



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:22 AM UTC

PDB ID : 8VH5 / pdb_00008vh5
EMDB ID : EMD-43235
Title : Cryo-EM structure of Rab12-LRRK2 complex in the LRRK2 dimer state
Authors : Zhu, H.; Sun, J.
Deposited on : 2023-12-30
Resolution : 4.00 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

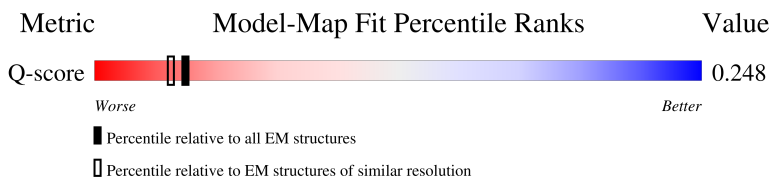
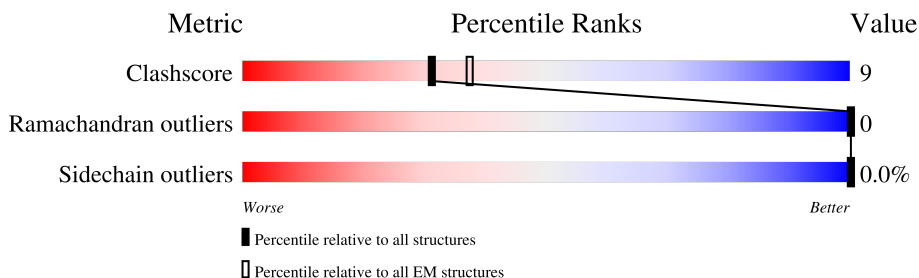
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	2527	9% 71% 16% 12%
1	C	2527	8% 72% 16% 12%
2	B	176	60% 75% 22% .
2	D	176	64% 74% 23% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33744 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 Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2221	Total	C	N	O	S	0	0
			15573	10054	2651	2783	85		
1	C	2221	Total	C	N	O	S	0	0
			15587	10060	2655	2787	85		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	HIS	ARG	conflict	UNP Q5S007
A	1647	THR	SER	conflict	UNP Q5S007
A	2397	THR	MET	conflict	UNP Q5S007
C	50	HIS	ARG	conflict	UNP Q5S007
C	1647	THR	SER	conflict	UNP Q5S007
C	2397	THR	MET	conflict	UNP Q5S007

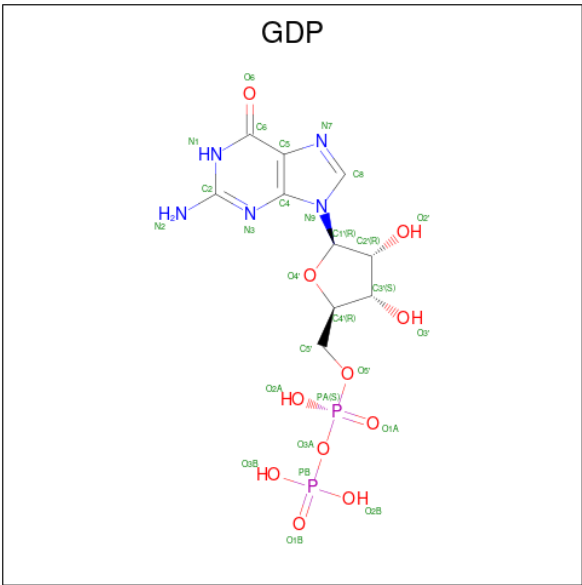
- Molecule 2 is a protein called Ras-related protein Rab-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	171	Total	C	N	O	S	0	0
			1200	775	199	220	6		
2	D	171	Total	C	N	O	S	0	0
			1200	775	199	220	6		

There are 2 discrepancies between the modelled and reference sequences:

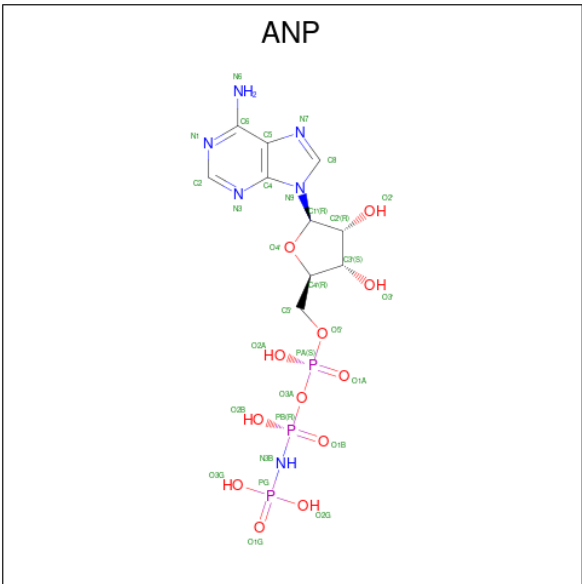
Chain	Residue	Modelled	Actual	Comment	Reference
B	101	LEU	GLN	conflict	UNP Q6IQ22
D	101	LEU	GLN	conflict	UNP Q6IQ22

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	C	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

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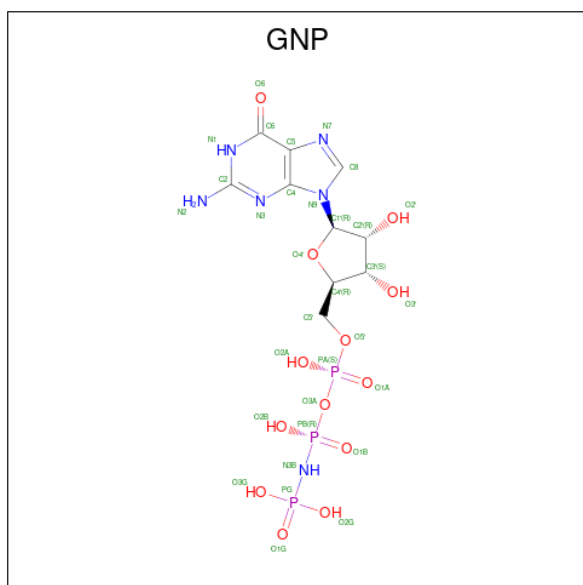
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Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			32	10	6	13	3	
6	D	1	Total	C	N	O	P	0
			32	10	6	13	3	

