	0.67
1:D:1016:TRP:CD1	1:D:1039:PHE:HZ	2.13	0.67
1:C:1714:VAL:HG22	1:C:1729:PHE:HZ	1.59	0.67
1:D:1200:GLN:HE22	1:D:1309:LEU:HB3	1.59	0.67
1:D:1734:ILE:HG12	1:D:1794:PHE:CE1	2.29	0.66
1:C:1160:TYR:HE1	2:C:2602:PLX:O2	1.77	0.66
1:A:1165:VAL:HG23	1:A:1289:PHE:HB3	1.76	0.66
1:A:2228:VAL:HG23	1:A:2321:TRP:CD1	2.30	0.66
1:D:1165:VAL:HG23	1:D:1289:PHE:HB3	1.77	0.66
1:C:1987:ASP:OD2	1:C:2027:GLN:NE2	2.28	0.66
1:C:2199:LEU:HG	1:A:2134:LEU:HD21	1.76	0.66
1:A:2109:PHE:CB	3:A:2603:PEE:C5	2.74	0.66
1:A:1537:GLU:O	1:A:1541:LEU:HG	1.96	0.66
1:A:2031:MET:HE1	3:A:2603:PEE:H63	1.78	0.66
1:A:2461:LEU:HG	1:A:2462:ALA:H	1.60	0.66
1:A:1016:TRP:CD1	1:A:1039:PHE:HZ	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2243:ALA:HB1	1:A:2247:SER:HB2	1.77	0.66
1:D:2243:ALA:HB1	1:D:2247:SER:HB2	1.75	0.66
1:C:2228:VAL:HG23	1:C:2321:TRP:CD1	2.30	0.66
1:D:1799:GLN:HA	2:D:2602:PLX:H1C1	1.78	0.66
1:D:2206:PRO:HG2	1:D:2470:TYR:HE1	1.61	0.66
1:C:2244:GLN:HB2	1:D:2318:ARG:CZ	2.26	0.65
1:C:1016:TRP:CD1	1:C:1039:PHE:HZ	2.15	0.65
1:D:996:LEU:HD11	1:D:1288:PHE:HB2	1.77	0.65
3:D:2603:PEE:H74	3:D:2603:PEE:C25	2.26	0.65
1:A:2228:VAL:HG23	1:A:2321:TRP:HD1	1.62	0.65
1:D:1157:VAL:CG1	4:D:2604:P5S:H21	2.27	0.65
1:C:1728:ARG:CB	2:C:2601:PLX:O7	2.45	0.65
1:C:2228:VAL:HG23	1:C:2321:TRP:HD1	1.61	0.65
1:C:2250:PRO:HA	1:C:2282:VAL:HG12	1.79	0.65
1:A:2223:PRO:HA	1:A:2325:ARG:HA	1.77	0.65
1:C:1163:TRP:CB	2:C:2602:PLX:H282	2.26	0.64
1:A:1799:GLN:HA	2:A:2602:PLX:H1C1	1.79	0.64
3:C:2603:PEE:H82	3:C:2603:PEE:C41	2.23	0.64
1:C:2135:ARG:CZ	3:C:2603:PEE:O1P	2.45	0.64
3:C:2603:PEE:H74	3:C:2603:PEE:C25	2.26	0.64
1:C:1981:PHE:HE2	3:C:2603:PEE:C14	2.11	0.64
1:C:2227:THR:HG23	1:C:2324:GLN:HE22	1.63	0.64
3:A:2603:PEE:H74	3:A:2603:PEE:C25	2.26	0.64
1:C:1981:PHE:CE2	3:C:2603:PEE:H16	2.32	0.64
1:C:1982:LEU:CD1	3:C:2603:PEE:H24	2.27	0.64
1:C:2434:LEU:HB2	1:C:2437:CYS:HB3	1.80	0.64
1:D:2387:VAL:HG12	1:D:2390:LEU:H	1.63	0.64
1:C:1989:ILE:HD11	3:C:2603:PEE:H33	1.79	0.63
2:C:2602:PLX:O1	2:C:2602:PLX:H1A2	1.98	0.63
1:C:2373:PRO:HB3	1:C:2398:TYR:CE1	2.33	0.63
1:A:1981:PHE:HD2	3:A:2603:PEE:H17	1.58	0.63
1:D:2135:ARG:CZ	3:D:2603:PEE:O1P	2.45	0.63
1:C:1799:GLN:HA	2:C:2602:PLX:H1C1	1.80	0.63
1:C:2460:PHE:HD1	1:C:2464:TYR:HE2	1.45	0.63
1:A:1981:PHE:HE2	3:A:2603:PEE:H17	1.25	0.63
1:D:2387:VAL:HG11	1:D:2390:LEU:HD23	1.80	0.63
1:D:1989:ILE:HD12	3:D:2603:PEE:H38	1.80	0.63
1:D:2227:THR:HG23	1:D:2324:GLN:HE22	1.63	0.63
2:D:2602:PLX:O1	2:D:2602:PLX:H1A2	1.98	0.63
1:C:2243:ALA:HB1	1:C:2247:SER:HB2	1.80	0.63
1:A:1153:LEU:CD1	4:A:2604:P5S:C49	2.67	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2602:PLX:O1	2:A:2602:PLX:H1A2	1.98	0.63
1:D:2109:PHE:CB	3:D:2603:PEE:H11	2.23	0.63
1:A:2387:VAL:HG12	1:A:2390:LEU:H	1.64	0.63
1:D:1160:TYR:HE1	2:D:2602:PLX:O2	1.82	0.63
1:D:1799:GLN:HA	2:D:2602:PLX:C1C	2.28	0.62
1:A:1296:ILE:HD11	4:A:2604:P5S:O18	1.99	0.62
1:A:1989:ILE:HD11	3:A:2603:PEE:H33	1.81	0.62
1:D:2250:PRO:HA	1:D:2282:VAL:HG12	1.81	0.62
1:A:1693:PHE:O	1:A:1697:LEU:HD23	2.00	0.62
1:C:2183:LYS:NZ	1:A:2147:LEU:O	2.24	0.62
4:C:2604:P5S:H48	4:C:2604:P5S:H26A	1.81	0.62
4:A:2604:P5S:H48	4:A:2604:P5S:H26A	1.81	0.62
1:D:1979:LEU:HB3	1:D:2092:LEU:HD13	1.82	0.62
1:D:1981:PHE:HE2	3:D:2603:PEE:C14	2.13	0.62
1:C:2318:ARG:NH2	1:A:2245:GLN:HG2	2.15	0.61
1:C:1698:ASN:ND2	1:C:1786:ASP:OD1	2.29	0.61
1:A:2387:VAL:HG11	1:A:2390:LEU:HD23	1.82	0.61
1:C:2318:ARG:NH2	1:A:2244:GLN:HB2	2.16	0.61
1:A:2318:ARG:CZ	1:D:2244:GLN:HB2	2.31	0.61
1:C:1415:PHE:HE2	1:C:2532:LEU:HD12	1.65	0.61
1:C:1675:LEU:HG	1:C:1676:LEU:HD12	1.82	0.61
1:A:2250:PRO:HA	1:A:2282:VAL:HG12	1.81	0.61
1:A:2458:LEU:HB3	1:A:2461:LEU:HD13	1.81	0.61
1:C:2387:VAL:HG12	1:C:2390:LEU:H	1.65	0.61
1:D:1989:ILE:HD11	3:D:2603:PEE:H33	1.81	0.61
1:A:2318:ARG:NH2	1:D:2244:GLN:HB2	2.15	0.61
1:D:1296:ILE:HD11	4:D:2604:P5S:O18	2.00	0.61
1:C:1980:MET:HB3	1:C:2092:LEU:HD11	1.83	0.61
1:C:1989:ILE:HD12	3:C:2603:PEE:H38	1.82	0.61
1:D:1352:ILE:HD11	1:D:2525:LEU:HD11	1.83	0.61
1:D:1795:PHE:HA	2:D:2602:PLX:H24	1.83	0.61
1:A:1727:LYS:O	1:A:1731:MET:HG2	2.01	0.61
1:A:2264:ASP:HA	1:A:2270:MET:SD	2.41	0.61
1:C:813:VAL:O	1:C:817:THR:HG23	2.01	0.60
1:C:1296:ILE:HD11	4:C:2604:P5S:O18	2.00	0.60
1:A:1692:TYR:O	1:A:1695:ILE:HG22	2.01	0.60
1:D:802:ARG:HH21	1:D:943:ARG:HE	1.48	0.60
1:A:1160:TYR:HE1	2:A:2602:PLX:O2	1.83	0.60
3:A:2603:PEE:H40	3:A:2603:PEE:C44	2.31	0.60
1:D:1728:ARG:CB	2:D:2601:PLX:O7	2.49	0.60
1:C:1153:LEU:HD12	4:C:2604:P5S:C49	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2604:P5S:H26A	4:D:2604:P5S:H48	1.81	0.60
1:A:1153:LEU:HD12	4:A:2604:P5S:C49	2.31	0.60
3:D:2603:PEE:H40	3:D:2603:PEE:C44	2.31	0.60
1:A:1152:MET:HA	1:A:1155:VAL:HG22	1.82	0.60
1:D:2458:LEU:HB3	1:D:2461:LEU:HD13	1.83	0.60
1:C:1981:PHE:HD2	3:C:2603:PEE:C13	2.07	0.60
1:A:1799:GLN:HA	2:A:2602:PLX:C1C	2.32	0.60
1:A:2407:ARG:HB3	1:A:2426:PHE:HB3	1.84	0.60
1:D:2407:ARG:HB3	1:D:2426:PHE:HB3	1.84	0.60
1:C:2461:LEU:HG	1:C:2462:ALA:H	1.66	0.59
1:A:2023:MET:HA	1:A:2026:VAL:HG22	1.84	0.59
1:A:2377:ARG:HA	1:A:2449:PHE:HB2	1.83	0.59
1:D:1039:PHE:HA	1:D:1042:LEU:HD12	1.84	0.59
1:A:2058:HIS:NE2	1:A:2083:TYR:OH	2.35	0.59
3:C:2603:PEE:H40	3:C:2603:PEE:C44	2.31	0.59
1:A:2536:PRO:HA	1:A:2539:MET:HG2	1.84	0.59
1:D:2023:MET:HA	1:D:2026:VAL:HG12	1.84	0.59
1:C:2289:SER:HA	1:C:2431:VAL:HG13	1.85	0.59
1:C:2318:ARG:HH12	1:A:2245:GLN:H	1.51	0.59
1:C:2244:GLN:HB2	1:D:2318:ARG:NH2	2.16	0.59
1:A:1989:ILE:HD12	3:A:2603:PEE:H38	1.82	0.59
1:C:2407:ARG:HB3	1:C:2426:PHE:HB3	1.84	0.59
1:A:1357:GLU:O	1:A:1361:GLN:HG2	2.02	0.59
1:A:1719:MET:HE1	1:A:2091:ALA:HA	1.84	0.59
1:D:1715:PHE:HZ	1:D:2087:CYS:HG	1.49	0.59
1:D:1152:MET:HA	1:D:1155:VAL:HG12	1.85	0.59
2:D:2602:PLX:H271	2:D:2602:PLX:O8	2.03	0.59
1:A:802:ARG:HH21	1:A:943:ARG:HE	1.51	0.59
1:A:2181:GLN:O	1:A:2183:LYS:N	2.35	0.59
1:A:2377:ARG:HH12	1:A:2379:PRO:HB3	1.68	0.59
1:C:2375:TYR:H	1:C:2391:GLN:HE22	1.50	0.58
1:A:2373:PRO:HB3	1:A:2398:TYR:CE1	2.38	0.58
1:D:2377:ARG:HH12	1:D:2379:PRO:HB3	1.68	0.58
1:C:1799:GLN:HA	2:C:2602:PLX:C1C	2.33	0.58
2:A:2602:PLX:O8	2:A:2602:PLX:H271	2.03	0.58
2:C:2602:PLX:O8	2:C:2602:PLX:H271	2.03	0.58
1:A:1728:ARG:CB	2:A:2601:PLX:O7	2.51	0.58
1:C:2377:ARG:HA	1:C:2449:PHE:HB2	1.85	0.58
1:A:998:ALA:HA	1:A:1100:LEU:HD12	1.85	0.58
1:A:1991:ILE:HD11	1:A:2023:MET:HG3	1.85	0.58
1:A:2145:THR:HG21	1:A:2152:TRP:HZ3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2377:ARG:HA	1:D:2449:PHE:HB2	1.84	0.58
1:C:1092:THR:O	1:C:1095:ILE:HG22	2.03	0.58
1:A:1981:PHE:HD2	3:A:2603:PEE:C11	2.07	0.58
1:A:2379:PRO:HD2	1:A:2384:ALA:HA	1.85	0.58
1:A:2135:ARG:CZ	3:A:2603:PEE:O1P	2.51	0.58
1:D:1987:ASP:OD2	1:D:2082:TRP:NE1	2.36	0.58
1:D:2497:LEU:HD12	1:D:2543:THR:HG21	1.85	0.58
1:C:1693:PHE:O	1:C:1697:LEU:HD23	2.02	0.58
1:C:2035:ARG:NE	3:C:2603:PEE:O5	2.37	0.58
1:A:1980:MET:HB2	1:A:2089:TYR:CD1	2.39	0.58
1:A:2031:MET:CE	3:A:2603:PEE:H56	2.34	0.58
1:D:2145:THR:HG21	1:D:2152:TRP:CZ3	2.39	0.58
1:A:1795:PHE:HA	2:A:2602:PLX:H24	1.85	0.58
1:D:1203:THR:HA	1:D:1206:GLN:NE2	2.19	0.58
1:D:1357:GLU:O	1:D:1361:GLN:HG2	2.03	0.58
1:D:1985:ILE:O	1:D:1989:ILE:HG12	2.04	0.58
1:C:1357:GLU:O	1:C:1361:GLN:HG2	2.03	0.57
1:A:2181:GLN:C	1:A:2183:LYS:H	2.06	0.57
1:D:1716:LEU:HD21	1:D:2054:VAL:HG11	1.85	0.57
1:D:998:ALA:HA	1:D:1100:LEU:HD12	1.86	0.57
1:D:2357:LEU:HD21	1:D:2405:LEU:HB2	1.86	0.57
1:D:2377:ARG:HH21	1:D:2385:ASN:HD21	1.53	0.57
1:C:1008:PHE:CE2	1:C:1080:LEU:HD23	2.40	0.57
1:C:2357:LEU:HD21	1:C:2405:LEU:HB2	1.86	0.57
1:C:2497:LEU:HD12	1:C:2543:THR:HG21	1.85	0.57
1:D:1092:THR:O	1:D:1095:ILE:HG22	2.04	0.57
1:D:1981:PHE:CE1	3:D:2603:PEE:H8	2.39	0.57
1:D:2145:THR:HG21	1:D:2152:TRP:HZ3	1.69	0.57
1:C:1352:ILE:HD11	1:C:2525:LEU:HD21	1.87	0.57
1:C:1152:MET:HA	1:C:1155:VAL:HG12	1.86	0.57
1:A:1981:PHE:CZ	3:A:2603:PEE:H8	2.38	0.57
1:D:2373:PRO:HB3	1:D:2398:TYR:CE1	2.39	0.57
1:C:1795:PHE:HA	2:C:2602:PLX:H24	1.87	0.57
1:A:2145:THR:HG22	1:A:2514:ARG:HD3	1.87	0.57
1:C:802:ARG:HH21	1:C:943:ARG:HE	1.50	0.57
1:D:1162:PHE:HE1	1:D:1210:TRP:HZ2	1.53	0.57
1:D:2379:PRO:HD2	1:D:2384:ALA:HA	1.86	0.57
1:C:1036:TYR:HA	1:C:1039:PHE:CE1	2.40	0.56
1:C:2025:LEU:HD23	1:D:2204:TRP:CZ2	2.40	0.56
1:A:1716:LEU:HD21	1:A:2054:VAL:HG11	1.86	0.56
1:D:1163:TRP:CB	2:D:2602:PLX:H282	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1163:TRP:HB3	2:C:2602:PLX:C28	2.28	0.56
1:A:2497:LEU:HD12	1:A:2543:THR:HG21	1.86	0.56
1:D:2408:GLU:HB3	1:D:2427:LEU:HB2	1.85	0.56
1:C:1327:ASN:OD1	1:C:1328:LEU:N	2.38	0.56
1:D:1714:VAL:HG22	1:D:1729:PHE:HZ	1.69	0.56
1:D:2231:LYS:NZ	1:D:2233:GLY:O	2.34	0.56
1:C:860:ILE:HD13	1:C:927:HIS:HE1	1.70	0.56
1:C:2325:ARG:HB2	1:C:2334:GLU:HG2	1.85	0.56
1:A:2357:LEU:HD21	1:A:2405:LEU:HB2	1.87	0.56
1:D:1206:GLN:HG3	1:D:1297:PHE:CE2	2.41	0.56
1:C:2318:ARG:CZ	1:A:2244:GLN:HB2	2.36	0.56
1:C:2509:ASP:HA	1:C:2512:LEU:HG	1.87	0.56
1:A:1092:THR:O	1:A:1095:ILE:HG22	2.05	0.56
1:D:1698:ASN:ND2	1:D:1786:ASP:OD1	2.35	0.56
1:D:2300:SER:O	1:D:2304:MET:HG2	2.06	0.56
1:C:2135:ARG:HA	1:C:2138:MET:HE2	1.87	0.56
1:C:2300:SER:O	1:C:2304:MET:HG2	2.05	0.56
1:A:2408:GLU:HB3	1:A:2427:LEU:HB2	1.87	0.56
1:C:998:ALA:HA	1:C:1100:LEU:HD12	1.87	0.56
1:C:2024:LEU:HD11	1:D:2204:TRP:HZ3	1.71	0.56
1:C:2241:MET:HE3	1:C:2291:GLY:HA2	1.87	0.56
1:C:1981:PHE:CE1	3:C:2603:PEE:H8	2.40	0.56
1:C:1989:ILE:HD11	3:C:2603:PEE:C21	2.35	0.56
1:A:2377:ARG:HH21	1:A:2385:ASN:HD21	1.53	0.56
1:A:2342:LEU:HD13	1:A:2371:LEU:HD23	1.87	0.56
3:D:2603:PEE:H68	3:D:2603:PEE:H78	1.86	0.56
1:D:1327:ASN:OD1	1:D:1328:LEU:N	2.39	0.56
1:A:1327:ASN:OD1	1:A:1328:LEU:N	2.39	0.55
1:A:1036:TYR:HA	1:A:1039:PHE:CE1	2.41	0.55
1:A:1714:VAL:HG22	1:A:1729:PHE:HZ	1.70	0.55
1:C:1981:PHE:HD2	3:C:2603:PEE:C11	2.11	0.55
1:C:2342:LEU:HD13	1:C:2371:LEU:HD23	1.88	0.55
1:C:2468:GLY:O	1:C:2471:VAL:HG12	2.07	0.55
1:D:2535:SER:HG	1:D:2538:THR:HG1	1.53	0.55
1:A:2031:MET:HE2	3:A:2603:PEE:C35	2.35	0.55
1:A:1989:ILE:HD11	3:A:2603:PEE:C21	2.37	0.55
1:C:2245:GLN:HG2	1:D:2318:ARG:NH2	2.22	0.55
1:C:2298:PRO:HB3	1:C:2301:ARG:HH21	1.72	0.55
1:C:2408:GLU:HB3	1:C:2427:LEU:HB2	1.89	0.55
1:A:1985:ILE:O	1:A:1989:ILE:HG12	2.06	0.55
1:C:2377:ARG:HH12	1:C:2379:PRO:HB3	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2285:GLN:HB3	1:D:2443:LEU:HD11	1.89	0.55
1:C:1056:PRO:HB3	1:C:1085:PHE:O	2.07	0.55
1:C:1987:ASP:OD2	1:C:2082:TRP:NE1	2.39	0.55
1:C:2191:MET:O	1:C:2194:LEU:HG	2.06	0.55
1:D:1036:TYR:HA	1:D:1039:PHE:CE1	2.42	0.55
1:D:2235:TYR:CD1	1:D:2304:MET:HE3	2.42	0.55
4:C:2604:P5S:H24A	4:C:2604:P5S:H45	1.89	0.54
1:A:1987:ASP:OD2	1:A:2082:TRP:NE1	2.39	0.54
1:D:2119:LEU:HD12	1:D:2167:CYS:HB3	1.89	0.54
1:D:2135:ARG:HD2	3:D:2603:PEE:H2	1.87	0.54
1:C:2239:PHE:CZ	1:C:2241:MET:HG2	2.42	0.54
1:A:1527:HIS:HA	1:A:1530:MET:HE3	1.87	0.54
4:D:2604:P5S:H45	4:D:2604:P5S:H24A	1.89	0.54
1:C:984:PHE:HB3	1:C:987:TYR:HB3	1.89	0.54
1:C:2181:GLN:O	1:C:2183:LYS:N	2.40	0.54
1:A:2318:ARG:NH2	1:D:2245:GLN:HG2	2.22	0.54
1:C:2231:LYS:NZ	1:C:2233:GLY:O	2.34	0.54
1:C:2377:ARG:HH21	1:C:2385:ASN:HD21	1.56	0.54
1:A:984:PHE:HB3	1:A:987:TYR:HB3	1.90	0.54
1:C:2379:PRO:HD2	1:C:2384:ALA:HA	1.88	0.54
1:A:2182:LYS:O	1:A:2182:LYS:HD3	2.07	0.54
4:A:2604:P5S:H24A	4:A:2604:P5S:H45	1.89	0.54
1:D:1019:ALA:O	1:D:1022:THR:OG1	2.20	0.54
1:D:2286:ILE:HG13	1:D:2444:LEU:HB2	1.90	0.54
1:D:2342:LEU:HD13	1:D:2371:LEU:HD23	1.87	0.54
1:D:2468:GLY:O	1:D:2471:VAL:HG12	2.07	0.54
1:C:1985:ILE:O	1:C:1989:ILE:HG12	2.07	0.54
1:C:2321:TRP:CH2	1:C:2373:PRO:HG2	2.32	0.54
1:D:2035:ARG:NE	3:D:2603:PEE:O5	2.40	0.54
3:A:2603:PEE:H68	3:A:2603:PEE:H78	1.86	0.54
1:C:1352:ILE:HD12	1:C:2509:ASP:HB3	1.89	0.54
1:C:2030:THR:HA	1:C:2033:ILE:HG22	1.90	0.54
1:C:2135:ARG:HD2	3:C:2603:PEE:H2	1.89	0.54
1:A:1019:ALA:O	1:A:1022:THR:OG1	2.21	0.54
1:D:2325:ARG:HB2	1:D:2334:GLU:HG2	1.89	0.54
1:A:2471:VAL:O	1:A:2475:LEU:HG	2.08	0.54
1:C:1153:LEU:CD1	4:C:2604:P5S:C49	2.70	0.53
1:A:2119:LEU:HD12	1:A:2167:CYS:HB3	1.90	0.53
1:D:1170:PHE:HB2	1:D:1188:CYS:SG	2.47	0.53
1:D:1981:PHE:HD2	3:D:2603:PEE:C11	2.09	0.53
1:C:2458:LEU:HB3	1:C:2461:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2183:LYS:HB2	1:D:2146:THR:HA	1.90	0.53
1:C:1170:PHE:HB2	1:C:1188:CYS:SG	2.49	0.53
1:A:631:LEU:O	1:A:634:VAL:N	2.38	0.53
1:C:1982:LEU:HD13	3:C:2603:PEE:H23	1.91	0.53
1:C:2361:ARG:HB2	1:C:2362:PRO:HD2	1.90	0.53
4:C:2604:P5S:H54	4:C:2604:P5S:H32A	1.91	0.53
1:C:2043:VAL:HG12	1:C:2101:TYR:HD2	1.74	0.53
1:C:2188:LYS:HG3	1:A:2140:TRP:CZ3	2.43	0.53
1:C:2305:LYS:HZ1	1:C:2359:GLU:HG3	1.73	0.53
1:A:2361:ARG:HB2	1:A:2362:PRO:HD2	1.90	0.53
1:C:2298:PRO:HD2	1:A:2429:TRP:CH2	2.43	0.53
4:A:2604:P5S:H54	4:A:2604:P5S:H32A	1.91	0.53
1:D:2194:LEU:O	1:D:2197:LEU:HG	2.09	0.53
1:A:1170:PHE:HB2	1:A:1188:CYS:SG	2.48	0.53
1:C:1157:VAL:HG11	4:C:2604:P5S:H44A	1.91	0.53
1:A:2285:GLN:HB3	1:A:2443:LEU:HD11	1.90	0.53
1:C:996:LEU:HD11	1:C:1288:PHE:HB2	1.91	0.52
1:C:2119:LEU:HD12	1:C:2167:CYS:HB3	1.90	0.52
3:C:2603:PEE:C45	3:C:2603:PEE:C41	2.86	0.52
1:D:984:PHE:HB3	1:D:987:TYR:HB3	1.92	0.52
1:D:1799:GLN:CA	2:D:2602:PLX:H1C1	2.38	0.52
1:D:2361:ARG:HB2	1:D:2362:PRO:HD2	1.90	0.52
1:D:2471:VAL:O	1:D:2475:LEU:HG	2.10	0.52
1:C:2285:GLN:HB3	1:C:2443:LEU:HD11	1.91	0.52
1:A:1199:LEU:HD22	1:A:1302:PHE:HZ	1.74	0.52
1:A:2286:ILE:HG13	1:A:2444:LEU:HB2	1.92	0.52
1:C:631:LEU:O	1:C:634:VAL:N	2.38	0.52
1:C:1692:TYR:O	1:C:1695:ILE:HG22	2.09	0.52
3:A:2603:PEE:C45	3:A:2603:PEE:C41	2.85	0.52
1:D:2298:PRO:HB3	1:D:2301:ARG:HH21	1.75	0.52
1:C:1192:LEU:HB3	1:C:1794:PHE:CE2	2.45	0.52
1:A:2147:LEU:HD23	1:A:2151:ASN:HB3	1.91	0.52
1:C:1162:PHE:O	1:C:1165:VAL:HG12	2.10	0.52
3:A:2603:PEE:C45	3:A:2603:PEE:C24	2.85	0.52
1:C:1406:VAL:HG11	1:C:2523:GLU:HG3	1.90	0.52
1:C:2404:GLN:HB3	1:C:2431:VAL:HB	1.92	0.52
1:C:1019:ALA:O	1:C:1022:THR:OG1	2.23	0.52
1:A:1734:ILE:HG12	1:A:1794:PHE:HE1	1.75	0.52
1:C:2535:SER:HG	1:C:2538:THR:HG1	1.57	0.52
3:C:2603:PEE:H68	3:C:2603:PEE:H78	1.86	0.52
1:D:2037:LEU:HD23	1:D:2046:LYS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2602:PLX:H291	2:C:2602:PLX:H6	1.93	0.51
1:A:1190:TYR:HD2	1:A:1191:LEU:HD22	1.75	0.51
1:A:2026:VAL:O	1:A:2030:THR:HG23	2.09	0.51
1:A:2324:GLN:HA	1:A:2334:GLU:O	2.10	0.51
1:D:2305:LYS:HZ1	1:D:2359:GLU:HG3	1.75	0.51
1:C:1221:ILE:HD11	1:C:1283:ASP:HB3	1.90	0.51
3:D:2603:PEE:C45	3:D:2603:PEE:C41	2.86	0.51
1:C:1219:THR:HA	1:C:1222:ILE:HG12	1.90	0.51
1:A:1988:ILE:O	1:A:1991:ILE:HG22	2.10	0.51
1:D:1162:PHE:O	1:D:1165:VAL:HG12	2.10	0.51
1:C:2162:ILE:HG22	1:C:2504:LEU:HD21	1.92	0.51
1:C:2527:ALA:HA	1:C:2530:ILE:HG22	1.93	0.51
2:D:2602:PLX:H6	2:D:2602:PLX:H291	1.92	0.51
1:C:1982:LEU:CD1	3:C:2603:PEE:C16	2.88	0.51
1:A:1406:VAL:HG11	1:A:2523:GLU:HG3	1.93	0.51
1:A:1713:LEU:O	1:A:1717:TRP:N	2.43	0.51
1:C:2271:GLN:HE22	1:C:2389:GLN:HE22	1.59	0.51
1:C:2286:ILE:HG13	1:C:2444:LEU:HB2	1.92	0.51
1:D:1989:ILE:HD11	3:D:2603:PEE:C21	2.41	0.51
1:C:2181:GLN:C	1:C:2183:LYS:H	2.13	0.51
2:A:2602:PLX:H291	2:A:2602:PLX:H6	1.93	0.51
1:D:1976:VAL:O	1:D:1976:VAL:HG13	2.11	0.51
1:C:2264:ASP:HA	1:C:2270:MET:SD	2.51	0.51
1:C:2429:TRP:CH2	1:D:2298:PRO:HD2	2.46	0.51
1:C:2387:VAL:HG11	1:C:2390:LEU:HD23	1.93	0.51
1:A:1743:THR:HA	1:A:1746:LEU:HG	1.92	0.51
1:C:2266:TYR:O	1:C:2270:MET:HG2	2.10	0.51
3:C:2603:PEE:C45	3:C:2603:PEE:C24	2.85	0.51
1:D:1157:VAL:HG22	4:D:2604:P5S:H23	1.94	0.51
4:D:2604:P5S:H28A	4:D:2604:P5S:H50	1.92	0.51
4:D:2604:P5S:H32A	4:D:2604:P5S:H54	1.91	0.51
1:A:2185:LYS:O	1:A:2188:LYS:HB3	2.11	0.50
1:A:2197:LEU:O	1:A:2201:ALA:N	2.40	0.50
1:D:1163:TRP:HB3	2:D:2602:PLX:C28	2.34	0.50
1:D:2138:MET:SD	1:D:2142:TRP:CD1	3.04	0.50
1:D:2294:TRP:CB	1:D:2429:TRP:HA	2.41	0.50
1:C:2471:VAL:O	1:C:2475:LEU:HG	2.11	0.50
1:A:996:LEU:HD11	1:A:1288:PHE:HB2	1.92	0.50
1:A:1107:GLN:O	1:A:1111:PHE:HB2	2.11	0.50
1:C:1008:PHE:CD2	1:C:1080:LEU:HD23	2.46	0.50
4:C:2604:P5S:H50	4:C:2604:P5S:H28A	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2197:LEU:O	1:D:2201:ALA:N	2.39	0.50
1:C:2146:THR:HG22	1:D:2181:GLN:HB3	1.94	0.50
1:A:1787:LEU:O	1:A:1791:MET:HG2	2.10	0.50
1:A:2509:ASP:HA	1:A:2512:LEU:HG	1.94	0.50
1:D:1190:TYR:HD2	1:D:1191:LEU:HD22	1.77	0.50
1:D:2321:TRP:CH2	1:D:2373:PRO:HG2	2.34	0.50
1:C:1044:LEU:HD13	1:C:1097:ASP:OD2	2.12	0.50
1:C:1734:ILE:HD11	1:C:1790:LEU:HD13	1.93	0.50
1:C:2085:VAL:O	1:C:2088:ILE:HG22	2.12	0.50
1:C:2294:TRP:CZ2	1:C:2296:ILE:HD12	2.46	0.50
1:D:1084:ASP:OD1	1:D:1086:PHE:N	2.44	0.50
1:D:2294:TRP:CZ2	1:D:2296:ILE:HD12	2.47	0.50
1:C:1107:GLN:O	1:C:1111:PHE:HB2	2.11	0.50
1:A:1163:TRP:HB3	2:A:2602:PLX:C28	2.32	0.50
4:A:2604:P5S:H50	4:A:2604:P5S:H28A	1.92	0.50
1:C:1981:PHE:HE2	3:C:2603:PEE:H20	1.75	0.50
1:D:1981:PHE:CZ	3:D:2603:PEE:H8	2.46	0.50
1:D:2535:SER:OG	1:D:2538:THR:OG1	2.27	0.50
1:C:1036:TYR:CZ	1:C:1040:LEU:HD11	2.47	0.50
1:C:1713:LEU:O	1:C:1717:TRP:N	2.43	0.50
1:A:2222:GLN:H	1:A:2329:LYS:HE3	1.77	0.50
1:C:1521:ARG:HE	1:C:1528:ARG:NH1	2.10	0.50
1:A:1991:ILE:CD1	1:A:2023:MET:HG3	2.42	0.50
1:A:2321:TRP:CH2	1:A:2373:PRO:HG2	2.37	0.49
1:D:1148:SER:OG	1:D:1151:ASP:OD2	2.24	0.49
1:C:2501:ASP:OD1	1:C:2502:ARG:N	2.44	0.49
1:A:1162:PHE:O	1:A:1165:VAL:HG12	2.12	0.49
1:A:2130:PHE:O	1:A:2134:LEU:HD12	2.12	0.49
1:D:1107:GLN:O	1:D:1111:PHE:HB2	2.11	0.49
1:D:1690:LEU:O	1:D:1694:ILE:HG12	2.12	0.49
1:C:2227:THR:HG22	1:C:2242:SER:HB3	1.93	0.49
1:C:2037:LEU:HD23	1:C:2046:LYS:HA	1.93	0.49
1:C:2151:ASN:O	1:C:2155:VAL:HG23	2.12	0.49
1:C:2271:GLN:NE2	1:C:2389:GLN:OE1	2.45	0.49
1:C:2389:GLN:O	1:C:2392:PRO:HD3	2.12	0.49
1:A:1211:ASP:HA	1:A:1214:ILE:HG12	1.94	0.49
1:A:1287:PHE:O	1:A:1291:LEU:HG	2.11	0.49
1:D:2135:ARG:NH2	3:D:2603:PEE:O1P	2.46	0.49
1:C:1148:SER:OG	1:C:1151:ASP:OD2	2.22	0.49
1:C:1289:PHE:HA	1:C:1292:LEU:HG	1.92	0.49
1:C:2245:GLN:H	1:D:2318:ARG:HH12	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2377:ARG:NH1	1:C:2379:PRO:HB3	2.28	0.49
1:A:822:LEU:HD13	1:A:1092:THR:HA	1.95	0.49
1:D:631:LEU:O	1:D:634:VAL:N	2.37	0.49
1:C:1153:LEU:O	1:C:1157:VAL:HG22	2.13	0.49
1:C:1353:ARG:O	1:C:1356:GLN:HG3	2.13	0.49
1:C:2147:LEU:HB3	1:C:2151:ASN:HB2	1.95	0.49
1:C:2395:GLU:HA	1:C:2398:TYR:CD2	2.47	0.49
1:A:1163:TRP:CB	2:A:2602:PLX:H282	2.33	0.49
1:A:1246:ILE:HA	1:A:1251:LEU:CD1	2.41	0.49
1:D:2148:SER:HB3	1:D:2151:ASN:ND2	2.28	0.49
1:D:2377:ARG:NH1	1:D:2379:PRO:HB3	2.27	0.49
1:C:1714:VAL:HG12	1:C:1719:MET:HE3	1.94	0.49
1:C:2183:LYS:NZ	1:A:2145:THR:OG1	2.46	0.49
1:C:2293:LEU:HB2	1:D:2295:ARG:HB2	1.95	0.49
1:C:2295:ARG:HB2	1:A:2293:LEU:HD12	1.94	0.49
1:C:1162:PHE:O	1:C:1166:LEU:HG	2.12	0.49
1:C:1695:ILE:HA	1:C:1789:GLN:HE21	1.77	0.49
1:C:1981:PHE:CE1	3:C:2603:PEE:H50	2.47	0.49
1:A:2318:ARG:HH12	1:D:2245:GLN:H	1.60	0.49
1:A:1224:LYS:NZ	1:A:1280:ILE:HD13	2.27	0.49
1:A:1976:VAL:O	1:A:1976:VAL:HG13	2.13	0.49
1:A:1353:ARG:O	1:A:1356:GLN:HG3	2.13	0.49
1:A:1695:ILE:HA	1:A:1789:GLN:HE21	1.77	0.49
1:D:1038:LEU:O	1:D:1041:THR:OG1	2.28	0.49
1:C:1243:CYS:HA	1:C:1246:ILE:HG12	1.94	0.48
1:C:2183:LYS:HE2	1:A:2145:THR:C	2.33	0.48
1:C:2295:ARG:HB2	1:A:2293:LEU:HB2	1.95	0.48
1:A:1157:VAL:CG1	4:A:2604:P5S:H23	2.43	0.48
1:A:1521:ARG:HE	1:A:1528:ARG:NH1	2.11	0.48
1:A:2295:ARG:HB2	1:D:2293:LEU:HD12	1.96	0.48
1:D:2227:THR:HG22	1:D:2242:SER:HB3	1.94	0.48
1:D:2389:GLN:O	1:D:2392:PRO:HD3	2.13	0.48
1:C:1734:ILE:HG12	1:C:1794:PHE:HE1	1.75	0.48
1:A:2231:LYS:NZ	1:A:2233:GLY:O	2.35	0.48
1:A:2496:GLU:HB2	1:D:2534:ARG:HE	1.78	0.48
1:C:2222:GLN:H	1:C:2329:LYS:HE3	1.76	0.48
1:C:2318:ARG:HH22	1:A:2245:GLN:HG2	1.78	0.48
3:C:2603:PEE:H40	3:C:2603:PEE:H77	1.95	0.48
1:A:2135:ARG:HD2	3:A:2603:PEE:H2	1.95	0.48
1:A:2239:PHE:CZ	1:A:2241:MET:HG2	2.49	0.48
1:A:2377:ARG:NH1	1:A:2379:PRO:HB3	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2460:PHE:HD2	1:A:2465:GLY:HA3	1.78	0.48
1:D:1713:LEU:O	1:D:1717:TRP:N	2.46	0.48
1:D:2374:LYS:NZ	1:D:2445:PRO:O	2.39	0.48
1:C:969:ARG:HG2	1:C:976:SER:HB2	1.95	0.48
1:C:2135:ARG:NH2	3:C:2603:PEE:O1P	2.46	0.48
1:C:2517:ARG:HG3	1:C:2517:ARG:O	2.13	0.48
1:A:1023:ARG:HD3	1:A:1028:ALA:HB1	1.95	0.48
1:A:1036:TYR:CZ	1:A:1040:LEU:HD11	2.48	0.48
1:A:2492:ILE:O	1:A:2496:GLU:HG2	2.13	0.48
1:D:1992:ILE:HG21	3:D:2603:PEE:C27	2.42	0.48
1:C:1692:TYR:HA	1:C:1695:ILE:HG22	1.94	0.48
1:C:2194:LEU:O	1:C:2197:LEU:HG	2.12	0.48
1:C:2257:GLU:O	1:C:2261:GLN:OE1	2.31	0.48
1:A:2471:VAL:HA	1:A:2474:VAL:HG12	1.96	0.48
1:D:2375:TYR:HD1	1:D:2391:GLN:HE22	1.60	0.48
1:C:2245:GLN:HG2	1:D:2318:ARG:CZ	2.43	0.48
1:A:1146:CYS:HA	1:A:1151:ASP:HB3	1.94	0.48
1:D:1961:PHE:O	1:D:1965:ILE:HG12	2.14	0.48
3:D:2603:PEE:C45	3:D:2603:PEE:C24	2.85	0.48
1:C:1799:GLN:CA	2:C:2602:PLX:H1C1	2.43	0.48
1:D:2235:TYR:CG	1:D:2304:MET:HE3	2.49	0.48
1:D:2529:LEU:HD11	1:D:2533:TYR:HE2	1.78	0.48
1:C:2197:LEU:O	1:C:2201:ALA:N	2.41	0.48
1:A:1992:ILE:HG21	3:A:2603:PEE:C27	2.44	0.48
1:A:2407:ARG:HB3	1:A:2426:PHE:CG	2.49	0.48
1:D:1406:VAL:HG11	1:D:2523:GLU:HG3	1.94	0.48
1:D:2222:GLN:H	1:D:2329:LYS:HE3	1.78	0.48
1:D:2407:ARG:HB3	1:D:2426:PHE:CG	2.49	0.48
1:C:1146:CYS:HA	1:C:1151:ASP:HB3	1.95	0.48
1:C:2293:LEU:HD12	1:D:2295:ARG:HB2	1.95	0.48
1:C:2347:ASN:O	1:C:2347:ASN:ND2	2.47	0.48
1:A:1961:PHE:O	1:A:1965:ILE:HG12	2.13	0.48
1:D:1521:ARG:HE	1:D:1528:ARG:NH1	2.11	0.48
1:D:2135:ARG:HB2	3:D:2603:PEE:H48	1.95	0.48
1:C:1961:PHE:O	1:C:1965:ILE:HG12	2.14	0.48
1:A:2210:MET:HE1	1:A:2466:ILE:HG23	1.95	0.48
1:A:2295:ARG:HB2	1:D:2293:LEU:HB2	1.96	0.48
1:D:1023:ARG:HD3	1:D:1028:ALA:HB1	1.95	0.48
1:D:1143:PHE:HE1	1:D:1155:VAL:HA	1.79	0.48
1:C:2140:TRP:HD1	1:C:2152:TRP:CE3	2.32	0.47
1:C:2372:PHE:HD2	1:C:2400:GLY:HA2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2603:PEE:H82	3:C:2603:PEE:H75	1.66	0.47
1:A:2325:ARG:HB2	1:A:2334:GLU:HG2	1.95	0.47
1:A:2363:ASP:CG	1:A:2406:ARG:HH22	2.17	0.47
1:A:2389:GLN:O	1:A:2392:PRO:HD3	2.14	0.47
1:A:2183:LYS:HD3	1:A:2183:LYS:C	2.35	0.47
1:A:2311:GLY:O	1:A:2351:ARG:NH1	2.47	0.47
1:A:2477:VAL:O	1:A:2481:VAL:HG23	2.14	0.47
1:D:1353:ARG:O	1:D:1356:GLN:HG3	2.14	0.47
1:C:978:LEU:O	1:C:982:ILE:HG12	2.13	0.47
1:C:1143:PHE:HE1	1:C:1155:VAL:HA	1.79	0.47
1:C:2380:ASN:ND2	1:C:2453:VAL:HA	2.26	0.47
1:C:2407:ARG:HB3	1:C:2426:PHE:CG	2.49	0.47
1:A:2347:ASN:O	1:A:2347:ASN:ND2	2.47	0.47
1:D:2147:LEU:HD23	1:D:2151:ASN:HB3	1.95	0.47
1:D:2477:VAL:O	1:D:2481:VAL:HG23	2.15	0.47
1:C:1160:TYR:CE1	2:C:2602:PLX:O2	2.62	0.47
1:C:2488:ILE:O	1:C:2488:ILE:HG13	2.14	0.47
1:A:1287:PHE:CE2	1:A:1291:LEU:HD11	2.50	0.47
1:A:1734:ILE:HD11	1:A:1790:LEU:HD13	1.96	0.47
1:A:2224:ILE:HG12	1:A:2326:ASP:HA	1.96	0.47
1:D:2093:SER:O	1:D:2097:ILE:HG13	2.14	0.47
1:D:2447:VAL:O	1:D:2448:ILE:HD13	2.15	0.47
1:C:1985:ILE:HG21	3:C:2603:PEE:H26	1.96	0.47
1:A:1521:ARG:O	1:A:1528:ARG:NH2	2.48	0.47
1:D:1036:TYR:CZ	1:D:1040:LEU:HD11	2.49	0.47
1:D:1695:ILE:HA	1:D:1789:GLN:HE21	1.80	0.47
1:C:1739:VAL:HA	1:C:1742:VAL:HG12	1.95	0.47
1:C:1982:LEU:HD13	3:C:2603:PEE:C16	2.45	0.47
1:C:2311:GLY:O	1:C:2351:ARG:NH1	2.48	0.47
1:C:2324:GLN:HA	1:C:2334:GLU:O	2.14	0.47
1:A:1799:GLN:CA	2:A:2602:PLX:H1C1	2.42	0.47
1:A:1985:ILE:HG21	3:A:2603:PEE:H26	1.95	0.47
1:A:2294:TRP:CZ2	1:A:2296:ILE:HD12	2.49	0.47
1:A:2473:ILE:HA	1:A:2476:VAL:HG22	1.97	0.47
1:D:1146:CYS:HA	1:D:1151:ASP:HB3	1.95	0.47
1:D:1218:VAL:HA	1:D:1221:ILE:HG22	1.97	0.47
1:D:2225:ASP:OD2	1:D:2324:GLN:NE2	2.48	0.47
1:D:2311:GLY:O	1:D:2351:ARG:NH1	2.47	0.47
1:C:1162:PHE:CE2	1:C:1166:LEU:HD11	2.50	0.47
1:C:1415:PHE:CE2	1:C:2532:LEU:HD12	2.47	0.47
1:C:1976:VAL:O	1:C:1976:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2496:GLU:O	1:A:2534:ARG:NH2	2.48	0.47
1:A:831:LEU:HD12	1:A:832:LEU:N	2.30	0.47
1:C:1162:PHE:HE1	1:C:1210:TRP:CZ2	2.33	0.47
1:C:2211:SER:HA	1:C:2214:ARG:HE	1.80	0.47
1:A:1977:TYR:OH	1:A:2034:ASP:OD1	2.31	0.47
1:D:2036:ALA:HA	1:D:2142:TRP:CD1	2.49	0.47
1:C:2225:ASP:OD2	1:C:2324:GLN:NE2	2.47	0.47
1:A:2031:MET:CE	3:A:2603:PEE:C35	2.92	0.47
1:D:1734:ILE:HG12	1:D:1794:PHE:HE1	1.75	0.47
1:C:1206:GLN:O	1:C:1210:TRP:HD1	1.98	0.46
1:C:2477:VAL:O	1:C:2481:VAL:HG23	2.15	0.46
1:A:2280:ASP:OD2	1:A:2452:LYS:HE3	2.15	0.46
1:A:2326:ASP:HB3	1:A:2329:LYS:HB2	1.97	0.46
1:C:1061:ASP:HA	1:C:1085:PHE:CE1	2.50	0.46
1:C:2193:GLY:O	1:C:2196:ILE:HG12	2.15	0.46
1:A:1718:ALA:HB2	1:A:1729:PHE:CZ	2.50	0.46
1:A:2373:PRO:HB3	1:A:2398:TYR:CD1	2.51	0.46
1:D:1739:VAL:HA	1:D:1742:VAL:HG12	1.97	0.46
1:D:2181:GLN:O	1:D:2183:LYS:N	2.48	0.46
1:C:1023:ARG:HD3	1:C:1028:ALA:HB1	1.96	0.46
1:C:1084:ASP:OD1	1:C:1086:PHE:N	2.46	0.46
1:C:2235:TYR:CG	1:C:2304:MET:HE3	2.50	0.46
1:A:1988:ILE:HA	1:A:1991:ILE:HG22	1.97	0.46
1:D:1734:ILE:HD11	1:D:1790:LEU:HD13	1.95	0.46
1:C:1980:MET:HB3	1:C:2092:LEU:CD1	2.44	0.46
1:D:1206:GLN:O	1:D:1210:TRP:HD1	1.99	0.46
1:C:2141:VAL:HA	1:D:2188:LYS:NZ	2.30	0.46
1:A:1218:VAL:HA	1:A:1221:ILE:HG22	1.98	0.46
1:A:1233:VAL:HG12	1:A:1233:VAL:O	2.16	0.46
3:A:2603:PEE:H1	3:A:2603:PEE:O2P	2.16	0.46
1:D:2182:LYS:HG2	1:D:2185:LYS:HG3	1.96	0.46
1:D:2363:ASP:CG	1:D:2406:ARG:HH22	2.18	0.46
1:D:2380:ASN:ND2	1:D:2453:VAL:HA	2.26	0.46
1:C:1233:VAL:HG12	1:C:1233:VAL:O	2.16	0.46
1:C:1992:ILE:HG21	3:C:2603:PEE:C27	2.46	0.46
1:C:2092:LEU:HD12	1:C:2093:SER:N	2.30	0.46
1:A:1337:ILE:HA	1:A:1340:LYS:HZ2	1.80	0.46
1:D:2342:LEU:HD22	1:D:2371:LEU:HG	1.97	0.46
1:C:1744:LYS:O	1:C:1748:GLN:HG2	2.16	0.46
1:A:1984:ASP:O	1:A:1988:ILE:HG12	2.16	0.46
1:D:2211:SER:HA	1:D:2214:ARG:HE	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2271:GLN:HE22	1:D:2389:GLN:HE22	1.63	0.46
1:C:2286:ILE:CG1	1:C:2444:LEU:HB2	2.46	0.46
1:C:2301:ARG:HH12	1:C:2424:SER:CA	2.29	0.46
1:A:1056:PRO:HB3	1:A:1085:PHE:O	2.16	0.46
1:A:2166:LYS:HB2	1:A:2504:LEU:HD11	1.97	0.46
1:A:2321:TRP:HH2	1:A:2373:PRO:CG	2.24	0.46
1:D:2305:LYS:HD2	1:D:2305:LYS:HA	1.81	0.46
1:D:2460:PHE:HB3	1:D:2465:GLY:HA3	1.98	0.46
1:C:857:THR:HA	1:C:860:ILE:HG22	1.98	0.46
1:C:2372:PHE:HB2	1:C:2399:LEU:O	2.15	0.46
1:C:2468:GLY:O	1:C:2471:VAL:N	2.49	0.46
1:A:2030:THR:HA	1:A:2033:ILE:HG12	1.96	0.46
1:D:1246:ILE:HA	1:D:1251:LEU:CD1	2.46	0.46
1:D:2139:ASP:O	1:D:2143:THR:OG1	2.30	0.46
1:D:2181:GLN:C	1:D:2183:LYS:H	2.18	0.46
1:D:2319:PHE:CE2	1:D:2321:TRP:NE1	2.78	0.46
1:C:2202:ILE:O	1:C:2206:PRO:HD3	2.16	0.46
1:C:2298:PRO:HD2	1:A:2429:TRP:CZ3	2.51	0.46
1:C:2363:ASP:CG	1:C:2406:ARG:HH22	2.18	0.46
1:C:2532:LEU:HD11	1:C:2542:TRP:CD1	2.51	0.46
1:A:1719:MET:CE	1:A:2094:ALA:HB3	2.46	0.46
1:A:2085:VAL:O	1:A:2088:ILE:HG22	2.16	0.46
1:C:2280:ASP:OD2	1:C:2452:LYS:HE3	2.16	0.45
1:C:2376:ILE:HA	1:C:2386:PRO:HA	1.98	0.45
1:C:2534:ARG:HG3	1:D:2496:GLU:OE1	2.15	0.45
1:A:2361:ARG:HH11	1:A:2364:GLN:HG2	1.81	0.45
1:A:2463:GLY:H	1:A:2467:VAL:HG21	1.81	0.45
1:D:2280:ASP:OD2	1:D:2452:LYS:HE3	2.16	0.45
3:D:2603:PEE:H1	3:D:2603:PEE:O2P	2.16	0.45
1:C:2535:SER:OG	1:C:2538:THR:OG1	2.28	0.45
1:A:1153:LEU:HD12	4:A:2604:P5S:C48	2.46	0.45
1:A:1719:MET:HE1	1:A:2094:ALA:HB3	1.97	0.45
1:D:1233:VAL:HG12	1:D:1233:VAL:O	2.15	0.45
1:D:2280:ASP:O	1:D:2450:SER:N	2.49	0.45
1:D:2405:LEU:HD11	1:D:2428:GLU:HB3	1.98	0.45
1:C:1162:PHE:HE1	1:C:1210:TRP:HZ2	1.62	0.45
1:C:1224:LYS:NZ	1:C:1280:ILE:HD13	2.31	0.45
1:C:2210:MET:HE1	1:C:2466:ILE:HG23	1.98	0.45
1:C:2301:ARG:O	1:C:2304:MET:HB2	2.16	0.45
1:A:1084:ASP:OD1	1:A:1086:PHE:N	2.47	0.45
1:A:1692:TYR:HA	1:A:1695:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2473:ILE:O	1:A:2477:VAL:HG12	2.17	0.45
1:D:2271:GLN:NE2	1:D:2389:GLN:OE1	2.48	0.45
1:D:2301:ARG:HH12	1:D:2424:SER:CA	2.29	0.45
1:C:2119:LEU:HD12	1:C:2167:CYS:CB	2.46	0.45
1:A:2308:LEU:HD22	1:A:2351:ARG:HG3	1.98	0.45
1:D:1280:ILE:HG22	1:D:1280:ILE:O	2.16	0.45
1:D:2324:GLN:HA	1:D:2334:GLU:O	2.17	0.45
1:C:2280:ASP:O	1:C:2450:SER:N	2.50	0.45
1:C:2305:LYS:HD2	1:C:2305:LYS:HA	1.81	0.45
3:C:2603:PEE:C24	3:C:2603:PEE:C44	2.95	0.45
1:A:2211:SER:HA	1:A:2214:ARG:HE	1.82	0.45
1:A:2271:GLN:NE2	1:A:2389:GLN:OE1	2.48	0.45
1:D:1296:ILE:CD1	4:D:2604:P5S:O18	2.65	0.45
1:A:1018:VAL:O	1:A:1022:THR:HG23	2.17	0.45
1:A:1215:LEU:O	1:A:1219:THR:HG23	2.17	0.45
1:A:1696:ILE:HD11	1:A:2083:TYR:CE2	2.52	0.45
1:A:2333:VAL:HG11	1:A:2382:PRO:HA	1.97	0.45
1:A:2375:TYR:CD2	1:A:2390:LEU:HB3	2.52	0.45
1:D:1215:LEU:O	1:D:1219:THR:HG23	2.17	0.45
1:D:2301:ARG:O	1:D:2304:MET:HB2	2.17	0.45
1:C:831:LEU:HD12	1:C:832:LEU:N	2.31	0.45
1:C:1192:LEU:HD23	1:C:1794:PHE:CD2	2.52	0.45
1:C:2204:TRP:CE2	1:A:2025:LEU:HD12	2.52	0.45
1:A:2280:ASP:O	1:A:2450:SER:N	2.50	0.45
1:D:2373:PRO:HB3	1:D:2398:TYR:CD1	2.52	0.45
1:C:2125:PHE:O	1:C:2128:VAL:HG12	2.17	0.45
1:C:2361:ARG:HH11	1:C:2364:GLN:HG2	1.81	0.45
1:C:2479:LYS:HE2	1:A:2480:PHE:CZ	2.52	0.45
1:A:1243:CYS:HA	1:A:1246:ILE:HG22	1.98	0.45
1:A:1739:VAL:HA	1:A:1742:VAL:HG12	1.99	0.45
1:A:2034:ASP:OD1	1:A:2035:ARG:N	2.49	0.45
1:A:2261:GLN:HA	1:A:2264:ASP:HB2	1.98	0.45
1:A:2510:ILE:HG12	1:A:2525:LEU:HB3	1.99	0.45
3:A:2603:PEE:H40	3:A:2603:PEE:H77	1.94	0.45
3:A:2603:PEE:C24	3:A:2603:PEE:C44	2.95	0.45
1:D:1162:PHE:HE1	1:D:1210:TRP:CZ2	2.34	0.45
3:D:2603:PEE:C25	3:D:2603:PEE:C44	2.95	0.45
1:C:2183:LYS:HG3	1:C:2184:LYS:HG2	1.99	0.45
1:C:2471:VAL:HA	1:C:2474:VAL:HG12	1.99	0.45
1:A:2405:LEU:HD11	1:A:2428:GLU:HB3	1.98	0.45
1:D:2119:LEU:HD12	1:D:2167:CYS:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:967:ARG:NH1	1:C:1116:THR:OG1	2.49	0.45
1:C:1981:PHE:CZ	3:C:2603:PEE:H8	2.52	0.45
1:C:2055:VAL:O	1:C:2059:ILE:HG12	2.17	0.45
1:D:2258:GLU:HA	1:D:2261:GLN:OE1	2.16	0.45
1:D:2321:TRP:HH2	1:D:2373:PRO:CG	2.22	0.45
1:C:1254:THR:HG23	1:C:1255:VAL:HG12	1.99	0.44
1:C:2294:TRP:CB	1:C:2429:TRP:HA	2.41	0.44
1:C:2325:ARG:NH1	1:C:2336:THR:OG1	2.47	0.44
1:A:2286:ILE:CG1	1:A:2444:LEU:HB2	2.46	0.44
1:A:2294:TRP:CB	1:A:2429:TRP:HA	2.41	0.44
1:A:2498:PRO:HD3	1:D:2534:ARG:NH2	2.26	0.44
1:D:2220:VAL:HG21	1:D:2280:ASP:HA	2.00	0.44
1:C:2318:ARG:CZ	1:A:2245:GLN:HG2	2.47	0.44
1:C:2319:PHE:CE2	1:C:2321:TRP:NE1	2.78	0.44
3:C:2603:PEE:H1	3:C:2603:PEE:O2P	2.16	0.44
1:A:2188:LYS:NZ	1:D:2140:TRP:O	2.40	0.44
1:D:1301:TYR:HA	1:D:1304:HIS:CD2	2.53	0.44
1:D:2376:ILE:HA	1:D:2386:PRO:HA	1.99	0.44
1:C:2241:MET:CE	1:C:2291:GLY:HA2	2.47	0.44
1:D:2325:ARG:NH1	1:D:2336:THR:OG1	2.47	0.44
1:C:2181:GLN:HB3	1:A:2146:THR:HG22	2.00	0.44
1:D:1243:CYS:HA	1:D:1246:ILE:HG22	1.99	0.44
1:C:1166:LEU:HB3	1:C:1192:LEU:HD11	1.99	0.44
1:A:2204:TRP:CH2	1:D:2025:LEU:HB2	2.52	0.44
1:A:2220:VAL:HG21	1:A:2280:ASP:HA	1.99	0.44
1:A:2258:GLU:HA	1:A:2261:GLN:OE1	2.18	0.44
1:D:792:ALA:O	1:D:796:ARG:HG2	2.17	0.44
1:D:1227:LEU:HD21	1:D:1251:LEU:HG	1.99	0.44
1:D:2193:GLY:HA2	1:D:2196:ILE:HG12	2.00	0.44
1:D:2324:GLN:HG3	1:D:2335:TYR:HD1	1.81	0.44
3:D:2603:PEE:C23	3:D:2603:PEE:H81	2.47	0.44
1:C:792:ALA:O	1:C:796:ARG:HG2	2.17	0.44
1:D:2162:ILE:HD11	1:D:2500:VAL:HB	1.99	0.44
1:D:2286:ILE:CG1	1:D:2444:LEU:HB2	2.47	0.44
1:A:2125:PHE:O	1:A:2128:VAL:HG12	2.17	0.44
1:C:1018:VAL:O	1:C:1022:THR:HG23	2.18	0.44
1:A:792:ALA:O	1:A:796:ARG:HG2	2.17	0.44
1:A:1143:PHE:HA	1:A:1151:ASP:OD1	2.17	0.44
1:A:2301:ARG:HH12	1:A:2424:SER:CA	2.31	0.44
1:D:2031:MET:HA	1:D:2034:ASP:OD2	2.18	0.44
1:D:2395:GLU:HA	1:D:2398:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2603:PEE:C24	3:D:2603:PEE:C44	2.95	0.44
1:C:1698:ASN:O	1:C:1703:ALA:HB3	2.18	0.44
1:C:1977:TYR:O	1:C:1980:MET:HG2	2.17	0.44
1:C:2375:TYR:H	1:C:2391:GLN:NE2	2.14	0.44
1:C:2407:ARG:HB3	1:C:2426:PHE:CD2	2.53	0.44
1:A:1715:PHE:HZ	1:A:2087:CYS:HG	1.65	0.44
1:A:2145:THR:HG21	1:A:2152:TRP:CZ3	2.50	0.44
1:A:2395:GLU:HA	1:A:2398:TYR:CD2	2.53	0.44
1:A:2406:ARG:HA	1:A:2406:ARG:HD3	1.80	0.44
1:A:2521:LEU:O	1:A:2525:LEU:HD23	2.17	0.44
3:A:2603:PEE:C25	3:A:2603:PEE:C44	2.95	0.44
1:D:2361:ARG:HH11	1:D:2364:GLN:HG2	1.82	0.44
3:D:2603:PEE:C24	3:D:2603:PEE:H77	2.48	0.44
1:C:2324:GLN:HG3	1:C:2335:TYR:HD1	1.82	0.43
1:C:2405:LEU:HD11	1:C:2428:GLU:HB3	1.99	0.43
1:C:2534:ARG:NH2	1:D:2498:PRO:HD3	2.29	0.43
1:A:967:ARG:NH1	1:A:1116:THR:OG1	2.51	0.43
1:C:2301:ARG:HH12	1:C:2424:SER:HA	1.82	0.43
3:C:2603:PEE:C25	3:C:2603:PEE:C44	2.95	0.43
1:A:1206:GLN:O	1:A:1210:TRP:HD1	2.01	0.43
1:D:1023:ARG:HB3	1:D:1028:ALA:HB3	1.99	0.43
1:D:2209:PHE:HD1	1:D:2212:LEU:HD21	1.84	0.43
1:D:2372:PHE:HB2	1:D:2399:LEU:O	2.19	0.43
1:D:2406:ARG:HA	1:D:2406:ARG:HD3	1.82	0.43
1:C:2220:VAL:HG21	1:C:2280:ASP:HA	2.00	0.43
1:A:2289:SER:HA	1:A:2431:VAL:HG13	2.00	0.43
1:A:2318:ARG:HH22	1:D:2245:GLN:HG2	1.83	0.43
1:A:2407:ARG:HB3	1:A:2426:PHE:CD2	2.53	0.43
1:A:2408:GLU:O	1:A:2426:PHE:HA	2.18	0.43
3:A:2603:PEE:C23	3:A:2603:PEE:H81	2.47	0.43
1:A:1300:HIS:CD2	4:A:2604:P5S:N	2.86	0.43
1:A:2231:LYS:HB3	1:A:2318:ARG:HB2	1.99	0.43
1:D:1157:VAL:CG2	4:D:2604:P5S:H23	2.48	0.43
1:D:1981:PHE:HD2	3:D:2603:PEE:C13	2.22	0.43
1:C:2204:TRP:CH2	1:A:2025:LEU:HB2	2.53	0.43
1:A:2496:GLU:O	1:D:2534:ARG:NH2	2.52	0.43
1:D:1160:TYR:CE1	2:D:2602:PLX:O2	2.67	0.43
1:D:2210:MET:HE1	1:D:2466:ILE:HG23	2.01	0.43
1:D:2375:TYR:HD1	1:D:2391:GLN:NE2	2.15	0.43
1:D:2473:ILE:O	1:D:2477:VAL:HG12	2.18	0.43
1:C:1292:LEU:O	1:C:1296:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2527:ALA:O	1:C:2530:ILE:HG22	2.18	0.43
1:A:2361:ARG:NH1	1:A:2364:GLN:HG2	2.34	0.43
1:A:2372:PHE:HB2	1:A:2399:LEU:O	2.19	0.43
2:A:2602:PLX:H202	2:A:2602:PLX:H171	1.90	0.43
1:D:967:ARG:NH1	1:D:1116:THR:OG1	2.51	0.43
1:C:1192:LEU:HD23	1:C:1794:PHE:CE2	2.53	0.43
1:C:2318:ARG:HH12	1:A:2245:GLN:N	2.13	0.43
1:C:2370:HIS:HB3	1:C:2398:TYR:O	2.18	0.43
1:A:1415:PHE:HE2	1:A:2532:LEU:HD13	1.83	0.43
1:A:2181:GLN:HB3	1:D:2146:THR:HG22	2.00	0.43
1:A:2376:ILE:HA	1:A:2386:PRO:HA	2.00	0.43
1:D:1018:VAL:O	1:D:1022:THR:HG23	2.18	0.43
1:C:967:ARG:HG2	1:C:980:TYR:CE1	2.54	0.43
3:C:2603:PEE:C24	3:C:2603:PEE:H77	2.48	0.43
1:A:1023:ARG:HB3	1:A:1028:ALA:HB3	2.00	0.43
1:A:2193:GLY:O	1:A:2196:ILE:HG12	2.17	0.43
1:A:2523:GLU:HG2	1:A:2524:GLU:N	2.33	0.43
1:D:1521:ARG:O	1:D:1528:ARG:NH2	2.50	0.43
1:D:2247:SER:O	1:D:2285:GLN:NE2	2.52	0.43
1:D:2257:GLU:O	1:D:2261:GLN:OE1	2.37	0.43
1:D:2471:VAL:HA	1:D:2474:VAL:HG12	2.00	0.43
1:D:2523:GLU:HG2	1:D:2524:GLU:N	2.34	0.43
1:C:2148:SER:HB3	1:C:2151:ASN:ND2	2.33	0.43
1:C:2512:LEU:O	1:C:2516:THR:HG23	2.19	0.43
3:C:2603:PEE:C23	3:C:2603:PEE:H81	2.47	0.43
1:A:2257:GLU:O	1:A:2261:GLN:OE1	2.37	0.43
1:A:2271:GLN:HE22	1:A:2389:GLN:HE22	1.67	0.43
1:D:1337:ILE:HA	1:D:1340:LYS:HZ2	1.83	0.43
1:D:2261:GLN:HA	1:D:2264:ASP:HB2	2.01	0.43
1:C:2093:SER:O	1:C:2097:ILE:HG13	2.18	0.43
1:C:2123:GLN:O	1:C:2127:LEU:HG	2.19	0.43
1:C:2202:ILE:HG23	1:C:2203:ILE:HG13	2.01	0.43
1:C:2231:LYS:HG3	1:C:2237:PRO:HA	2.01	0.43
1:A:1296:ILE:CD1	4:A:2604:P5S:O18	2.65	0.43
1:A:2161:ASN:O	1:A:2164:ILE:HG22	2.19	0.43
1:A:2182:LYS:HD3	1:A:2185:LYS:H	1.84	0.43
1:D:1350:LYS:HE3	1:D:1350:LYS:HB3	1.91	0.43
1:D:2301:ARG:HH12	1:D:2424:SER:HA	1.83	0.43
1:D:2407:ARG:HB3	1:D:2426:PHE:CD2	2.53	0.43
1:C:1521:ARG:O	1:C:1528:ARG:NH2	2.52	0.42
1:C:2052:VAL:HG13	1:C:2053:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2227:THR:CG2	1:C:2324:GLN:HE22	2.32	0.42
1:C:2357:LEU:CD2	1:C:2405:LEU:HB2	2.48	0.42
1:A:1300:HIS:HD2	4:A:2604:P5S:N	2.16	0.42
1:A:1695:ILE:HD11	1:A:1710:LEU:CG	2.46	0.42
1:A:1980:MET:HB2	1:A:2089:TYR:HD1	1.83	0.42
1:A:2119:LEU:HD12	1:A:2167:CYS:CB	2.48	0.42
1:D:2161:ASN:O	1:D:2164:ILE:HG22	2.19	0.42
1:C:2210:MET:HG3	1:C:2214:ARG:NH2	2.33	0.42
1:C:2220:VAL:O	1:C:2329:LYS:HD2	2.19	0.42
1:A:2342:LEU:HD22	1:A:2371:LEU:HG	2.00	0.42
1:D:1192:LEU:HB3	1:D:1794:PHE:CE2	2.54	0.42
1:C:1056:PRO:HA	1:C:1085:PHE:HB3	2.01	0.42
1:C:2375:TYR:HD1	1:C:2447:VAL:HB	1.84	0.42
1:D:2206:PRO:O	1:D:2210:MET:HB2	2.19	0.42
1:D:2468:GLY:O	1:D:2471:VAL:N	2.53	0.42
1:C:2025:LEU:HD12	1:C:2026:VAL:N	2.34	0.42
1:C:2188:LYS:HE2	1:A:2141:VAL:O	2.19	0.42
1:C:2388:LYS:NZ	1:C:2392:PRO:O	2.53	0.42
1:A:2247:SER:O	1:A:2285:GLN:NE2	2.51	0.42
1:A:2325:ARG:HB2	1:A:2334:GLU:HB3	2.01	0.42
4:A:2604:P5S:H51A	4:A:2604:P5S:H30	2.01	0.42
1:D:2357:LEU:CD2	1:D:2405:LEU:HB2	2.49	0.42
1:D:2388:LYS:NZ	1:D:2392:PRO:O	2.53	0.42
1:D:2407:ARG:HB3	1:D:2426:PHE:CB	2.49	0.42
3:D:2603:PEE:H38	3:D:2603:PEE:H43	1.83	0.42
1:C:1300:HIS:HD2	4:C:2604:P5S:N	2.18	0.42
1:C:1354:ALA:O	1:C:1357:GLU:HG3	2.19	0.42
1:C:2326:ASP:OD2	1:C:2329:LYS:NZ	2.42	0.42
1:A:967:ARG:HG2	1:A:980:TYR:CE1	2.53	0.42
1:A:2404:GLN:OE1	1:A:2406:ARG:NH2	2.53	0.42
1:D:2408:GLU:O	1:D:2426:PHE:HA	2.18	0.42
1:C:1157:VAL:HG12	4:C:2604:P5S:H23	1.96	0.42
1:C:1296:ILE:CD1	4:C:2604:P5S:O18	2.67	0.42
1:C:2169:ARG:O	1:C:2173:LYS:HG3	2.20	0.42
1:C:2408:GLU:O	1:C:2426:PHE:HA	2.18	0.42
1:A:1981:PHE:HE2	3:A:2603:PEE:H20	1.82	0.42
1:C:802:ARG:HH21	1:C:943:ARG:HH21	1.67	0.42
1:A:1537:GLU:O	1:A:1540:LEU:HG	2.20	0.42
1:A:2169:ARG:O	1:A:2173:LYS:HG3	2.20	0.42
3:A:2603:PEE:C24	3:A:2603:PEE:H77	2.48	0.42
1:D:2030:THR:HA	1:D:2033:ILE:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:791:SER:O	1:C:795:THR:HG23	2.20	0.42
1:C:2145:THR:HG1	1:C:2152:TRP:HZ3	1.68	0.42
1:A:840:LEU:HD23	1:A:840:LEU:HA	1.90	0.42
1:A:1148:SER:OG	1:A:1151:ASP:OD2	2.20	0.42
1:A:1698:ASN:O	1:A:1703:ALA:HB3	2.20	0.42
1:A:2031:MET:HA	1:A:2034:ASP:OD2	2.20	0.42
1:A:2109:PHE:CB	3:A:2603:PEE:H11	2.48	0.42
1:A:2388:LYS:NZ	1:A:2392:PRO:O	2.52	0.42
1:A:2502:ARG:HH22	1:A:2546:ARG:CZ	2.33	0.42
1:D:967:ARG:HG2	1:D:980:TYR:CE1	2.55	0.42
1:D:2438:LYS:HE2	1:D:2438:LYS:HB3	1.89	0.42
1:C:1169:VAL:HG22	1:C:1286:CYS:SG	2.60	0.42
1:C:1184:TYR:HE2	1:C:1283:ASP:OD1	2.03	0.42
1:C:1196:THR:O	1:C:1200:GLN:HG2	2.20	0.42
1:C:2145:THR:HG21	1:C:2152:TRP:CZ3	2.55	0.42
1:C:2287:GLU:HB3	1:C:2290:SER:HB3	2.02	0.42
1:A:1041:THR:HA	1:A:1101:LEU:HD11	2.02	0.42
1:A:1251:LEU:HD12	1:A:1251:LEU:H	1.84	0.42
1:A:2231:LYS:HG3	1:A:2237:PRO:HA	2.02	0.42
1:A:2318:ARG:CZ	1:D:2245:GLN:HG2	2.50	0.42
1:D:1041:THR:HA	1:D:1101:LEU:HD11	2.02	0.42
1:D:2231:LYS:HG3	1:D:2237:PRO:HA	2.02	0.42
1:D:2289:SER:HA	1:D:2431:VAL:HG13	2.01	0.42
1:D:2404:GLN:N	1:D:2431:VAL:O	2.52	0.42
1:D:2468:GLY:O	1:D:2472:GLU:OE1	2.37	0.42
3:D:2603:PEE:H82	3:D:2603:PEE:H75	1.66	0.42
1:C:1301:TYR:HA	1:C:1304:HIS:CD2	2.55	0.42
1:C:1989:ILE:HD13	3:C:2603:PEE:H37	1.92	0.42
1:C:2036:ALA:HA	1:C:2142:TRP:CD1	2.55	0.42
1:C:2183:LYS:O	1:C:2184:LYS:C	2.58	0.42
1:C:2261:GLN:HA	1:C:2264:ASP:HB2	2.01	0.42
1:C:2447:VAL:O	1:C:2448:ILE:HD13	2.20	0.42
1:A:1183:GLY:HA2	1:A:1186:LEU:HG	2.02	0.42
1:A:1196:THR:O	1:A:1200:GLN:HG2	2.20	0.42
1:A:1353:ARG:NH2	1:A:2518:GLU:OE2	2.53	0.42
1:A:2082:TRP:O	1:A:2086:LYS:HG2	2.20	0.42
1:D:2169:ARG:O	1:D:2173:LYS:HG3	2.20	0.42
1:D:2361:ARG:NH1	1:D:2364:GLN:HG2	2.35	0.42
4:D:2604:P5S:H51A	4:D:2604:P5S:H30	2.01	0.42
1:C:1153:LEU:HD12	4:C:2604:P5S:C48	2.50	0.41
1:C:1300:HIS:CD2	4:C:2604:P5S:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2209:PHE:HD1	1:C:2212:LEU:HD21	1.84	0.41
1:C:2342:LEU:HD22	1:C:2371:LEU:HG	2.01	0.41
1:A:791:SER:O	1:A:795:THR:HG23	2.20	0.41
1:A:1157:VAL:HG11	4:A:2604:P5S:H23	2.01	0.41
1:A:1973:ALA:O	1:A:2102:PRO:HB3	2.20	0.41
1:A:2322:ASN:OD1	1:A:2324:GLN:NE2	2.53	0.41
1:D:2256:TYR:OH	1:D:2273:ILE:O	2.31	0.41
1:C:2023:MET:HA	1:C:2026:VAL:HG22	2.02	0.41
1:C:2361:ARG:NH1	1:C:2364:GLN:HG2	2.34	0.41
1:A:1552:ARG:O	1:A:1555:VAL:HG22	2.20	0.41
1:A:1731:MET:HA	1:A:1734:ILE:HG22	2.03	0.41
1:A:1739:VAL:O	1:A:1743:THR:HG23	2.20	0.41
1:A:2318:ARG:HD2	1:A:2318:ARG:HA	1.85	0.41
1:D:2220:VAL:O	1:D:2329:LYS:HD2	2.21	0.41
1:C:1164:LEU:O	1:C:1168:VAL:HG23	2.21	0.41
1:C:1981:PHE:CD1	3:C:2603:PEE:H8	2.55	0.41
1:C:2373:PRO:HB3	1:C:2398:TYR:CD1	2.54	0.41
4:C:2604:P5S:H51A	4:C:2604:P5S:H30	2.01	0.41
1:A:1192:LEU:HB3	1:A:1794:PHE:CE2	2.54	0.41
1:A:2357:LEU:HD23	1:A:2405:LEU:HD22	2.01	0.41
1:D:791:SER:O	1:D:795:THR:HG23	2.21	0.41
1:D:990:GLY:HA3	1:D:1107:GLN:OE1	2.20	0.41
1:D:1056:PRO:HA	1:D:1085:PHE:HB3	2.01	0.41
1:D:2161:ASN:O	1:D:2165:ILE:HG12	2.21	0.41
1:D:2210:MET:HG3	1:D:2214:ARG:CZ	2.50	0.41
1:C:996:LEU:HD22	1:C:1287:PHE:HE1	1.84	0.41
1:C:1337:ILE:HA	1:C:1340:LYS:HZ2	1.84	0.41
1:C:1727:LYS:O	1:C:1731:MET:HG2	2.20	0.41
1:C:1988:ILE:HA	1:C:1991:ILE:HG22	2.02	0.41
1:A:802:ARG:HH21	1:A:943:ARG:HH21	1.67	0.41
1:A:1280:ILE:HG13	1:A:1283:ASP:HB3	2.01	0.41
1:A:2301:ARG:HH12	1:A:2424:SER:HA	1.85	0.41
1:A:2319:PHE:CE2	1:A:2321:TRP:NE1	2.78	0.41
1:C:1023:ARG:HB3	1:C:1028:ALA:HB3	2.01	0.41
1:C:1024:ARG:HH12	1:C:1211:ASP:CG	2.24	0.41
1:C:2530:ILE:HG13	1:D:2496:GLU:OE2	2.21	0.41
1:A:1243:CYS:O	1:A:1246:ILE:HG22	2.19	0.41
1:A:2305:LYS:HZ1	1:A:2359:GLU:HG3	1.84	0.41
1:D:1552:ARG:O	1:D:1555:VAL:HG22	2.20	0.41
1:D:2207:LEU:O	1:D:2210:MET:HB3	2.21	0.41
1:D:2357:LEU:HD23	1:D:2405:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1216:TYR:HA	1:C:1219:THR:HG22	2.02	0.41
1:A:2407:ARG:HB3	1:A:2426:PHE:CB	2.49	0.41
1:D:1746:LEU:HD23	1:D:1746:LEU:HA	1.90	0.41
1:D:2318:ARG:HA	1:D:2318:ARG:HD2	1.83	0.41
1:C:1977:TYR:OH	1:C:2035:ARG:HD2	2.21	0.41
1:C:2247:SER:O	1:C:2285:GLN:NE2	2.54	0.41
1:A:2251:PHE:CE2	1:A:2281:ILE:HG22	2.55	0.41
1:A:2325:ARG:NH1	1:A:2336:THR:OG1	2.49	0.41
1:D:1196:THR:O	1:D:1200:GLN:HG2	2.20	0.41
1:D:1973:ALA:O	1:D:2102:PRO:HB3	2.20	0.41
1:D:1981:PHE:HE2	3:D:2603:PEE:H20	1.83	0.41
1:D:1985:ILE:HG21	3:D:2603:PEE:H26	2.01	0.41
1:C:1695:ILE:HA	1:C:1789:GLN:NE2	2.36	0.41
1:C:2380:ASN:ND2	1:C:2453:VAL:HG12	2.36	0.41
1:A:2209:PHE:HD1	1:A:2212:LEU:HD21	1.86	0.41
1:C:967:ARG:H	1:C:967:ARG:HG3	1.64	0.41
1:C:981:PHE:HZ	4:C:2604:P5S:C41	2.09	0.41
1:C:991:LEU:HD12	1:C:992:GLU:N	2.36	0.41
1:C:1693:PHE:CE1	1:C:1697:LEU:HD21	2.56	0.41
1:C:1695:ILE:HD13	1:C:1714:VAL:HG21	2.03	0.41
1:C:1973:ALA:O	1:C:2102:PRO:HB3	2.20	0.41
1:C:2140:TRP:HD1	1:C:2152:TRP:CD2	2.39	0.41
1:C:2253:PRO:O	1:C:2256:TYR:HB3	2.21	0.41
1:C:2258:GLU:HA	1:C:2261:GLN:OE1	2.20	0.41
1:C:2269:ALA:O	1:C:2273:ILE:HG13	2.20	0.41
1:C:2357:LEU:HD23	1:C:2405:LEU:HD22	2.02	0.41
1:C:2404:GLN:N	1:C:2431:VAL:O	2.54	0.41
1:A:1160:TYR:CE1	2:A:2602:PLX:O2	2.68	0.41
1:A:1301:TYR:HA	1:A:1304:HIS:CD2	2.55	0.41
1:A:1690:LEU:O	1:A:1694:ILE:HG12	2.21	0.41
1:A:2161:ASN:O	1:A:2165:ILE:HG12	2.20	0.41
1:A:2317:LEU:HD12	1:A:2319:PHE:HB2	2.03	0.41
1:A:2536:PRO:O	1:A:2539:MET:HG2	2.21	0.41
4:A:2604:P5S:H2	4:A:2604:P5S:H39	1.48	0.41
1:D:1226:MET:SD	1:D:1227:LEU:N	2.94	0.41
1:D:1246:ILE:HA	1:D:1251:LEU:HD12	2.01	0.41
1:D:1292:LEU:O	1:D:1296:ILE:HG12	2.21	0.41
1:D:1300:HIS:HD2	4:D:2604:P5S:N	2.19	0.41
1:D:1300:HIS:CD2	4:D:2604:P5S:N	2.89	0.41
1:D:1354:ALA:O	1:D:1357:GLU:HG3	2.20	0.41
1:D:2071:ARG:O	1:D:2076:ASN:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2227:THR:CG2	1:D:2324:GLN:HE22	2.32	0.41
1:D:2251:PHE:CE2	1:D:2281:ILE:HG22	2.56	0.41
2:D:2601:PLX:O1	2:D:2601:PLX:H1A2	2.21	0.41
3:D:2603:PEE:H82	3:D:2603:PEE:C40	2.51	0.41
1:C:1552:ARG:O	1:C:1555:VAL:HG22	2.20	0.41
1:C:2141:VAL:O	1:D:2188:LYS:NZ	2.42	0.41
1:C:2510:ILE:HG12	1:C:2525:LEU:HB3	2.03	0.41
1:A:990:GLY:HA3	1:A:1107:GLN:OE1	2.21	0.41
1:A:1299:SER:HB2	1:A:1301:TYR:HD1	1.85	0.41
1:A:2226:VAL:HG23	1:A:2323:PHE:HD1	1.86	0.41
1:A:2339:LYS:HE3	1:A:2339:LYS:HB3	1.95	0.41
1:D:2230:LEU:HD23	1:D:2238:LEU:HB2	2.03	0.41
1:D:2308:LEU:HD22	1:D:2351:ARG:HG3	2.03	0.41
1:D:2322:ASN:HA	1:D:2337:ASN:HB3	2.03	0.41
1:D:2463:GLY:H	1:D:2467:VAL:HG21	1.86	0.41
1:D:2510:ILE:HG12	1:D:2525:LEU:HB3	2.03	0.41
1:C:840:LEU:HD23	1:C:840:LEU:HA	1.90	0.40
1:A:1164:LEU:O	1:A:1168:VAL:HG23	2.21	0.40
1:A:1292:LEU:O	1:A:1296:ILE:HG12	2.21	0.40
1:A:2257:GLU:O	1:A:2260:SER:HB2	2.20	0.40
1:A:2269:ALA:O	1:A:2273:ILE:HG13	2.21	0.40
1:A:2538:THR:O	1:A:2542:TRP:N	2.54	0.40
1:D:2277:SER:HB2	1:D:2278:PRO:HD2	2.03	0.40
1:C:2071:ARG:O	1:C:2076:ASN:N	2.33	0.40
1:C:2161:ASN:O	1:C:2165:ILE:HG12	2.21	0.40
1:C:2253:PRO:O	1:C:2257:GLU:OE1	2.38	0.40
1:A:1030:ALA:HB2	1:A:1111:PHE:HE2	1.86	0.40
1:A:1168:VAL:HG12	1:A:1286:CYS:SG	2.61	0.40
1:A:1337:ILE:O	1:A:1340:LYS:HG2	2.21	0.40
1:A:2077:ALA:O	1:A:2080:GLN:HG2	2.22	0.40
1:D:2020:PHE:HA	1:D:2023:MET:HG2	2.04	0.40
1:D:2321:TRP:HZ3	1:D:2376:ILE:HD12	1.86	0.40
1:C:1211:ASP:O	1:C:1215:LEU:HG	2.21	0.40
1:C:1299:SER:HB2	1:C:1301:TYR:HD1	1.86	0.40
1:A:2527:ALA:HA	1:A:2530:ILE:HG22	2.03	0.40
1:D:2061:MET:N	1:D:2061:MET:SD	2.94	0.40
1:D:2380:ASN:ND2	1:D:2453:VAL:HG12	2.36	0.40
1:D:2526:TYR:O	1:D:2530:ILE:HG12	2.21	0.40
1:C:2135:ARG:HB2	3:C:2603:PEE:H48	2.03	0.40
1:C:2321:TRP:HZ3	1:C:2376:ILE:HD12	1.86	0.40
1:C:2321:TRP:O	1:C:2337:ASN:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2601:PLX:O1	2:C:2601:PLX:H1A2	2.21	0.40
3:C:2603:PEE:H82	3:C:2603:PEE:C40	2.51	0.40
1:A:1084:ASP:OD1	1:A:1087:ARG:N	2.41	0.40
1:A:1354:ALA:O	1:A:1357:GLU:HG3	2.21	0.40
1:A:2318:ARG:HH12	1:D:2245:GLN:N	2.19	0.40
1:A:800:PHE:O	1:A:804:LEU:HG	2.22	0.40
1:A:1734:ILE:HD13	1:A:1793:LEU:HB2	2.03	0.40
1:A:2211:SER:HA	1:A:2214:ARG:HH21	1.87	0.40
1:D:1024:ARG:HH12	1:D:1211:ASP:CG	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1312/2547 (52%)	1241 (95%)	69 (5%)	2 (0%)	44	76
1	C	1312/2547 (52%)	1245 (95%)	66 (5%)	1 (0%)	48	81
1	D	1312/2547 (52%)	1241 (95%)	69 (5%)	2 (0%)	44	76
All	All	3936/7641 (52%)	3727 (95%)	204 (5%)	5 (0%)	50	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2182	LYS
1	A	2182	LYS
1	D	2182	LYS
1	A	2183	LYS
1	D	2183	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	869/2246 (39%)	866 (100%)	3 (0%)	91	92
1	C	870/2246 (39%)	869 (100%)	1 (0%)	92	95
1	D	872/2246 (39%)	871 (100%)	1 (0%)	92	95
All	All	2611/6738 (39%)	2606 (100%)	5 (0%)	91	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1152	MET
1	A	1152	MET
1	A	2303	GLN
1	A	2391	GLN
1	D	1152	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1300	HIS
1	C	1789	GLN
1	C	2222	GLN
1	C	2271	GLN
1	C	2285	GLN
1	C	2380	ASN
1	C	2389	GLN
1	A	1300	HIS
1	A	1789	GLN
1	A	2271	GLN
1	A	2285	GLN
1	A	2380	ASN
1	A	2389	GLN
1	D	1200	GLN
1	D	1300	HIS
1	D	1789	GLN