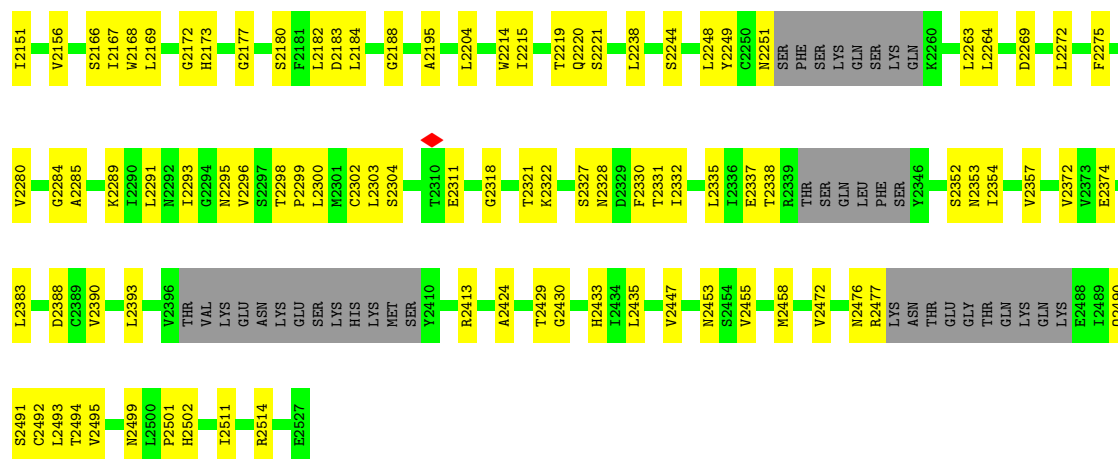
LEU	Q1087	N1305	Y1415	VAL	ARG	D1883	A2040	L2238	N2328	G2430
ALA	L1090	D1317	Y1419	GLU	GLU	L1870	V2043	S2244	D2329	H2433
SER	L1092	L1322	P1433	CYS	ALA	N1872	G2070	V2245	T2330	I2434
ARG	M1093	N1333	W1434	PRO	LEU	N1873	C2101	L2248	I2332	L2435
E982	G1116	L1337	M1437	LYS	ARG	E1882	L2110	V2249	L2335	V2447
Y983	K1138	M1338	K1439	GLY	ARG	F1883	L2124	C2250	E2336	N2453
1984	E1146	V1340	A1440	PHE	LEU	L1884	S2125	N2251	T2338	S2454
T985	N1147	G1341	R1441	VAL	THR	L1885	A2126	SER	R2339	V2455
S986	P1169	N1342	V1447	GLU	SER	Y1889	L2127	PHE	SER	N2458
1987	P1172	T1348	I1448	LYS	GLN	V1905	Q2127	LYS	GLN	V2472
D988	P1176	T1349	T1452	LEU	LYS	N1909	Q2128	GLN	SER	N2476
S990	M1175	T1357	D1455	SER	LYS	T1912	L2137	V2260	Y2346	D2477
A991	I1177	LYS	V1456	ARG	ARG	E1920	R2143	L2263	S2352	LYS
1992	A1191	GLY	S1457	PHE	PHE	H1758	L2146	L2264	N2353	ASN
D998	I1192	Q1365	K1463	P1642	P1659	L1763	L2151	L2269	I2354	THR
A999	N1193	T1368	GLN	A1659	LEU	H1755	V2156	L2272	V2357	GLN
L1000	N1195	V1369	ARG	LEU	PRO	E1929	L2166	F2275	S2372	LYS
C1004	L1198	T1374	ASP	LEU	ILE	L1932	S2167	L2277	V2373	ASN
C1005	R1199	V1376	LYS	LEU	CYS	E1939	L2168	L2290	E2374	THR
I1006	S1200	P1377	GLY	LEU	GLY	G1942	L2169	L2291	V2379	GLY
S1007	L1237	I1378	E1492	LEU	GLU	R1944	L2172	L2292	V2383	GLY
L1010	L1237	R1381	T1491	LEU	GLY	L1945	G2172	L2293	L2388	THR
L1013	H1251	ASP	E1505	LEU	GLY	V1946	H2173	L2294	D2389	GLN
F1014	M1255	LYS	M1506	LEU	GLY	L1956	G2177	L2295	C2389	GLN
K1015	M1260	L1388	N1510	LEU	GLY	D1956	S2180	L2296	V2390	LYS
N1021	D1274	V1389	E1512	LEU	GLY	L1959	F2181	L2297	L2393	GLU
F1026	M1278	L1390	K1512	LEU	GLY	R1968	D2182	L2298	V2396	SER
L1034	N1281	N1391	L1517	LEU	GLY	D1980	L2184	L2299	L2299	ASN
L1037	L1282	V1392	V1518	LEU	GLY	R1983	G2188	L2300	L2301	LYS
D1041	S1283	W1393	V1519	LEU	GLY	D1994	A2195	L2302	L2302	GLU
L1042	M1286	W1393	C1526	LEU	GLY	P1997	L2204	L2303	L2303	SER
S1043	E1287	V1394	W1541	LEU	GLY	A2021	W2214	L2304	L2304	THR
N1045	K1290	F1395	I1548	LEU	GLY	Q2022	I2215	T2310	T2310	VAL
S1052	F1408	D1394	L1564	LEU	GLY	TTR	T2219	E2311	R2413	LYS
Y1053	T1410	R1398	K1601	LEU	GLY	CYS	Q2220	G2318	V2414	LYS
S1058	D1077	F1395	T1612	LEU	GLY	ARG	G2222	T2321	K2415	GLY
C1059		F1395	VAL	LEU	GLY	GLY		K2322	A2424	ASN
N1062		R1398	LYS	LEU	GLY	ILE		S2327	T2429	ASP
R1067		F1408		LEU	GLY	LYS				TRP
I1070		T1410		LEU	GLY	LYS				GLY
D1077		D1077		LEU	GLY	LYS				ASP

• Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

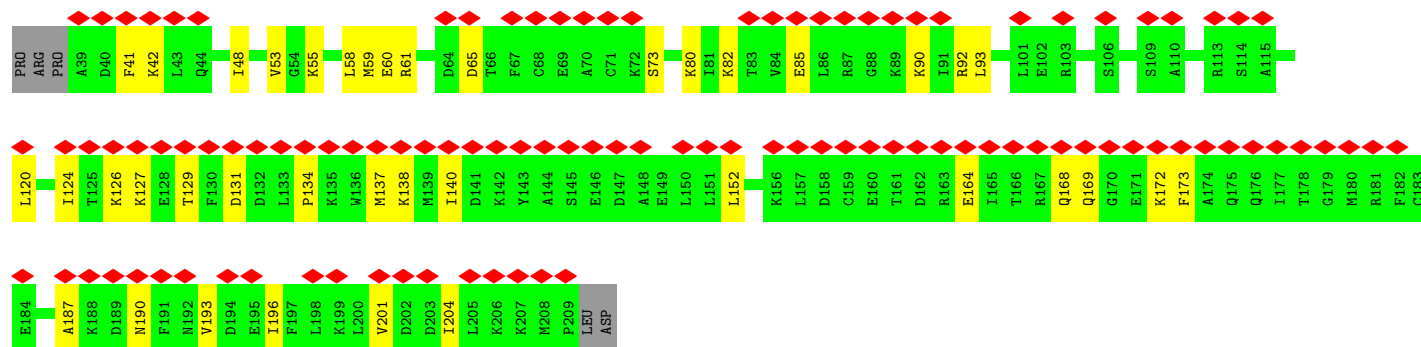
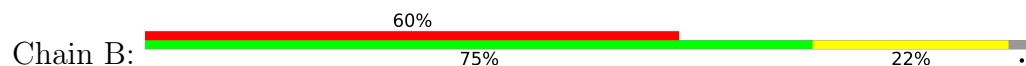


MET	ALA	SER	GLY	SER	CYS	GLN	GLY	CYS	GLU	GLU	D12	E13	E14	T15	L16	K17	K18	L19	I20	V21	R22	L23	L24	N25	VAL	GLN	GLU	G29	K30	Q31	I32	E33	T34	L35	V36	I38	L39	E40	D41	L42	L43	V44	F45	T46	Y47	S48	ASN	ASP	TRP	GLY	VAL	LEU	G113	V114	H115	Q116	L117	I118	L119	K120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						

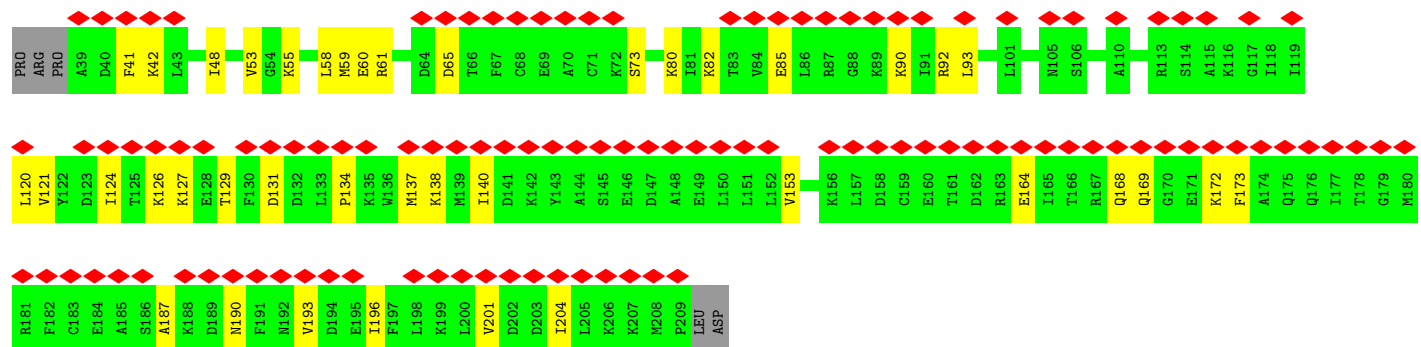
E1920	H1768	P1642	ARG	GLY	P189	A999	TRP	L762	L559	V414	I266	C181	M121
H1929	L1763	A1659	K1463	THR	E190	L1000	THR	R767	Q560	F415	I273	L184	L122
P1930	P1768	LEU	P1480	ILE	A191	S1001	PHE	R772	Q566	Q416	L274	H185	T123
S1931	K1772	ILE	D1484	V1369	I1192	C1004	PRO	R790	V566	N420	H275	H186	V124
L1932	K1775	GLY	T1491	V1373	I1193	I1006	ASP	L791	S568	L426	R276	L187	H125
G1939	I1775	GLU	E1492	K1374	L1195	S1007	SER	R792	S569	N429	I285	R190	N126
P1942	L1787	THR	I1505	W1376	L1198	L1010	MET	R793	D575	V430	V291	V191	S128
R1943	M1668	LEU	N1506	P1377	S1200	L1013	SER	R801	E578	R433	V295	S192	N129
M1944	H1701	L1668	N1506	I1378	S1200	L1013	VAL	R802	M579	R434	V299	E193	N130
L1945	H1684	L1668	N1506	I1378	S1200	L1013	PHE	R803	L582	T435	V299	E194	L131
V1946	F1511	R1381	N1506	I1378	S1200	L1013	ALA	R804	A585	K439	L316	Q195	V133
D1956	E1689	ASP	F1511	R1381	L1226	L1034	GLN	G807	A588	K439	T320	L196	V133
L1959	L1694	ASP	F1511	R1381	L1226	L1034	ASP	R808	S588	K439	T320	T197	I134
D1980	L1694	ASP	F1511	R1381	L1226	L1034	LEU	C809	L582	K439	T320	E198	G135
R1983	L1694	ASP	F1511	R1381	L1226	L1034	ASP	V813	L582	K439	T320	F199	G135
P1997	L1694	ASP	F1511	R1381	L1226	L1034	SER	E814	L582	K439	T320	V200	L136
H1998	L1694	ASP	F1511	R1381	L1226	L1034	GLY	P815	L582	K439	T320	E201	K137
A2021	L1694	ASP	F1511	R1381	L1226	L1034	SER	P820	L582	K439	T320	N202	T138
Q2022	L1694	ASP	F1511	R1381	L1226	L1034	GLY	D824	L582	K439	T320	D203	L139
CYS	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	K204	D140
CYS	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	Y205	L141
ARG	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	M206	L142
MET	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	L207	L143
GLY	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	L208	T144
ILE	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	L209	S145
LYS	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	G146	G146
T2031	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S210	K147
A2040	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	A211	I148
V2043	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	L212	T149
G2070	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	T213	L150
V2107	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	N214	L151
L2110	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	F215	I152
T2124	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	K216	L153
S2125	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	D217	D154
A2126	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	E218	E155
Q2127	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	E219	E156
V2128	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	E220	S157
L2137	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	I221	D158
T2141	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	V225	I159
R2142	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	L229	F160
R2143	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	H230	M161
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	L234	L162
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	H408	I163
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	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	D165
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	A166
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	M167
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	H168
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	M257
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	K258
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	A259
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	F170
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	P171
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	A172
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	M262
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	D174
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	E175
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	V176
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	Q177
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	K178
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	L179
	L1694	ASP	F1511	R1381	L1226	L1034	GLY	L824	L582	K439	T320	S411	G180



• Molecule 2: Ras-related protein Rab-12



• Molecule 2: Ras-related protein Rab-12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	77265	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	77.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.547	Depositor
Minimum map value	-1.169	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	508.288, 508.288, 508.288	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.444, 1.444, 1.444	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, ANP, GDP, MG