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Mol	Chain	Res	Type
1	D	2271	GLN
1	D	2285	GLN
1	D	2380	ASN
1	D	2389	GLN
1	D	2391	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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	P5S	A	2604	-	52,53,53	0.37	0	56,60,60	0.45	0
4	P5S	D	2604	-	52,53,53	0.37	0	56,60,60	0.45	0
3	PEE	C	2603	-	50,50,50	1.17	6 (12%)	53,55,55	1.25	6 (11%)
3	PEE	A	2603	-	50,50,50	1.17	7 (14%)	53,55,55	1.25	6 (11%)
3	PEE	D	2603	-	50,50,50	1.17	6 (12%)	53,55,55	1.25	6 (11%)
4	P5S	C	2604	-	52,53,53	0.37	0	56,60,60	0.45	0
2	PLX	A	2602	-	51,51,51	0.65	0	55,59,59	0.71	1 (1%)
2	PLX	A	2601	-	51,51,51	0.62	0	55,59,59	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLX	D	2602	-	51,51,51	0.65	0	55,59,59	0.71	1 (1%)
2	PLX	C	2602	-	51,51,51	0.65	0	55,59,59	0.71	1 (1%)
2	PLX	D	2601	-	51,51,51	0.62	0	55,59,59	0.68	0
2	PLX	C	2601	-	51,51,51	0.62	0	55,59,59	0.68	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	P5S	A	2604	-	-	16/59/59/59	-
4	P5S	D	2604	-	-	16/59/59/59	-
3	PEE	C	2603	-	-	29/54/54/54	-
3	PEE	A	2603	-	-	29/54/54/54	-
3	PEE	D	2603	-	-	29/54/54/54	-
4	P5S	C	2604	-	-	16/59/59/59	-
2	PLX	A	2602	-	-	10/55/55/55	-
2	PLX	A	2601	-	-	5/55/55/55	-
2	PLX	D	2602	-	-	10/55/55/55	-
2	PLX	C	2602	-	-	10/55/55/55	-
2	PLX	D	2601	-	-	5/55/55/55	-
2	PLX	C	2601	-	-	5/55/55/55	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2603	PEE	C39-C38	3.68	1.53	1.31
3	A	2603	PEE	C39-C38	3.68	1.53	1.31
3	C	2603	PEE	C39-C38	3.67	1.53	1.31
3	A	2603	PEE	C18-C19	3.47	1.51	1.31
3	C	2603	PEE	C18-C19	3.47	1.51	1.31
3	D	2603	PEE	C18-C19	3.47	1.51	1.31
3	D	2603	PEE	P-O4P	3.05	1.71	1.59
3	C	2603	PEE	P-O4P	3.04	1.71	1.59
3	A	2603	PEE	P-O4P	3.04	1.71	1.59
3	A	2603	PEE	O3-C3	-2.68	1.39	1.45
3	C	2603	PEE	O3-C3	-2.67	1.39	1.45
3	D	2603	PEE	O3-C3	-2.66	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2603	PEE	O4P-C4	-2.36	1.35	1.44
3	C	2603	PEE	O4P-C4	-2.36	1.35	1.44
3	C	2603	PEE	O3-C30	2.35	1.40	1.33
3	D	2603	PEE	O4P-C4	-2.35	1.35	1.44
3	D	2603	PEE	O3-C30	2.35	1.40	1.33
3	A	2603	PEE	O3-C30	2.32	1.40	1.33
3	A	2603	PEE	O2-C2	-2.01	1.41	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2603	PEE	O2P-P-O1P	3.30	128.56	112.24
3	D	2603	PEE	O2P-P-O1P	3.30	128.56	112.24
3	A	2603	PEE	O2P-P-O1P	3.30	128.55	112.24
3	C	2603	PEE	O4P-P-O1P	-2.38	99.75	109.07
3	D	2603	PEE	O4P-P-O1P	-2.38	99.76	109.07
3	A	2603	PEE	O4P-P-O1P	-2.38	99.76	109.07
3	C	2603	PEE	C2-O2-C10	2.28	123.41	117.79
3	A	2603	PEE	C2-O2-C10	2.28	123.41	117.79
3	D	2603	PEE	C2-O2-C10	2.28	123.40	117.79
3	D	2603	PEE	C3-O3-C30	-2.22	108.89	117.12
3	C	2603	PEE	C3-O3-C30	-2.22	108.90	117.12
3	A	2603	PEE	C3-O3-C30	-2.22	108.90	117.12
3	A	2603	PEE	C12-C11-C10	-2.19	105.67	113.62
3	C	2603	PEE	C12-C11-C10	-2.18	105.68	113.62
3	D	2603	PEE	C12-C11-C10	-2.18	105.68	113.62
2	D	2602	PLX	C5-C4-C3	-2.11	106.80	111.79
2	C	2602	PLX	C5-C4-C3	-2.10	106.82	111.79
2	A	2602	PLX	C5-C4-C3	-2.10	106.82	111.79
3	D	2603	PEE	O2-C2-C1	2.04	115.78	108.40
3	C	2603	PEE	O2-C2-C1	2.04	115.77	108.40
3	A	2603	PEE	O2-C2-C1	2.03	115.77	108.40