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	0.30	1/15858 (0.0%)	0.52	9/21732 (0.0%)
1	C	0.29	0/15871	0.50	7/21745 (0.0%)
2	B	0.25	0/1219	0.42	0/1662
2	D	0.25	0/1219	0.42	0/1662
All	All	0.29	1/34167 (0.0%)	0.51	16/46801 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	THR	C-O	5.33	1.30	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	THR	CA-C-N	-9.31	105.17	120.72
1	A	213	THR	C-N-CA	-9.31	105.17	120.72
1	C	210	SER	CA-C-N	-7.65	108.22	122.60
1	C	210	SER	C-N-CA	-7.65	108.22	122.60
1	C	179	LEU	N-CA-C	-7.30	104.34	113.18
1	A	204	ASP	N-CA-C	-7.07	102.70	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ILE	N-CA-C	-6.71	103.16	113.16
1	C	148	ILE	N-CA-C	-6.68	103.20	113.16
1	A	184	LEU	N-CA-C	-6.11	105.08	112.54
1	A	210	SER	CA-C-N	-5.96	112.33	120.44
1	A	210	SER	C-N-CA	-5.96	112.33	120.44
1	A	209	LEU	CA-C-N	-5.61	113.15	120.44
1	A	209	LEU	C-N-CA	-5.61	113.15	120.44
1	C	213	THR	CA-C-N	-5.60	111.34	121.14
1	C	213	THR	C-N-CA	-5.60	111.34	121.14
1	C	204	ASP	N-CA-C	-5.09	105.73	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	LEU	Mainchain
1	A	986	SER	Peptide
1	C	172	ALA	Mainchain
1	C	986	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15573	0	14262	254	0
1	C	15587	0	14299	263	0
2	B	1200	0	1080	25	0
2	D	1200	0	1080	25	0
3	A	28	0	12	0	0
3	C	28	0	12	0	0
4	A	31	0	13	1	0
4	C	31	0	13	2	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	32	0	13	3	0
6	D	32	0	13	3	0
All	All	33744	0	30797	569	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (569) 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:C:173:ASN:ND2	1:C:176:VAL:HG23	1.25	1.48
1:C:173:ASN:ND2	1:C:176:VAL:CG2	1.92	1.32
1:C:173:ASN:HD22	1:C:176:VAL:CG2	1.61	1.05
1:C:133:VAL:HG12	1:C:176:VAL:HG22	1.52	0.89
1:A:813:VAL:HG21	1:A:989:LEU:HD21	1.55	0.87
1:C:221:ILE:O	1:C:225:VAL:HG23	1.76	0.85
1:A:221:ILE:O	1:A:225:VAL:HG23	1.76	0.85
1:C:813:VAL:HG21	1:C:989:LEU:HD21	1.55	0.85
1:C:173:ASN:HD21	1:C:176:VAL:HG23	0.83	0.84
1:C:173:ASN:HD21	1:C:176:VAL:CG2	1.75	0.80
1:C:173:ASN:HD22	1:C:176:VAL:HG21	1.49	0.75
1:C:133:VAL:HG12	1:C:176:VAL:CG2	2.16	0.74
1:A:170:PHE:HB2	1:A:176:VAL:HG11	1.68	0.73
1:C:801:ASN:HB3	1:C:984:ILE:HA	1.71	0.71
1:A:801:ASN:HB3	1:A:984:ILE:HA	1.71	0.71
1:C:2220:GLN:NE2	1:C:2244:SER:CB	2.55	0.69
1:A:2220:GLN:NE2	1:A:2244:SER:CB	2.55	0.69
2:B:55:LYS:NZ	6:B:302:GNP:O3G	2.27	0.68
2:D:55:LYS:NZ	6:D:302:GNP:O3G	2.27	0.67
1:A:575:ASP:O	1:A:579:MET:N	2.28	0.67
1:C:1070:ILE:H	1:C:1093:ASN:HB3	1.61	0.66
1:A:1959:LEU:HD13	1:A:2070:GLY:HA3	1.77	0.66
1:A:1070:ILE:H	1:A:1093:ASN:HB3	1.60	0.66
1:A:1457:SER:HG	1:A:1463:LYS:N	1.94	0.66
1:C:1959:LEU:HD13	1:C:2070:GLY:HA3	1.77	0.65
1:C:1172:PRO:HD2	1:C:1175:MET:HE2	1.79	0.65
1:A:1172:PRO:HD2	1:A:1175:MET:HE2	1.79	0.64
1:C:173:ASN:ND2	1:C:176:VAL:CB	2.61	0.64
1:A:2238:LEU:HD12	1:A:2285:ALA:H	1.62	0.63
1:A:502:LEU:HD23	1:A:559:ILE:HG23	1.81	0.63
1:C:2238:LEU:HD12	1:C:2285:ALA:H	1.63	0.63
1:A:553:PHE:O	1:A:560:GLN:NE2	2.32	0.62
1:C:575:ASP:O	1:C:579:MET:N	2.28	0.62
1:A:990:SER:O	1:A:1021:ASN:ND2	2.33	0.62
1:C:502:LEU:HD23	1:C:559:ILE:HG23	1.81	0.62
1:C:990:SER:O	1:C:1021:ASN:ND2	2.33	0.62
1:C:1346:GLY:H	1:C:1452:THR:HG21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:SER:OG	1:A:744:LEU:N	2.34	0.61
1:C:743:SER:OG	1:C:744:LEU:N	2.34	0.61
1:A:1346:GLY:H	1:A:1452:THR:HG21	1.65	0.61
1:C:553:PHE:O	1:C:560:GLN:NE2	2.32	0.61
1:C:807:GLY:HA2	1:C:991:ALA:HB3	1.81	0.60
1:A:807:GLY:HA2	1:A:991:ALA:HB3	1.82	0.60
1:C:1195:LEU:HD12	1:C:1198:LEU:HD12	1.83	0.60
1:A:350:LEU:HD22	1:A:384:LEU:HD12	1.83	0.60
1:C:1457:SER:HG	1:C:1463:LYS:N	1.99	0.60
1:C:1980:ASP:OD1	1:C:1983:ARG:NH2	2.35	0.60
1:A:230:HIS:O	1:A:276:ARG:NH1	2.35	0.60
1:C:350:LEU:HD22	1:C:384:LEU:HD12	1.83	0.60
1:A:713:LEU:HD22	1:A:733:ALA:HB1	1.84	0.60
2:B:48:ILE:HG13	2:B:120:LEU:HD13	1.84	0.60
2:D:48:ILE:HG13	2:D:120:LEU:HD13	1.84	0.60
1:C:992:ASN:O	1:C:1021:ASN:ND2	2.35	0.59
1:C:2272:LEU:HB3	1:C:2291:LEU:HB2	1.83	0.59