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2602	PLX	O7-C6-O6-C4
2	C	2602	PLX	C2-O1-P1-O4
2	C	2602	PLX	C2-O1-P1-O2
2	A	2602	PLX	O7-C6-O6-C4
2	A	2602	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
2	A	2602	PLX	C2-O1-P1-O2
2	D	2602	PLX	O7-C6-O6-C4
2	D	2602	PLX	C2-O1-P1-O4
2	D	2602	PLX	C2-O1-P1-O2
3	C	2603	PEE	C2-C1-O3P-P
3	C	2603	PEE	C4-O4P-P-O3P
3	C	2603	PEE	C4-O4P-P-O1P
3	A	2603	PEE	C2-C1-O3P-P
3	A	2603	PEE	C4-O4P-P-O3P
3	A	2603	PEE	C4-O4P-P-O1P
3	D	2603	PEE	C2-C1-O3P-P
3	D	2603	PEE	C4-O4P-P-O3P
3	D	2603	PEE	C4-O4P-P-O1P
4	C	2604	P5S	O-C-CA-CB
4	C	2604	P5S	OXT-C-CA-CB
4	C	2604	P5S	CA-CB-OG-P12
4	C	2604	P5S	CB-OG-P12-O16
4	C	2604	P5S	C3-O16-P12-O15
4	C	2604	P5S	C39-C38-O37-C2
4	C	2604	P5S	O47-C38-O37-C2
4	A	2604	P5S	O-C-CA-CB
4	A	2604	P5S	OXT-C-CA-CB
4	A	2604	P5S	CA-CB-OG-P12
4	A	2604	P5S	CB-OG-P12-O16
4	A	2604	P5S	C3-O16-P12-O15
4	A	2604	P5S	C39-C38-O37-C2
4	A	2604	P5S	O47-C38-O37-C2
4	D	2604	P5S	O-C-CA-CB
4	D	2604	P5S	OXT-C-CA-CB
4	D	2604	P5S	CA-CB-OG-P12
4	D	2604	P5S	CB-OG-P12-O16
4	D	2604	P5S	C3-O16-P12-O15
4	D	2604	P5S	C39-C38-O37-C2
4	D	2604	P5S	O47-C38-O37-C2
3	C	2603	PEE	C41-C42-C43-C44
3	A	2603	PEE	C41-C42-C43-C44
3	D	2603	PEE	C41-C42-C43-C44
3	C	2603	PEE	C1-O3P-P-O4P
3	A	2603	PEE	C1-O3P-P-O4P
3	D	2603	PEE	C1-O3P-P-O4P
4	C	2604	P5S	C3-O16-P12-OG
4	A	2604	P5S	C3-O16-P12-OG