1:A:1195:LEU:HD12	1:A:1198:LEU:HD12	1.83	0.59
1:A:1980:ASP:OD1	1:A:1983:ARG:NH2	2.35	0.59
1:A:992:ASN:O	1:A:1021:ASN:ND2	2.35	0.59
1:C:713:LEU:HD22	1:C:733:ALA:HB1	1.84	0.59
1:C:792:ARG:NH2	1:C:820:PRO:O	2.36	0.59
1:A:2272:LEU:HB3	1:A:2291:LEU:HB2	1.83	0.59
1:C:1817:ASN:ND2	1:C:1820:GLU:O	2.35	0.59
1:A:792:ARG:NH2	1:A:820:PRO:O	2.36	0.59
1:C:230:HIS:O	1:C:276:ARG:NH1	2.35	0.58
1:A:1817:ASN:ND2	1:A:1820:GLU:O	2.35	0.58
1:C:1062:ASN:HA	1:C:1087:GLN:HB2	1.85	0.58
1:C:2107:VAL:HB	1:C:2137:LEU:HD11	1.85	0.58
1:C:1695:TYR:HB2	1:C:1763:LEU:HB3	1.86	0.58
1:A:1062:ASN:HA	1:A:1087:GLN:HB2	1.85	0.58
1:C:2238:LEU:HA	1:C:2284:GLY:H	1.69	0.58
1:A:2107:VAL:HB	1:A:2137:LEU:HD11	1.85	0.58
1:A:1283:SER:HA	1:A:1305:ASN:HD21	1.68	0.58
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	1.86	0.58
1:A:2374:GLU:HB3	1:A:2383:LEU:HD21	1.86	0.57
1:A:2238:LEU:HA	1:A:2284:GLY:H	1.69	0.57
1:A:1041:ASP:N	1:A:1041:ASP:OD1	2.37	0.57
1:A:1433:PRO:O	1:A:1437:ASN:ND2	2.36	0.57
1:C:1283:SER:HA	1:C:1305:ASN:HD21	1.68	0.57
2:B:126:LYS:O	2:B:129:THR:OG1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1433:PRO:O	1:C:1437:ASN:ND2	2.36	0.57
1:C:2321:THR:OG1	1:C:2352:SER:O	2.21	0.57
1:C:2374:GLU:HB3	1:C:2383:LEU:HD21	1.86	0.57
1:A:1929:HIS:HB3	1:A:1932:LEU:HD23	1.86	0.57
1:C:1287:GLU:O	1:C:1290:LYS:NZ	2.36	0.57
1:C:1929:HIS:HB3	1:C:1932:LEU:HD23	1.86	0.57
1:A:426:LEU:O	1:A:433:ARG:NH2	2.38	0.57
1:C:426:LEU:O	1:C:433:ARG:NH2	2.38	0.57
1:C:1146:GLU:HA	1:C:1169:PRO:HB2	1.87	0.56
1:A:1373:VAL:HB	1:A:1601:LYS:HB3	1.86	0.56
1:A:2151:ILE:H	1:A:2173:HIS:HB3	1.70	0.56
4:A:2602:ANP:O2A	4:A:2602:ANP:O1B	2.23	0.56
1:C:173:ASN:HD22	1:C:176:VAL:CB	2.16	0.56
1:C:1373:VAL:HB	1:C:1601:LYS:HB3	1.86	0.56
1:C:1512:LYS:HA	1:C:1517:LEU:H	1.70	0.56
1:C:2151:ILE:H	1:C:2173:HIS:HB3	1.70	0.56
1:A:2322:LYS:HG3	1:A:2337:GLU:HA	1.88	0.56
1:C:2151:ILE:O	1:C:2172:GLY:N	2.33	0.56
1:C:793:ARG:O	1:C:793:ARG:NH1	2.37	0.56
1:A:1177:ILE:HG22	1:A:1200:SER:HB3	1.88	0.56
1:A:1146:GLU:HA	1:A:1169:PRO:HB2	1.87	0.56
1:A:316:LEU:HB3	1:A:349:TRP:HE1	1.70	0.55
1:C:1772:LYS:HA	1:C:1775:ILE:HD12	1.88	0.55
1:A:2289:LYS:NZ	1:A:2330:PHE:O	2.37	0.55
1:C:2322:LYS:HG3	1:C:2337:GLU:HA	1.88	0.55
1:A:194:GLU:O	1:A:198:GLU:N	2.40	0.55
1:C:194:GLU:O	1:C:198:GLU:N	2.40	0.55
1:C:316:LEU:HB3	1:C:349:TRP:HE1	1.70	0.55
1:A:211:ALA:CB	1:A:225:VAL:HG21	2.36	0.55
1:A:1772:LYS:HA	1:A:1775:ILE:HD12	1.88	0.55
1:C:230:HIS:HA	1:C:273:LEU:HD13	1.87	0.55
1:C:737:GLN:HE21	1:C:744:LEU:HD13	1.72	0.55
1:C:744:LEU:O	1:C:748:VAL:HG23	2.07	0.55
1:C:2458:MET:HG3	1:C:2472:VAL:HG22	1.87	0.55
1:A:2458:MET:HG3	1:A:2472:VAL:HG22	1.87	0.55
4:C:2602:ANP:O1B	4:C:2602:ANP:O2A	2.23	0.55
1:A:210:SER:O	1:A:214:ASN:N	2.34	0.55
1:A:495:GLU:OE1	1:A:495:GLU:N	2.33	0.55
1:A:1512:LYS:HA	1:A:1517:LEU:H	1.70	0.55
1:C:1177:ILE:HG22	1:C:1200:SER:HB3	1.88	0.55
1:A:548:ALA:HA	1:A:551:ASN:HD22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:GLN:HE21	1:A:744:LEU:HD13	1.72	0.55
1:C:1541:VAL:HG21	1:C:1548:ILE:HD11	1.89	0.55
1:A:230:HIS:HA	1:A:273:LEU:HD13	1.87	0.54
1:A:1871:ASN:ND2	1:A:1873:ASP:OD1	2.40	0.54
1:C:548:ALA:HA	1:C:551:ASN:HD22	1.72	0.54
1:C:1871:ASN:ND2	1:C:1873:ASP:OD1	2.40	0.54
1:C:2289:LYS:NZ	1:C:2330:PHE:O	2.37	0.54
1:A:2263:LEU:HB3	1:A:2275:PHE:HB2	1.90	0.54
1:A:538:PHE:HE1	1:A:543:HIS:HB3	1.73	0.54
1:A:744:LEU:O	1:A:748:VAL:HG23	2.06	0.54
1:A:1394:ASP:OD1	1:A:1394:ASP:N	2.40	0.54
1:A:1415:TYR:HB2	1:A:1447:VAL:HG22	1.90	0.54
2:B:59:MET:HG2	2:B:80:LYS:HD2	1.90	0.54
1:C:1041:ASP:N	1:C:1041:ASP:OD1	2.37	0.54
1:C:1415:TYR:HB2	1:C:1447:VAL:HG22	1.90	0.53
1:C:2263:LEU:HB3	1:C:2275:PHE:HB2	1.90	0.53
1:C:1956:ASP:HB3	1:C:1997:PRO:HB2	1.90	0.53
1:A:1044:SER:H	1:A:1067:ARG:HB2	1.72	0.53
1:A:2299:PRO:HD2	1:A:2353:ASN:HD21	1.74	0.53
1:C:1044:SER:H	1:C:1067:ARG:HB2	1.72	0.53
1:C:1260:ILE:HG12	1:C:1281:LEU:HD11	1.91	0.53
1:C:1394:ASP:OD1	1:C:1394:ASP:N	2.40	0.53
1:A:1368:THR:O	1:A:1398:ARG:NH2	2.40	0.53
1:A:1956:ASP:HB3	1:A:1997:PRO:HB2	1.90	0.53
1:A:2352:SER:OG	1:A:2353:ASN:N	2.42	0.53
1:A:1541:VAL:HG21	1:A:1548:ILE:HD11	1.89	0.53
1:C:2299:PRO:HD2	1:C:2353:ASN:HD21	1.73	0.53
1:C:1368:THR:O	1:C:1398:ARG:NH2	2.40	0.53
1:C:1448:ILE:HG23	1:C:1484:ASP:HB3	1.90	0.53
2:D:85:GLU:HA	2:D:90:LYS:HA	1.91	0.53
2:D:134:PRO:O	2:D:138:LYS:N	2.42	0.53
1:A:1448:ILE:HG23	1:A:1484:ASP:HB3	1.90	0.53
2:B:193:VAL:HA	2:B:196:ILE:HD12	1.91	0.53
2:D:59:MET:HG2	2:D:80:LYS:HD2	1.90	0.52
1:A:1043:HIS:O	1:A:1045:ASN:ND2	2.43	0.52
1:C:1317:ASP:OD1	1:C:1317:ASP:N	2.41	0.52
2:B:60:GLU:O	2:B:65:ASP:N	2.42	0.52
1:C:173:ASN:ND2	1:C:176:VAL:HG21	2.06	0.52
1:A:1317:ASP:OD1	1:A:1317:ASP:N	2.41	0.52
1:A:2151:ILE:O	1:A:2172:GLY:N	2.33	0.52
2:B:85:GLU:HA	2:B:90:LYS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:PRO:O	2:B:138:LYS:N	2.42	0.52
1:A:211:ALA:HB1	1:A:225:VAL:HG21	1.91	0.52
1:A:566:VAL:O	1:A:569:SER:OG	2.21	0.52
1:A:1260:ILE:HG12	1:A:1281:LEU:HD11	1.91	0.52
1:C:1004:CYS:SG	1:C:1005:CYS:N	2.83	0.52
1:C:1863:ASP:OD1	1:C:1863:ASP:N	2.42	0.52
2:D:60:GLU:O	2:D:65:ASP:N	2.42	0.52
2:D:193:VAL:HA	2:D:196:ILE:HD12	1.91	0.52
2:B:41:PHE:O	2:B:92:ARG:N	2.37	0.52
1:A:762:LEU:HD11	1:A:790:LEU:HD23	1.91	0.52
1:C:762:LEU:HD11	1:C:790:LEU:HD23	1.91	0.52
2:D:126:LYS:O	2:D:129:THR:OG1	2.21	0.52
1:A:2291:LEU:HD22	1:A:2293:ILE:HD11	1.92	0.51
1:A:1734:TRP:CD1	1:A:1736:GLN:H	2.29	0.51
1:A:1863:ASP:OD1	1:A:1863:ASP:N	2.42	0.51
1:C:1882:GLU:HG3	1:C:1885:LEU:HD23	1.92	0.51
1:A:1190:GLU:O	1:A:1194:ASN:ND2	2.43	0.51
1:A:2300:LEU:HD21	1:A:2303:LEU:HD21	1.93	0.51
1:C:133:VAL:CG1	1:C:176:VAL:CG2	2.88	0.51
1:C:1375:ASP:OD1	1:C:1375:ASP:N	2.43	0.51
1:C:2291:LEU:HD22	1:C:2293:ILE:HD11	1.92	0.51
1:A:748:VAL:HG21	1:A:761:LEU:HD22	1.92	0.51
1:C:1052:SER:OG	1:C:1077:ASP:OD1	2.27	0.51
1:A:2318:GLY:HA3	1:A:2354:ILE:HD13	1.93	0.51
1:A:2453:ASN:OD1	1:A:2477:ARG:N	2.41	0.51
1:C:416:GLN:OE1	1:C:420:ASN:ND2	2.44	0.51
1:C:667:VAL:O	1:C:715:ARG:NH2	2.44	0.51
1:C:1190:GLU:O	1:C:1194:ASN:ND2	2.43	0.51
1:C:1347:LYS:NZ	1:C:1395:PHE:O	2.42	0.51
1:C:2300:LEU:HD21	1:C:2303:LEU:HD21	1.93	0.51
1:C:2318:GLY:HA3	1:C:2354:ILE:HD13	1.93	0.51
1:A:219:GLU:HG3	1:A:266:ILE:HD11	1.93	0.51
1:C:1043:HIS:O	1:C:1045:ASN:ND2	2.43	0.51
1:A:1287:GLU:O	1:A:1290:LYS:NZ	2.36	0.51
1:C:1734:TRP:CD1	1:C:1736:GLN:H	2.29	0.51
1:C:2352:SER:OG	1:C:2353:ASN:N	2.42	0.51
1:C:2293:ILE:HD12	1:C:2332:ILE:HD11	1.93	0.51
1:A:667:VAL:O	1:A:715:ARG:NH2	2.44	0.51
1:C:1077:ASP:OD1	1:C:1077:ASP:N	2.44	0.51
1:C:2304:SER:OG	1:C:2357:VAL:O	2.29	0.51
1:A:416:GLN:OE1	1:A:420:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LEU:HD11	1:A:542:ILE:HG12	1.93	0.50
1:A:2304:SER:OG	1:A:2357:VAL:O	2.29	0.50
1:C:538:PHE:HE1	1:C:543:HIS:HB3	1.73	0.50
1:A:1004:CYS:SG	1:A:1005:CYS:N	2.83	0.50
1:C:1255:ASN:O	1:C:1278:ASN:ND2	2.45	0.50
1:C:1338:MET:HE1	1:C:1410:THR:H	1.76	0.50
1:C:2413:ARG:O	1:C:2430:GLY:N	2.45	0.50
2:D:41:PHE:O	2:D:92:ARG:N	2.37	0.50
1:C:488:LEU:HD11	1:C:542:ILE:HG12	1.93	0.50
1:A:1882:GLU:HG3	1:A:1885:LEU:HD23	1.92	0.50
1:A:2219:THR:HG23	1:A:2221:SER:H	1.77	0.50
1:C:748:VAL:HG21	1:C:761:LEU:HD22	1.92	0.50
1:A:2413:ARG:O	1:A:2430:GLY:N	2.45	0.50
1:A:1255:ASN:O	1:A:1278:ASN:ND2	2.45	0.50
1:A:1338:MET:HE1	1:A:1410:THR:H	1.76	0.50
1:C:2219:THR:HG23	1:C:2221:SER:H	1.77	0.50
1:C:495:GLU:OE1	1:C:495:GLU:N	2.33	0.49
1:A:1375:ASP:OD1	1:A:1375:ASP:N	2.43	0.49
1:A:2293:ILE:HD12	1:A:2332:ILE:HD11	1.93	0.49
1:C:1375:ASP:HA	1:C:1391:ASN:HA	1.95	0.49
2:B:137:MET:HA	2:B:140:ILE:HB	1.95	0.49
1:C:12:ASP:O	1:C:15:THR:OG1	2.30	0.49
1:C:607:LEU:HD21	1:C:648:GLY:HA2	1.94	0.49
1:A:1077:ASP:OD1	1:A:1077:ASP:N	2.44	0.49
1:A:706:ASP:O	1:A:710:ASN:ND2	2.46	0.49
1:A:1733:TYR:HB3	1:A:1738:ILE:HA	1.95	0.49
2:D:137:MET:HA	2:D:140:ILE:HB	1.95	0.49
1:A:1694:LEU:HB2	1:A:1811:TRP:HB2	1.95	0.49
2:B:168:GLN:O	2:B:172:LYS:N	2.44	0.49
1:A:793:ARG:O	1:A:793:ARG:NH1	2.37	0.49
1:A:1369:VAL:HG22	1:A:1398:ARG:HH22	1.78	0.49