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Mol	Chain	Res	Type	Atoms
4	D	2604	P5S	C3-O16-P12-OG
3	C	2603	PEE	C31-C30-O3-C3
3	A	2603	PEE	C31-C30-O3-C3
3	D	2603	PEE	C31-C30-O3-C3
3	C	2603	PEE	C11-C10-O2-C2
3	A	2603	PEE	C11-C10-O2-C2
3	D	2603	PEE	C11-C10-O2-C2
3	C	2603	PEE	C1-C2-O2-C10
3	A	2603	PEE	C1-C2-O2-C10
3	D	2603	PEE	C1-C2-O2-C10
3	C	2603	PEE	O5-C30-O3-C3
3	A	2603	PEE	O5-C30-O3-C3
3	D	2603	PEE	O5-C30-O3-C3
3	C	2603	PEE	C43-C44-C45-C46
3	A	2603	PEE	C43-C44-C45-C46
3	D	2603	PEE	C43-C44-C45-C46
3	C	2603	PEE	C31-C32-C33-C34
3	A	2603	PEE	C31-C32-C33-C34
3	D	2603	PEE	C31-C32-C33-C34
3	C	2603	PEE	O4-C10-O2-C2
3	A	2603	PEE	O4-C10-O2-C2
3	D	2603	PEE	O4-C10-O2-C2
3	C	2603	PEE	C12-C13-C14-C15
3	D	2603	PEE	C12-C13-C14-C15
3	A	2603	PEE	C12-C13-C14-C15
3	C	2603	PEE	C17-C18-C19-C20
3	A	2603	PEE	C17-C18-C19-C20
3	D	2603	PEE	C17-C18-C19-C20
3	C	2603	PEE	C44-C45-C46-C47
3	A	2603	PEE	C44-C45-C46-C47
3	D	2603	PEE	C44-C45-C46-C47
3	C	2603	PEE	C14-C15-C16-C17
3	A	2603	PEE	C14-C15-C16-C17
3	D	2603	PEE	C14-C15-C16-C17
3	C	2603	PEE	O2-C2-C3-O3
3	A	2603	PEE	O2-C2-C3-O3
3	D	2603	PEE	O2-C2-C3-O3
2	D	2602	PLX	C13-C14-C15-C16
2	C	2602	PLX	C13-C14-C15-C16
2	A	2602	PLX	C13-C14-C15-C16
2	C	2602	PLX	C20-C21-C22-C23
2	A	2602	PLX	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	D	2602	PLX	C20-C21-C22-C23
4	C	2604	P5S	O19-C1-C2-C3
4	A	2604	P5S	O19-C1-C2-C3
4	D	2604	P5S	O19-C1-C2-C3
3	C	2603	PEE	C42-C43-C44-C45
3	A	2603	PEE	C42-C43-C44-C45
3	D	2603	PEE	C42-C43-C44-C45
4	C	2604	P5S	C2-C3-O16-P12
4	A	2604	P5S	C2-C3-O16-P12
4	D	2604	P5S	C2-C3-O16-P12
2	C	2602	PLX	C19-C20-C21-C22
2	A	2602	PLX	C19-C20-C21-C22
2	D	2602	PLX	C19-C20-C21-C22
4	C	2604	P5S	O19-C1-C2-O37
4	A	2604	P5S	O19-C1-C2-O37
4	D	2604	P5S	O19-C1-C2-O37
3	C	2603	PEE	C15-C16-C17-C18
3	A	2603	PEE	C15-C16-C17-C18
3	D	2603	PEE	C15-C16-C17-C18
4	C	2604	P5S	N-CA-CB-OG
4	A	2604	P5S	N-CA-CB-OG
4	D	2604	P5S	N-CA-CB-OG
3	C	2603	PEE	C1-O3P-P-O1P
3	A	2603	PEE	C1-O3P-P-O1P
3	D	2603	PEE	C1-O3P-P-O1P
4	C	2604	P5S	CB-OG-P12-O15
4	A	2604	P5S	CB-OG-P12-O15
4	D	2604	P5S	CB-OG-P12-O15
3	C	2603	PEE	C38-C39-C40-C41
3	A	2603	PEE	C38-C39-C40-C41
3	D	2603	PEE	C38-C39-C40-C41
4	C	2604	P5S	O37-C2-C3-O16
4	A	2604	P5S	O37-C2-C3-O16
4	D	2604	P5S	O37-C2-C3-O16
3	C	2603	PEE	C13-C14-C15-C16
3	A	2603	PEE	C13-C14-C15-C16
3	D	2603	PEE	C13-C14-C15-C16
2	C	2601	PLX	C3-O4-P1-O1
2	C	2601	PLX	C2-O1-P1-O4
2	C	2602	PLX	C3-O4-P1-O1
2	A	2601	PLX	C3-O4-P1-O1
2	A	2601	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
2	A	2602	PLX	C3-O4-P1-O1
2	D	2601	PLX	C3-O4-P1-O1
2	D	2601	PLX	C2-O1-P1-O4
2	D	2602	PLX	C3-O4-P1-O1
3	C	2603	PEE	C1-C2-C3-O3
3	A	2603	PEE	C1-C2-C3-O3
3	D	2603	PEE	C1-C2-C3-O3
3	C	2603	PEE	C40-C41-C42-C43
3	A	2603	PEE	C40-C41-C42-C43
3	D	2603	PEE	C40-C41-C42-C43
3	C	2603	PEE	C33-C34-C35-C36
3	A	2603	PEE	C33-C34-C35-C36
3	D	2603	PEE	C33-C34-C35-C36
2	C	2602	PLX	O8-C24-C25-C26
2	A	2602	PLX	O8-C24-C25-C26
2	D	2602	PLX	O8-C24-C25-C26
4	C	2604	P5S	C1-C2-C3-O16
4	A	2604	P5S	C1-C2-C3-O16
4	D	2604	P5S	C1-C2-C3-O16
2	C	2601	PLX	O7-C6-C7-C8
2	A	2601	PLX	O7-C6-C7-C8
2	D	2601	PLX	O7-C6-C7-C8
4	A	2604	P5S	C29-C30-C31-C32
4	D	2604	P5S	C29-C30-C31-C32
4	C	2604	P5S	C29-C30-C31-C32
2	C	2601	PLX	C3-O4-P1-O2
2	A	2601	PLX	C3-O4-P1-O2
2	D	2601	PLX	C3-O4-P1-O2
2	C	2601	PLX	O4-C3-C4-C5
2	A	2601	PLX	O4-C3-C4-C5
2	D	2601	PLX	O4-C3-C4-C5
3	C	2603	PEE	O4P-C4-C5-N
3	A	2603	PEE	O4P-C4-C5-N
3	D	2603	PEE	O4P-C4-C5-N
2	A	2602	PLX	C9-C10-C11-C12
2	C	2602	PLX	C9-C10-C11-C12
2	D	2602	PLX	C9-C10-C11-C12
3	C	2603	PEE	C16-C17-C18-C19
3	A	2603	PEE	C16-C17-C18-C19
3	D	2603	PEE	C16-C17-C18-C19
3	C	2603	PEE	O4-C10-C11-C12
3	A	2603	PEE	O4-C10-C11-C12