1:A:1375:ASP:HA	1:A:1391:ASN:HA	1.95	0.49
1:C:2166:SER:OG	1:C:2182:LEU:O	2.25	0.49
1:C:219:GLU:HG3	1:C:266:ILE:HD11	1.93	0.48
1:C:1694:LEU:HB2	1:C:1811:TRP:HB2	1.95	0.48
1:C:2327:SER:OG	1:C:2328:ASN:N	2.46	0.48
1:C:137:LYS:HA	1:C:179:LEU:HD13	1.95	0.48
1:A:1905:VAL:HG12	1:A:1946:VAL:HG22	1.94	0.48
1:C:706:ASP:O	1:C:710:ASN:ND2	2.46	0.48
2:D:73:SER:OG	6:D:302:GNP:O1G	2.22	0.48
1:A:209:LEU:O	1:A:210:SER:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2249:TYR:N	1:A:2264:LEU:O	2.45	0.48
1:C:1733:TYR:HB3	1:C:1738:ILE:HA	1.95	0.48
1:A:1419:TYR:HB2	1:A:1451:GLY:HA2	1.96	0.48
1:A:1439:LYS:HB2	1:A:1480:PRO:HD3	1.95	0.48
1:A:2166:SER:OG	1:A:2182:LEU:O	2.25	0.48
1:C:1905:VAL:HG12	1:C:1946:VAL:HG22	1.94	0.48
1:C:1455:ASP:OD1	1:C:1455:ASP:N	2.46	0.48
1:C:1980:ASP:OD2	1:C:2514:ARG:NH1	2.47	0.48
1:C:2124:THR:HG23	1:C:2127:GLN:H	1.79	0.48
1:A:1870:LEU:HB2	1:A:1939:GLY:HA3	1.95	0.48
1:A:2492:CYS:SG	1:A:2493:LEU:N	2.87	0.48
1:C:149:THR:HA	1:C:152:ILE:HD12	1.95	0.48
1:C:1393:TRP:HZ3	1:C:1408:PHE:HB3	1.79	0.48
1:A:1980:ASP:OD2	1:A:2514:ARG:NH1	2.47	0.48
1:C:2321:THR:O	1:C:2338:THR:OG1	2.31	0.48
1:A:435:ILE:O	1:A:439:LYS:N	2.46	0.48
1:C:1870:LEU:HB2	1:C:1939:GLY:HA3	1.95	0.48
1:A:607:LEU:HD21	1:A:648:GLY:HA2	1.94	0.48
1:C:512:ILE:HD11	1:C:566:VAL:HG13	1.95	0.48
1:C:1369:VAL:HG22	1:C:1398:ARG:HH22	1.78	0.48
1:A:2321:THR:O	1:A:2338:THR:OG1	2.31	0.47
1:C:2249:TYR:N	1:C:2264:LEU:O	2.45	0.47
1:A:182:LYS:O	1:A:185:HIS:HB3	2.14	0.47
1:A:2220:GLN:HE21	1:A:2244:SER:CB	2.26	0.47
1:A:2390:VAL:HA	1:A:2393:LEU:HG	1.97	0.47
1:C:1439:LYS:HB2	1:C:1480:PRO:HD3	1.95	0.47
1:C:2302:CYS:SG	1:C:2303:LEU:N	2.87	0.47
1:A:86:CYS:HB2	1:A:138:THR:HG22	1.96	0.47
1:A:2321:THR:OG1	1:A:2352:SER:O	2.21	0.47
1:A:2327:SER:OG	1:A:2328:ASN:N	2.46	0.47
1:A:149:THR:HA	1:A:152:ILE:HD12	1.95	0.47
1:A:460:GLU:HG2	1:A:500:VAL:HA	1.96	0.47
1:A:1333:ASN:ND2	1:A:1519:VAL:O	2.43	0.47
1:C:435:ILE:O	1:C:439:LYS:N	2.47	0.47
1:C:2492:CYS:SG	1:C:2493:LEU:N	2.87	0.47
1:C:2499:ASN:OD1	1:C:2502:HIS:ND1	2.44	0.47
1:A:12:ASP:O	1:A:15:THR:OG1	2.30	0.47
1:A:512:ILE:HD11	1:A:566:VAL:HG13	1.95	0.47
1:A:1393:TRP:HZ3	1:A:1408:PHE:HB3	1.79	0.47
1:A:1058:SER:OG	1:A:1059:CYS:N	2.47	0.47
1:C:204:ASP:O	1:C:208:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:GLU:HG2	1:C:500:VAL:HA	1.96	0.47
1:C:1419:TYR:HB2	1:C:1451:GLY:HA2	1.95	0.47
1:C:2220:GLN:HE21	1:C:2244:SER:CB	2.26	0.47
1:A:1341:GLY:O	1:A:1434:TRP:NE1	2.48	0.47
1:A:2295:ASN:N	1:A:2298:THR:OG1	2.44	0.47
2:B:168:GLN:HG3	2:B:172:LYS:HD3	1.97	0.47
1:C:208:LEU:HD21	1:C:229:LEU:HD21	1.97	0.47
1:C:998:ASP:O	1:C:1001:SER:OG	2.27	0.47
2:D:58:LEU:HG	2:D:187:ALA:HB2	1.97	0.47
2:D:168:GLN:HG3	2:D:172:LYS:HD3	1.97	0.47
1:C:2390:VAL:HA	1:C:2393:LEU:HG	1.96	0.47
1:A:1920:GLU:HG2	1:A:2021:ALA:HB1	1.97	0.47
1:C:86:CYS:HB2	1:C:138:THR:HG22	1.96	0.47
1:A:1052:SER:OG	1:A:1077:ASP:OD1	2.27	0.47
1:A:2302:CYS:SG	1:A:2303:LEU:N	2.87	0.47
1:C:1341:GLY:O	1:C:1434:TRP:NE1	2.48	0.47
1:C:2295:ASN:N	1:C:2298:THR:OG1	2.44	0.47
1:C:2453:ASN:OD1	1:C:2477:ARG:N	2.40	0.47
2:B:53:VAL:N	6:B:302:GNP:O1B	2.47	0.46
1:C:1058:SER:OG	1:C:1059:CYS:N	2.47	0.46
1:A:1339:ILE:HB	1:A:1394:ASP:HA	1.96	0.46
1:A:2499:ASN:OD1	1:A:2502:HIS:ND1	2.44	0.46
1:C:133:VAL:CG1	1:C:176:VAL:HG22	2.33	0.46
1:C:2455:VAL:HG11	1:C:2458:MET:HE3	1.97	0.46
2:D:127:LYS:O	2:D:131:ASP:N	2.48	0.46
1:A:1455:ASP:OD1	1:A:1455:ASP:N	2.46	0.46
1:A:203:LYS:C	1:A:205:TYR:N	2.70	0.46
1:A:2110:LEU:HD11	1:A:2128:VAL:HG23	1.98	0.46
2:B:58:LEU:HG	2:B:187:ALA:HB2	1.97	0.46
2:B:169:GLN:O	2:B:173:PHE:N	2.49	0.46
1:A:1909:ASN:OD1	1:A:1909:ASN:N	2.48	0.46
1:A:2124:THR:HG23	1:A:2127:GLN:H	1.79	0.46
2:B:61:ARG:HH21	2:B:190:ASN:HB2	1.81	0.46
2:D:82:LYS:O	2:D:93:LEU:N	2.47	0.46
1:A:1347:LYS:NZ	1:A:1395:PHE:O	2.42	0.46
2:D:201:VAL:HA	2:D:204:ILE:HB	1.97	0.46
1:C:566:VAL:O	1:C:569:SER:OG	2.21	0.46
1:C:1339:ILE:HB	1:C:1394:ASP:HA	1.96	0.46
1:A:2332:ILE:HD13	1:A:2335:LEU:HD13	1.98	0.46