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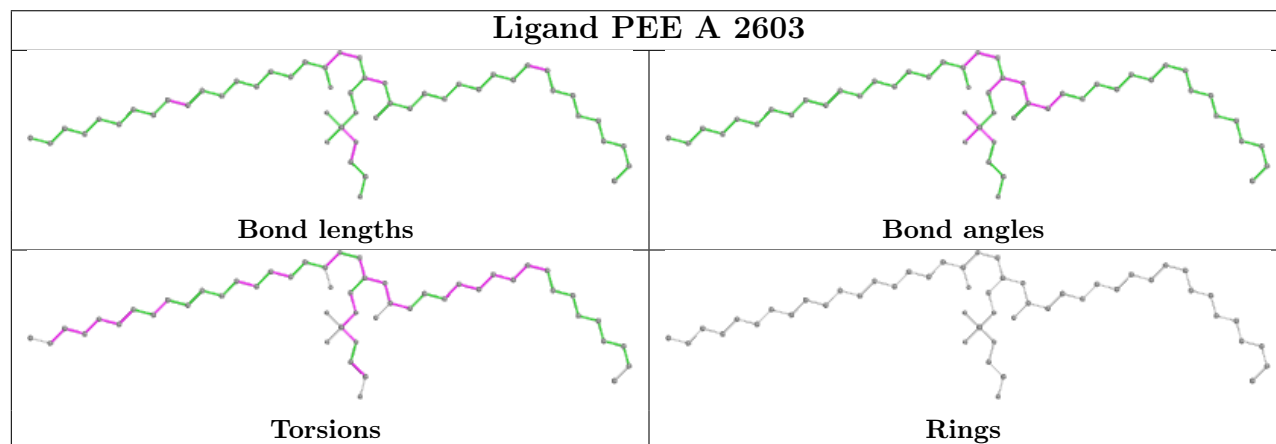
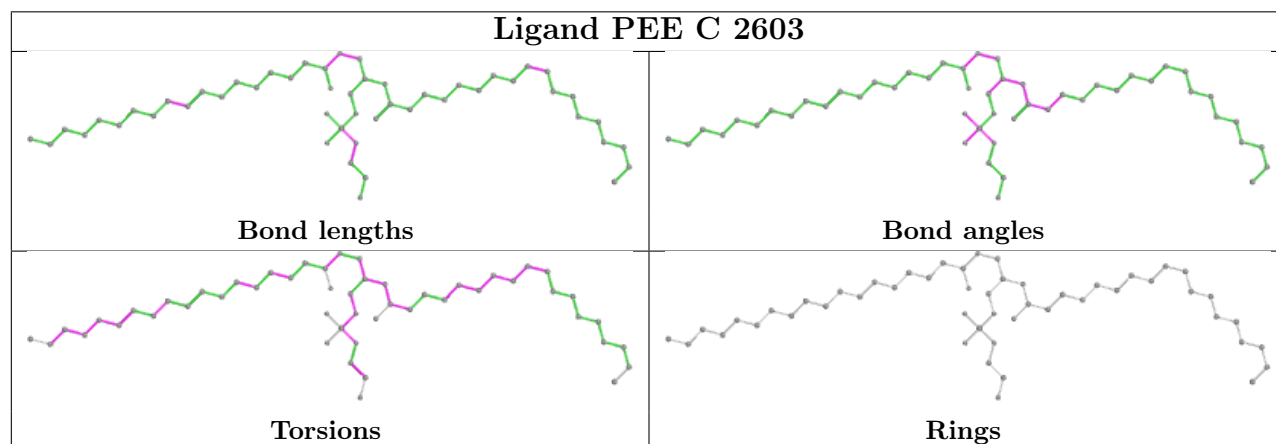
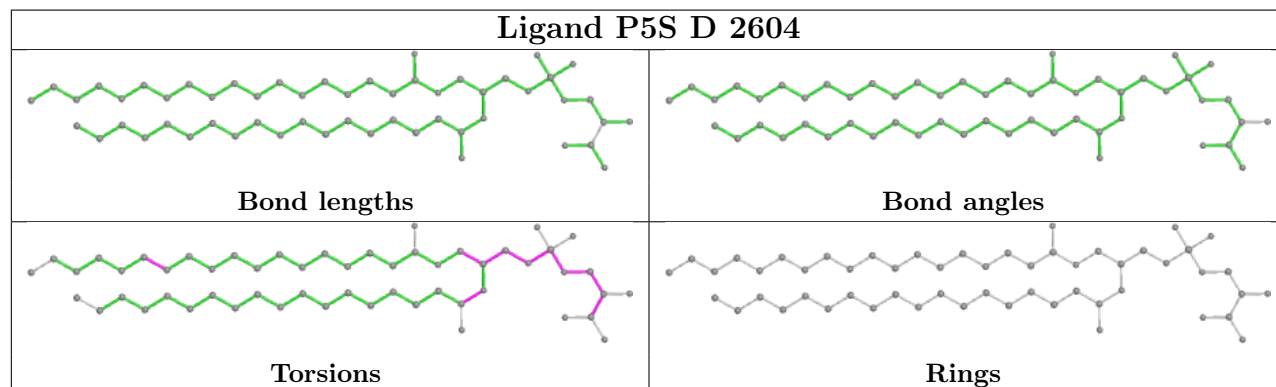
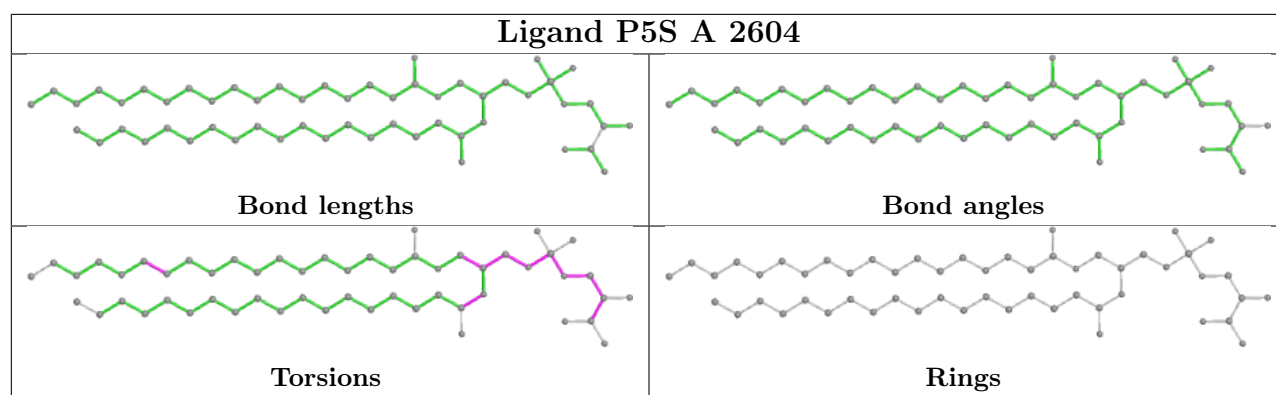
Mol	Chain	Res	Type	Atoms
3	D	2603	PEE	O4-C10-C11-C12
3	C	2603	PEE	O2-C10-C11-C12
3	A	2603	PEE	O2-C10-C11-C12
3	D	2603	PEE	O2-C10-C11-C12
2	C	2602	PLX	C14-C15-C16-C17
2	A	2602	PLX	C14-C15-C16-C17
2	D	2602	PLX	C14-C15-C16-C17

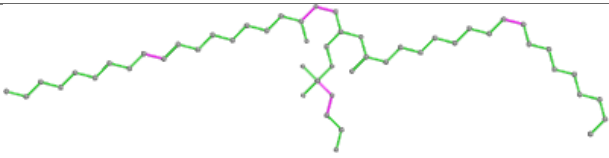
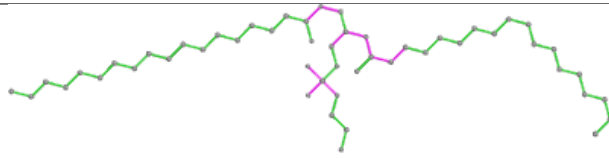
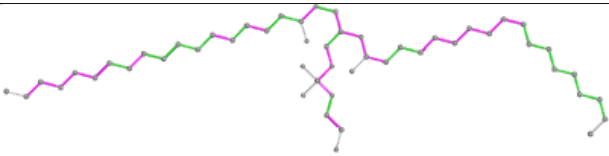
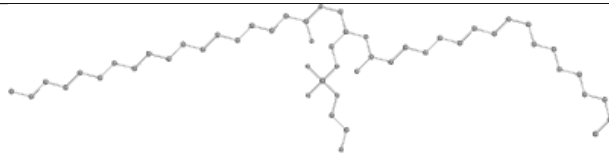
There are no ring outliers.

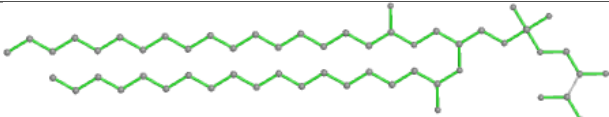
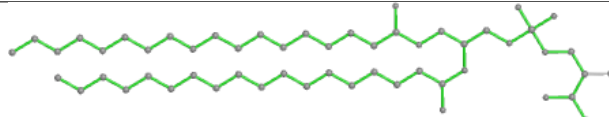
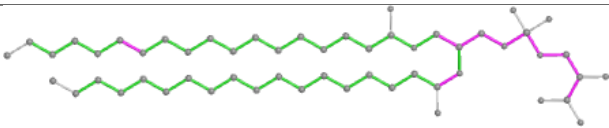
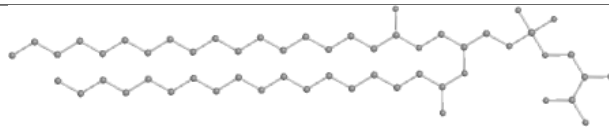
12 monomers are involved in 302 short contacts:

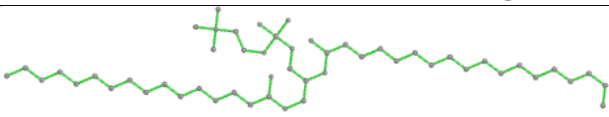
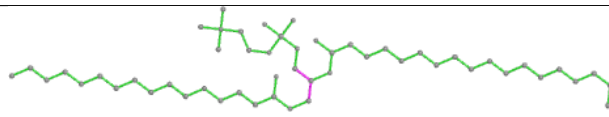
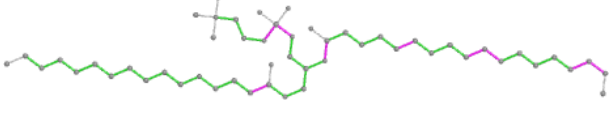
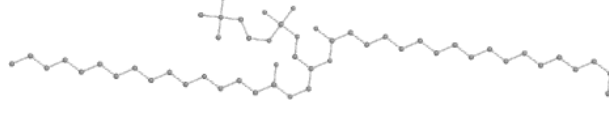
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2604	P5S	24	0
4	D	2604	P5S	17	0
3	C	2603	PEE	70	0
3	A	2603	PEE	60	0
3	D	2603	PEE	64	0
4	C	2604	P5S	25	0
2	A	2602	PLX	13	0
2	A	2601	PLX	1	0
2	D	2602	PLX	12	0
2	C	2602	PLX	12	0
2	D	2601	PLX	2	0
2	C	2601	PLX	2	0

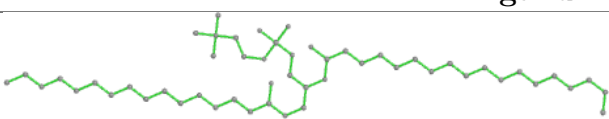
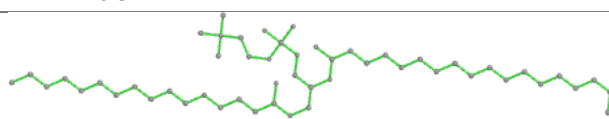
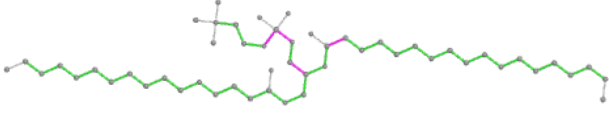
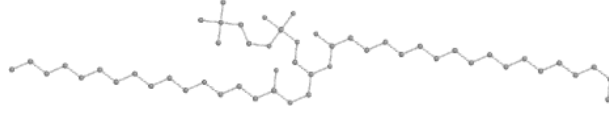
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

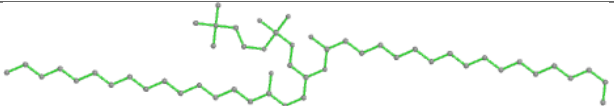
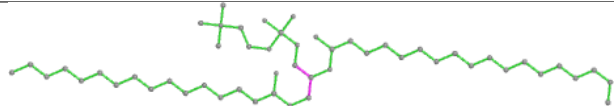
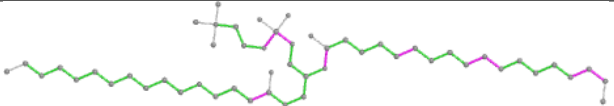
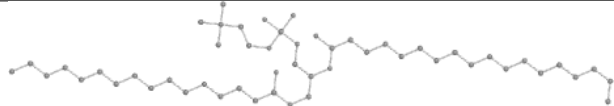


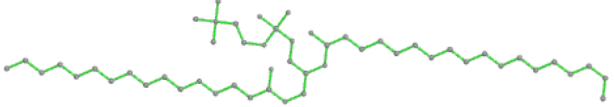
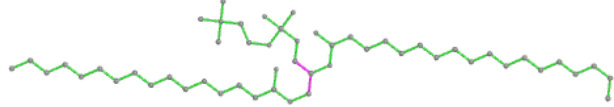
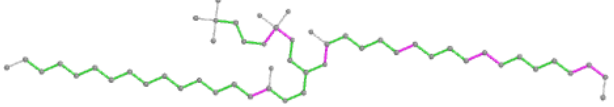
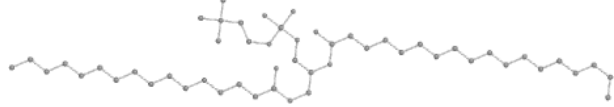
Ligand PEE D 2603	
	
Bond lengths	Bond angles
	
Torsions	Rings

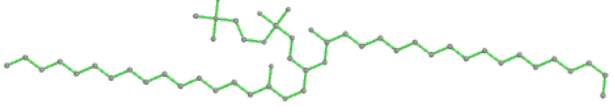
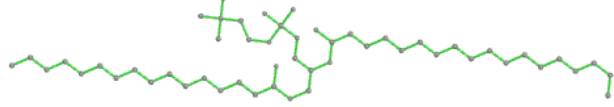
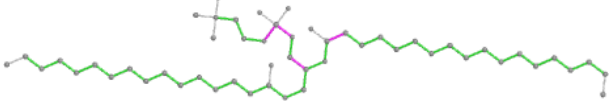
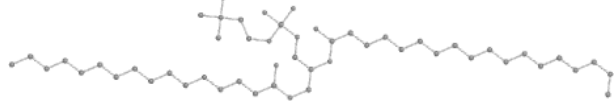
Ligand P5S C 2604	
	
Bond lengths	Bond angles
	
Torsions	Rings

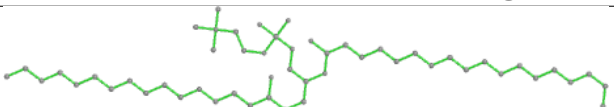
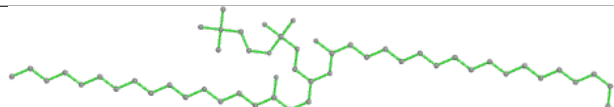
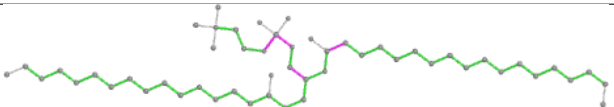
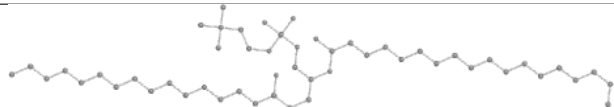
Ligand PLX A 2602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX A 2601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX D 2602	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand PLX C 2602	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand PLX D 2601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand PLX C 2601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

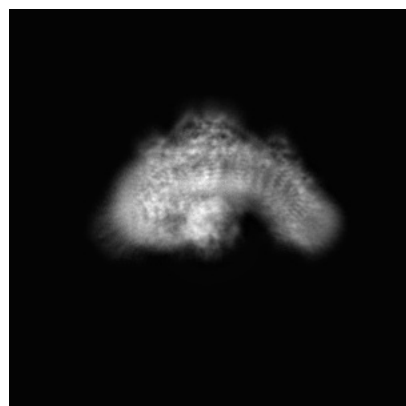
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35799. These allow visual inspection of the internal detail of the map and identification of artifacts.

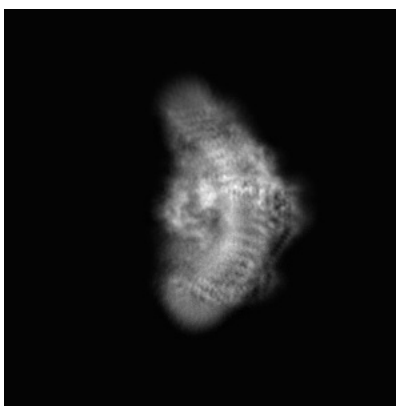
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

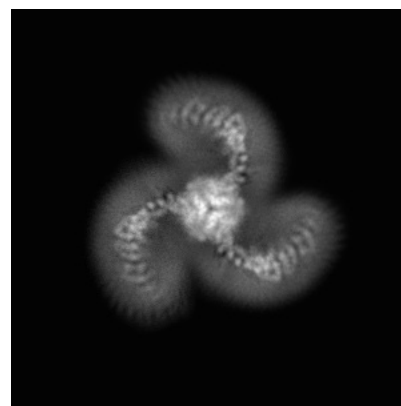
6.1.1 Primary map



X

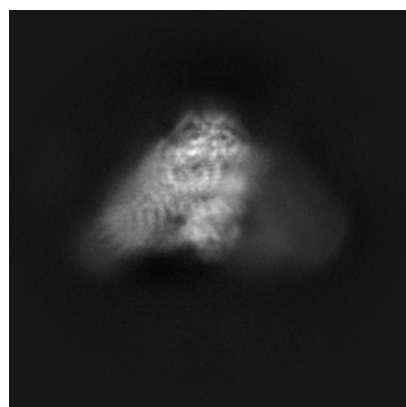


Y

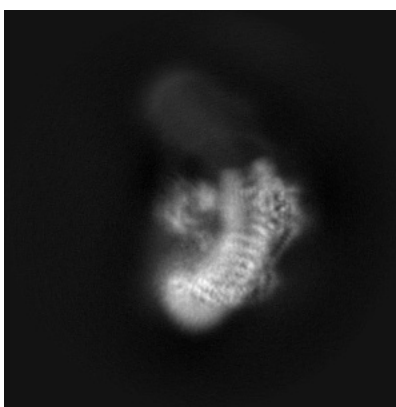


Z

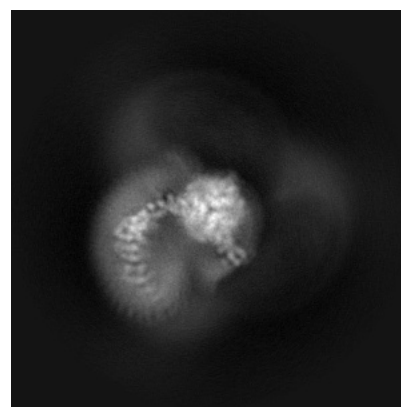
6.1.2 Raw map



X



Y

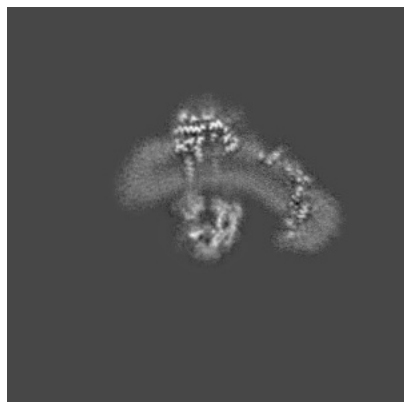


Z

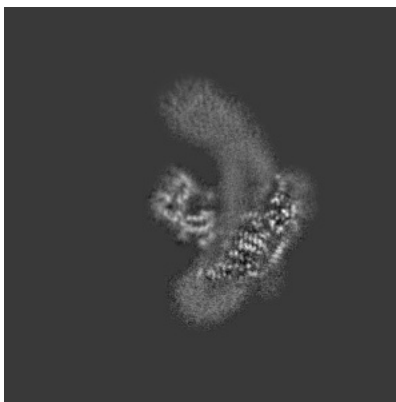
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

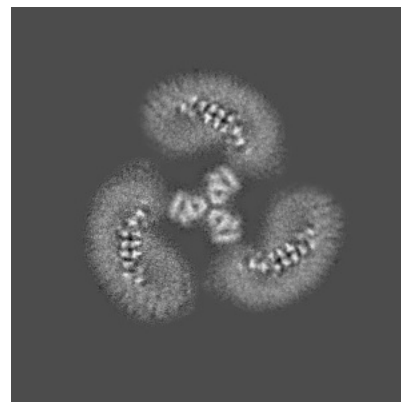
6.2.1 Primary map



X Index: 184

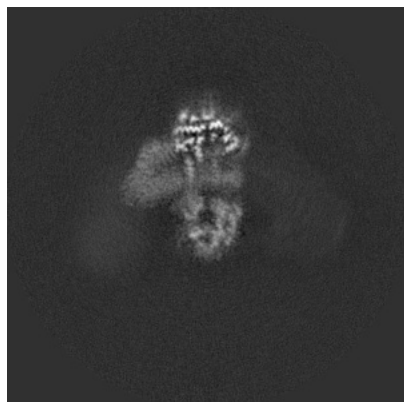


Y Index: 184

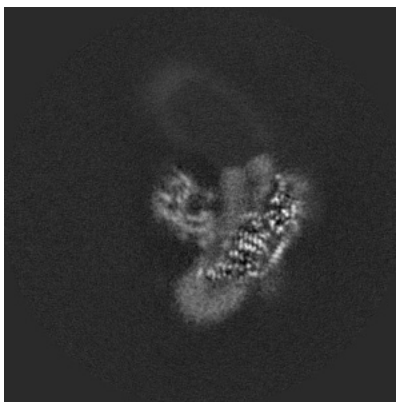


Z Index: 184

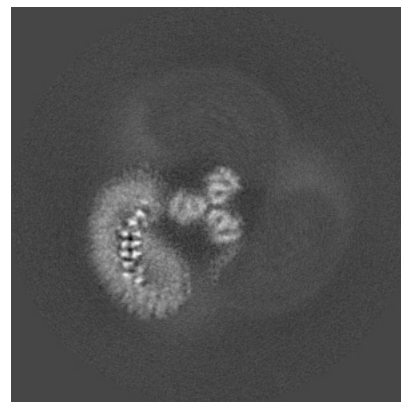
6.2.2 Raw map



X Index: 184



Y Index: 184

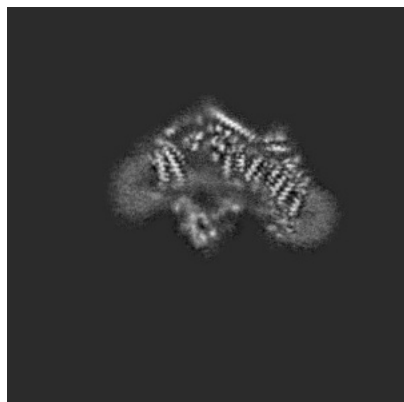


Z Index: 184

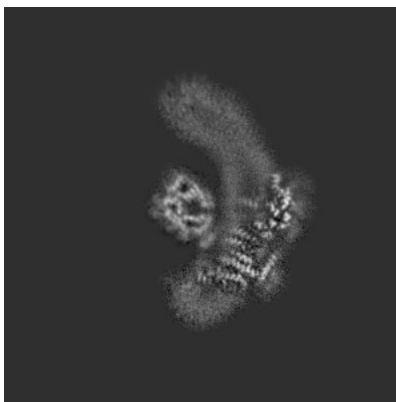
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

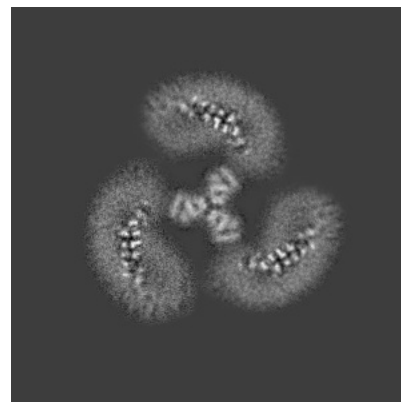
6.3.1 Primary map



X Index: 202

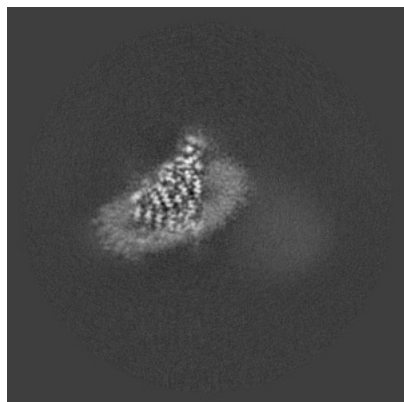


Y Index: 179

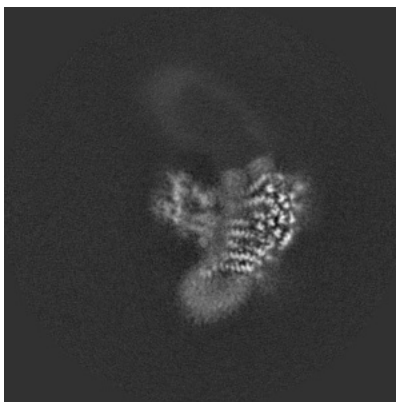


Z Index: 185

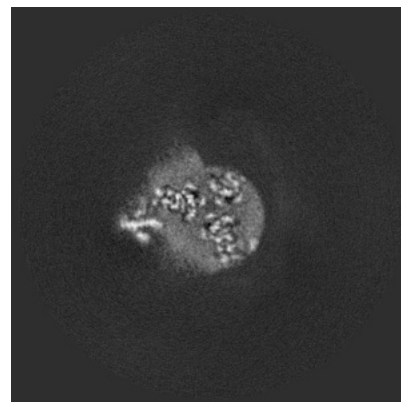
6.3.2 Raw map



X Index: 111



Y Index: 189

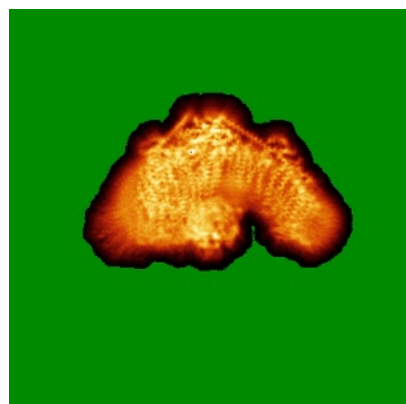


Z Index: 236

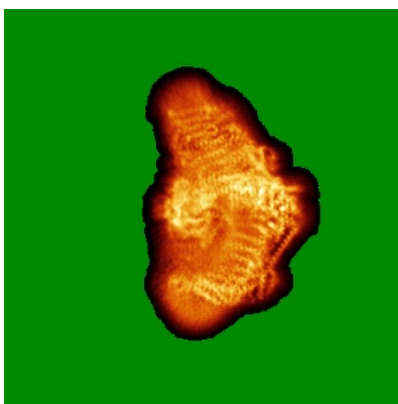
The images above show the largest variance slices of the map in three orthogonal directions.

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

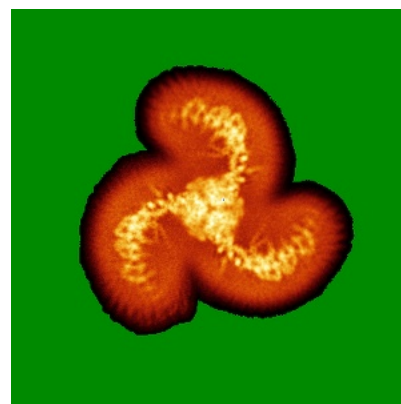
6.4.1 Primary map



X

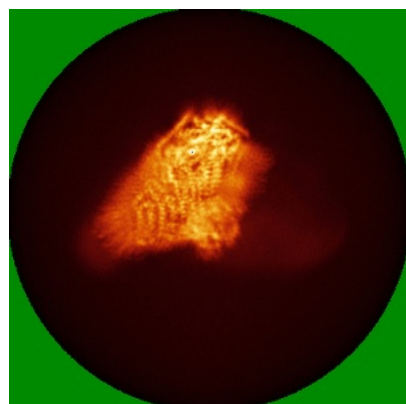


Y

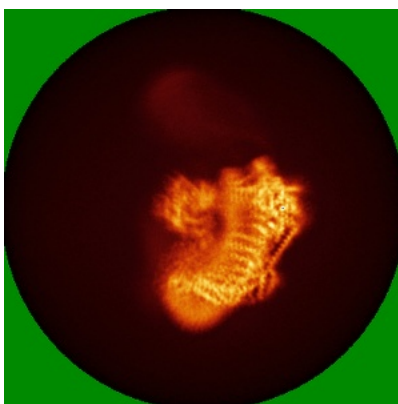


Z

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.

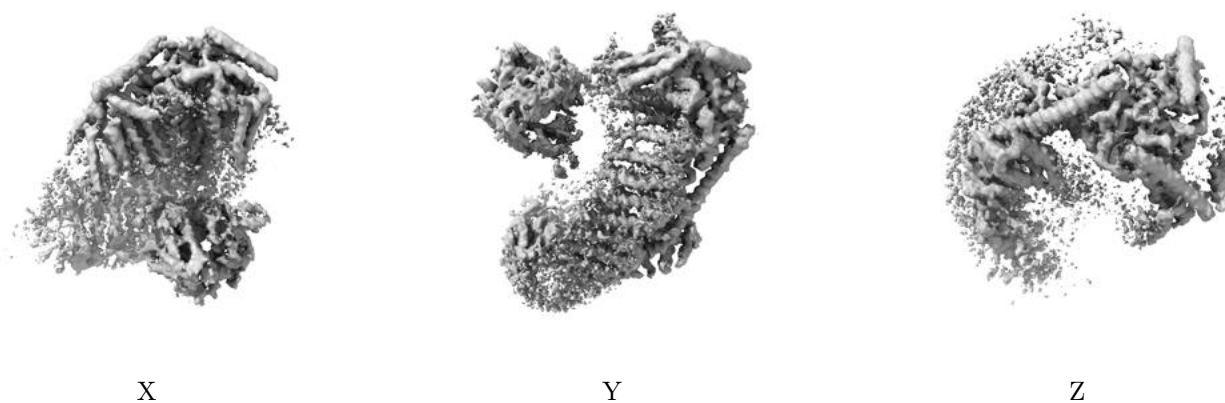
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 8.23. 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



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

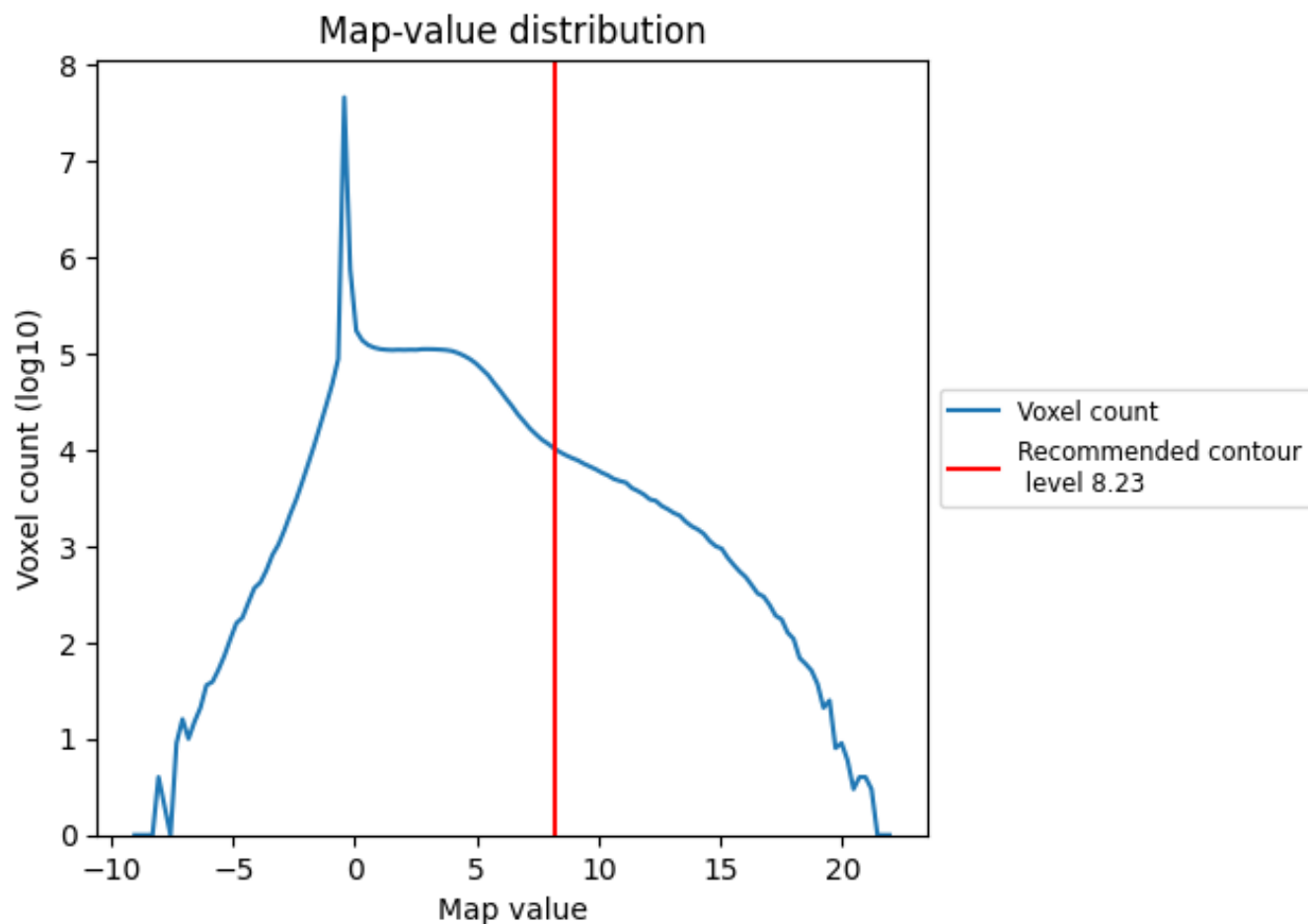
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

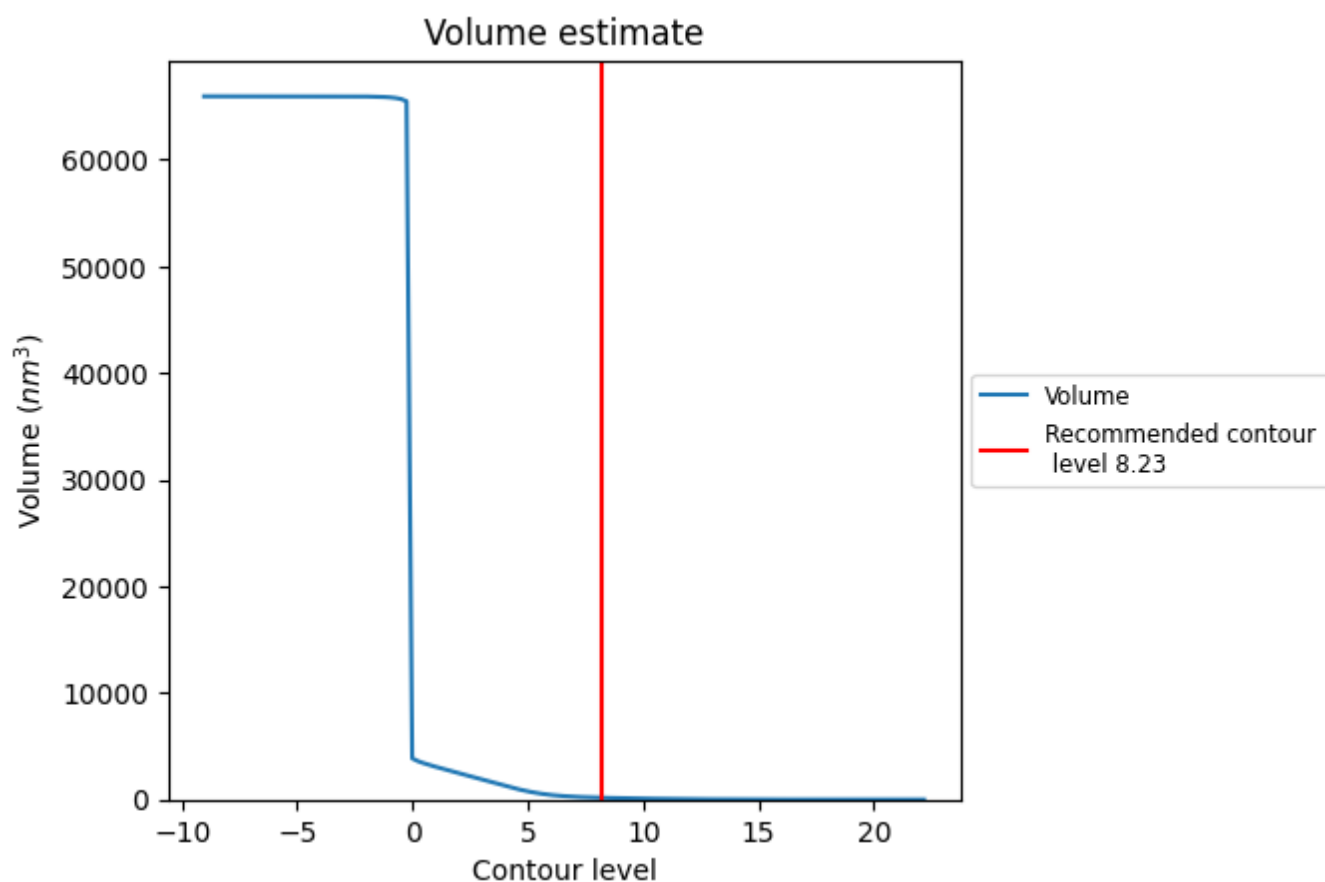
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

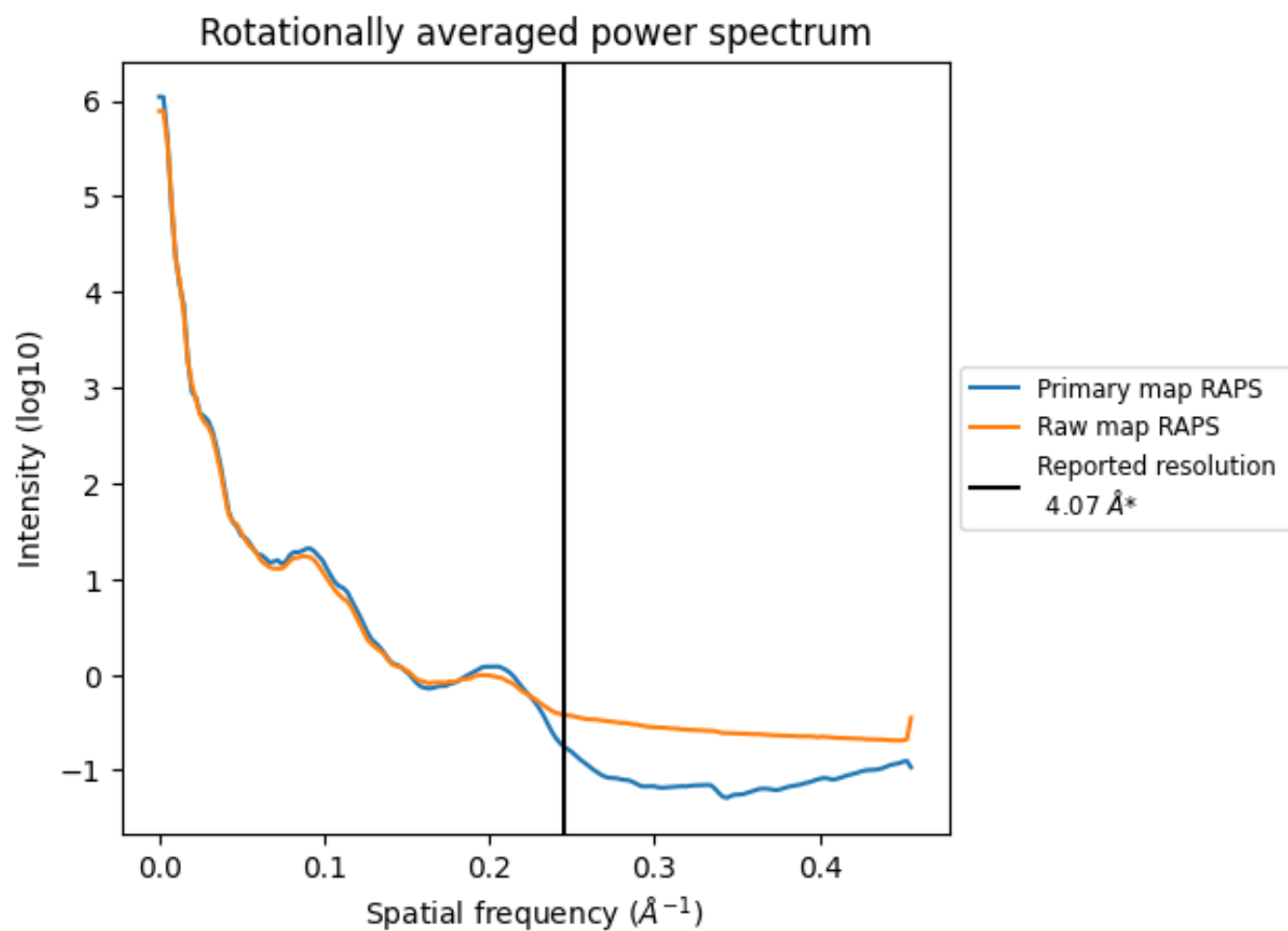
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 154 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

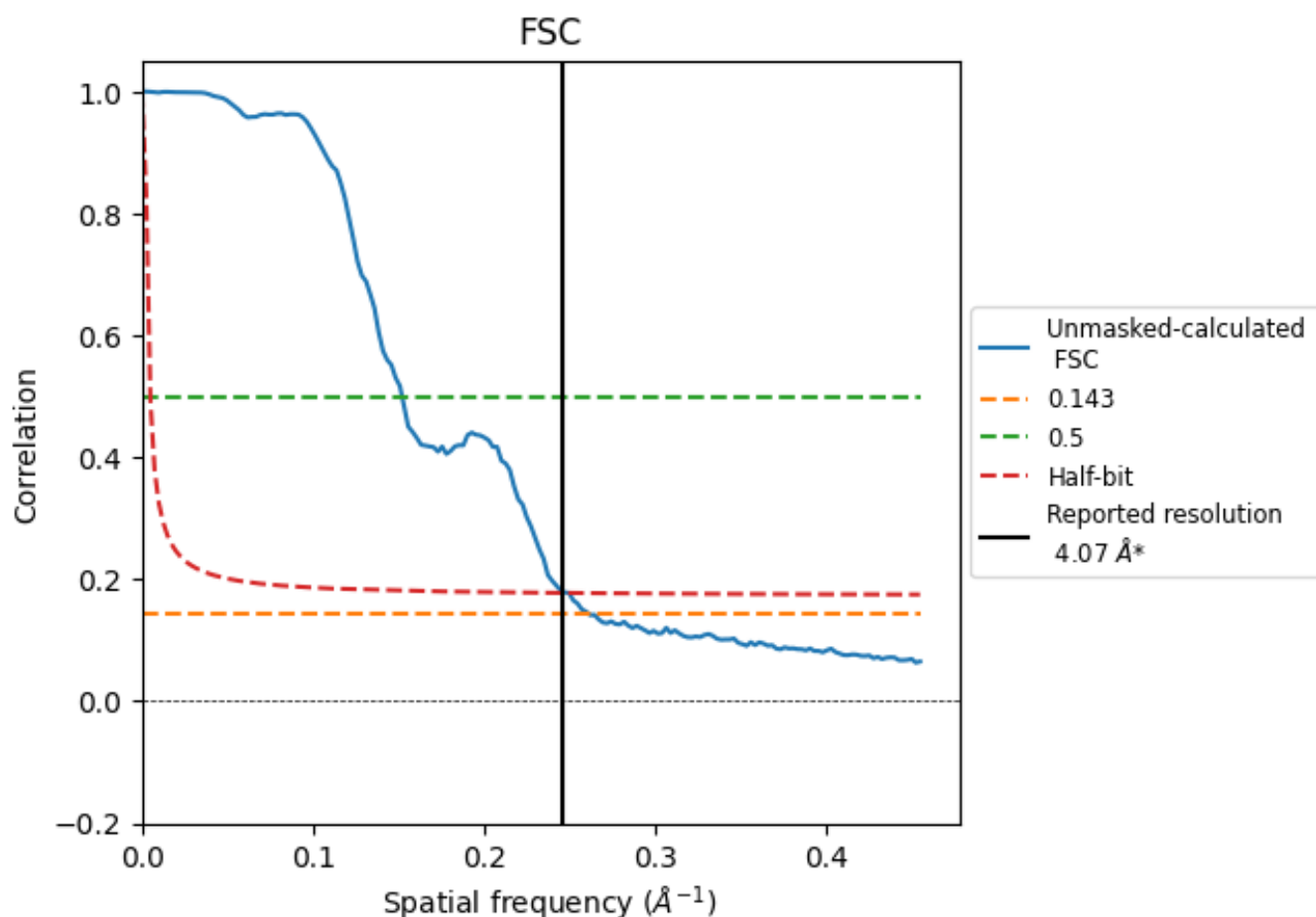


*Reported resolution corresponds to spatial frequency of 0.246 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.246 \AA^{-1}

8.2 Resolution estimates [i](#)

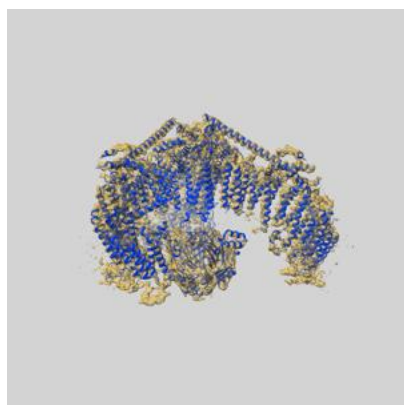
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	6.57	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

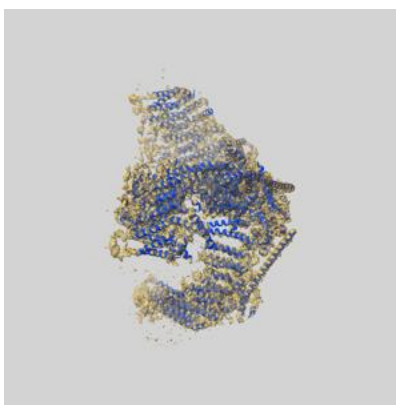
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35799 and PDB model 8IXN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

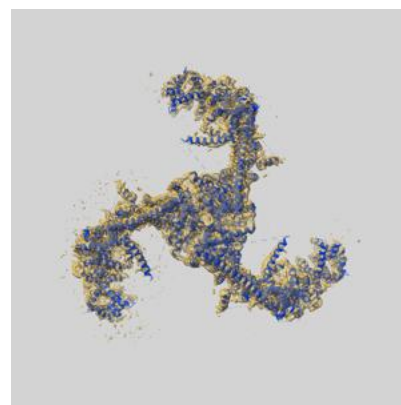
9.1 Map-model overlay [i](#)



X



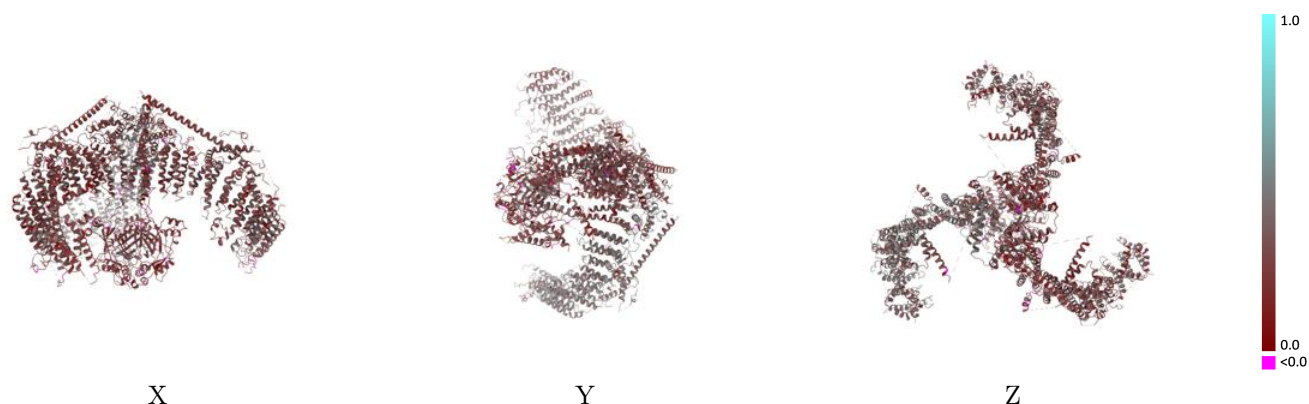
Y



Z

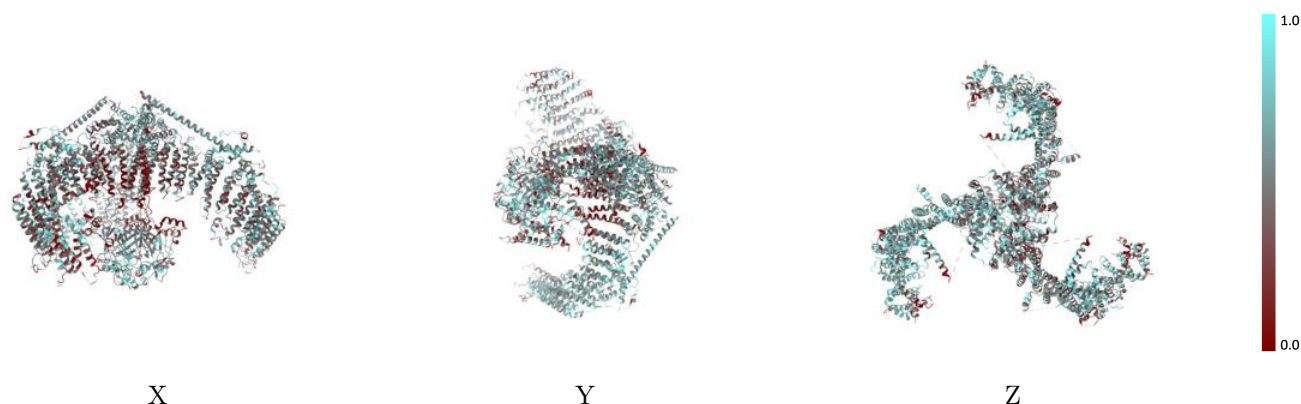
The images above show the 3D surface view of the map at the recommended contour level 8.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



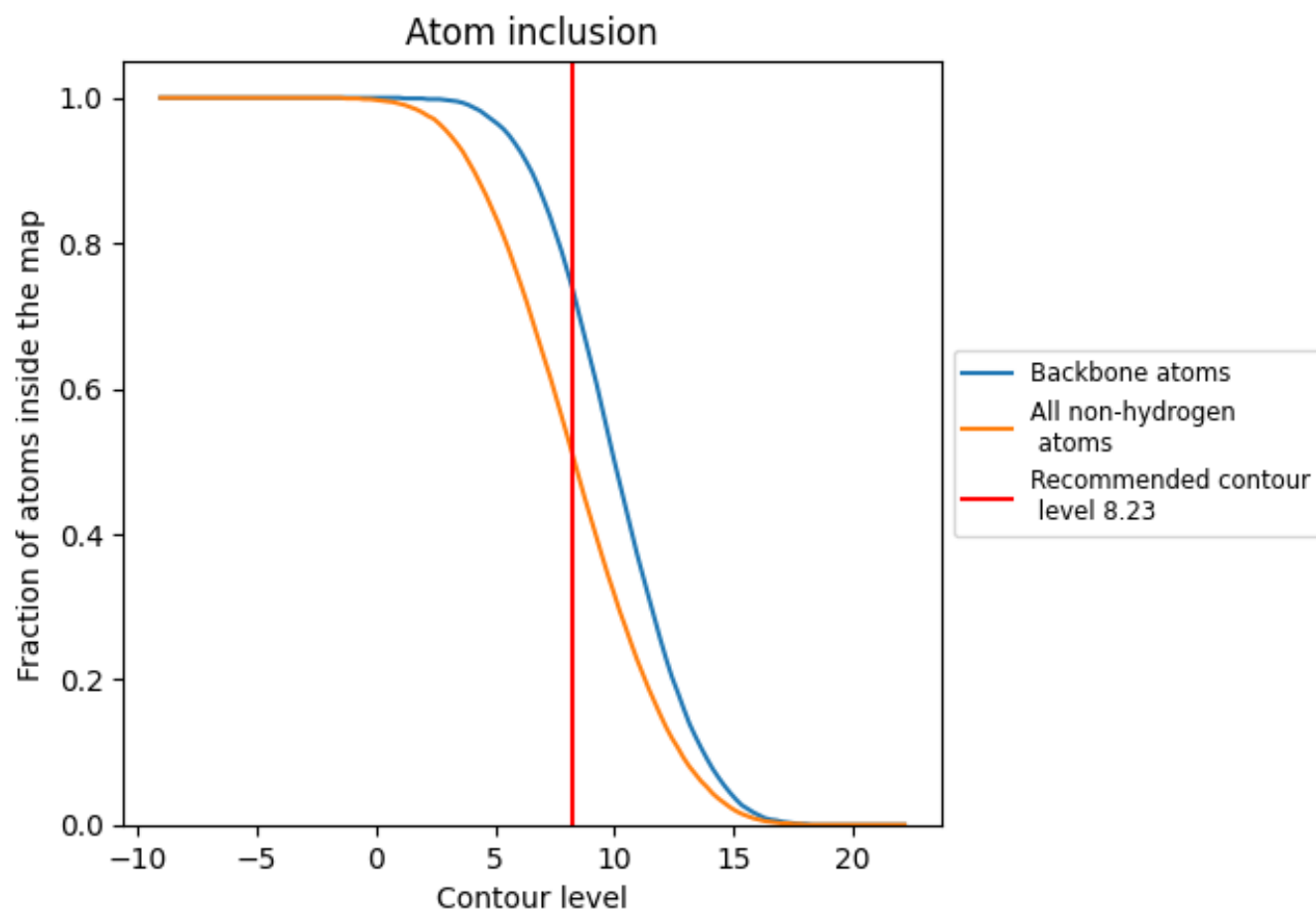
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 51% 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 (8.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5120	<div></div> 0.3010
A	<div></div> 0.4980	<div></div> 0.2760
C	<div></div> 0.4770	<div></div> 0.2610
D	<div></div> 0.5600	<div></div> 0.3640