1:A:2455:VAL:HG11	1:A:2458:MET:HE3	1.98	0.46
1:C:1441:ARG:NH1	1:C:1791:TRP:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1755:LEU:HB3	1:C:1758:HIS:HB2	1.98	0.46
1:C:1920:GLU:HG2	1:C:2021:ALA:HB1	1.97	0.46
1:C:585:ALA:O	1:C:588:SER:OG	2.34	0.45
1:C:1090:LEU:HD12	1:C:1090:LEU:HA	1.84	0.45
1:C:2169:LEU:O	1:C:2180:SER:N	2.42	0.45
2:D:61:ARG:HH21	2:D:190:ASN:HB2	1.81	0.45
2:B:201:VAL:HA	2:B:204:ILE:HB	1.97	0.45
1:C:1601:LYS:HE3	1:C:1601:LYS:HB2	1.76	0.45
1:C:2110:LEU:HD11	1:C:2128:VAL:HG23	1.98	0.45
1:C:2291:LEU:HD23	1:C:2291:LEU:HA	1.85	0.45
1:A:987:LEU:HB3	1:A:1013:LEU:HD21	1.98	0.45
1:C:2214:TRP:HE1	1:C:2280:VAL:HG12	1.81	0.45
2:D:168:GLN:O	2:D:172:LYS:N	2.44	0.45
1:A:2183:ASP:HB3	1:A:2188:GLY:H	1.81	0.45
1:C:1092:TYR:HB3	1:C:1883:PHE:CE2	2.52	0.45
1:A:990:SER:OG	1:A:991:ALA:N	2.50	0.45
1:A:1755:LEU:HB3	1:A:1758:HIS:HB2	1.98	0.45
1:A:1845:GLN:HB2	1:A:1847:ARG:HD2	1.97	0.45
1:C:1377:PRO:HA	1:C:1389:VAL:HA	1.99	0.45
1:C:2183:ASP:HB3	1:C:2188:GLY:H	1.81	0.45
1:C:2220:GLN:HE22	1:C:2244:SER:CB	2.30	0.45
1:A:320:THR:HA	1:A:323:ILE:HG22	1.98	0.45
1:A:1116:GLY:HA2	1:A:1138:LYS:HB2	1.99	0.45
1:A:1090:LEU:HD12	1:A:1090:LEU:HA	1.84	0.45
1:A:2143:ARG:HG2	1:A:2494:THR:HG22	1.99	0.45
1:A:2491:SER:O	1:A:2491:SER:OG	2.35	0.45
1:C:187:LEU:HD12	1:C:187:LEU:HA	1.83	0.45
1:C:987:LEU:HB3	1:C:1013:LEU:HD21	1.98	0.45
1:C:1034:LEU:HD13	1:C:1037:LEU:HD11	1.99	0.45
1:C:2248:LEU:HD23	1:C:2263:LEU:HD21	1.98	0.45
1:A:1034:LEU:HD13	1:A:1037:LEU:HD11	1.99	0.45
1:C:990:SER:OG	1:C:991:ALA:N	2.50	0.45
1:A:460:GLU:HB2	1:A:500:VAL:HG12	1.99	0.45
1:A:1506:ASN:O	1:A:1510:ASN:ND2	2.49	0.45
1:A:2248:LEU:HD23	1:A:2263:LEU:HD21	1.98	0.45
1:C:320:THR:HA	1:C:323:ILE:HG22	1.99	0.45
1:C:2302:CYS:SG	1:C:2304:SER:OG	2.73	0.45
1:C:985:THR:O	1:C:985:THR:OG1	2.28	0.44
1:C:1116:GLY:HA2	1:C:1138:LYS:HB2	1.99	0.44
1:C:1225:LEU:HB3	1:C:1227:PHE:HE2	1.82	0.44
1:C:2143:ARG:HG2	1:C:2494:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1942:PRO:HD2	1:A:1944:MET:HE3	1.99	0.44
1:C:1388:LEU:HD21	1:C:1390:LEU:HD23	1.99	0.44
1:C:1845:GLN:HB2	1:C:1847:ARG:HD2	1.97	0.44
1:C:1909:ASN:OD1	1:C:1909:ASN:N	2.48	0.44
1:A:1092:TYR:HB3	1:A:1883:PHE:CE2	2.52	0.44
1:A:1441:ARG:NH1	1:A:1791:TRP:O	2.49	0.44
1:A:1956:ASP:N	1:A:1956:ASP:OD1	2.50	0.44
1:C:729:LEU:HD23	1:C:733:ALA:HB3	1.99	0.44
1:C:1833:LYS:HD3	1:C:1859:LEU:HD22	1.99	0.44
2:D:53:VAL:N	6:D:302:GNP:O1B	2.47	0.44
1:A:285:ILE:HG23	1:A:291:VAL:HG11	1.99	0.44
1:A:1225:LEU:HB3	1:A:1227:PHE:HE2	1.82	0.44
1:C:2332:ILE:HD13	1:C:2335:LEU:HD13	1.98	0.44
2:D:169:GLN:O	2:D:173:PHE:N	2.49	0.44
1:A:1833:LYS:HD3	1:A:1859:LEU:HD22	1.99	0.44
1:A:2214:TRP:HE1	1:A:2280:VAL:HG12	1.81	0.44
1:C:150:LEU:HA	1:C:153:LEU:HD12	1.99	0.44
1:C:285:ILE:HG23	1:C:291:VAL:HG11	1.99	0.44
1:C:295:VAL:O	1:C:299:VAL:HG23	2.18	0.44
1:C:499:PRO:HA	1:C:502:LEU:HB2	2.00	0.44
1:C:1506:ASN:O	1:C:1510:ASN:ND2	2.49	0.44
1:A:2372:VAL:HA	1:A:2388:ASP:HA	2.00	0.44
2:B:82:LYS:O	2:B:93:LEU:N	2.47	0.44
1:A:681:SER:O	1:A:685:GLU:N	2.43	0.44
1:A:1337:LEU:HD22	1:A:1392:VAL:HG12	2.00	0.44
1:A:1684:HIS:HD2	1:A:1689:GLU:HG3	1.82	0.44
1:A:2435:LEU:HD13	1:A:2447:VAL:HG22	2.00	0.44
1:C:1942:PRO:HD2	1:C:1944:MET:HE3	1.99	0.44
1:C:2219:THR:OG1	1:C:2220:GLN:N	2.51	0.44
1:C:1755:LEU:HD12	1:C:1755:LEU:HA	1.83	0.44
1:A:2272:LEU:HD23	1:A:2291:LEU:HD12	2.00	0.44
1:C:1885:LEU:HD13	1:C:1894:TYR:CZ	2.53	0.44
1:A:499:PRO:HA	1:A:502:LEU:HB2	2.00	0.43
1:A:2219:THR:OG1	1:A:2220:GLN:N	2.51	0.43
2:B:73:SER:OG	6:B:302:GNP:O1G	2.22	0.43
1:C:460:GLU:HB2	1:C:500:VAL:HG12	1.99	0.43
1:C:667:VAL:HA	1:C:671:PHE:H	1.83	0.43
1:C:809:CYS:HA	1:C:992:ASN:HA	2.00	0.43
1:C:2141:THR:OG1	1:C:2495:VAL:O	2.31	0.43
1:A:429:ASN:OD1	1:A:430:VAL:N	2.51	0.43
1:A:1701:PRO:HG2	1:A:1704:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1885:LEU:HD13	1:A:1894:TYR:CZ	2.53	0.43
1:A:2220:GLN:HE22	1:A:2244:SER:CB	2.30	0.43
1:C:1337:LEU:HD22	1:C:1392:VAL:HG12	2.00	0.43
1:C:1684:HIS:HD2	1:C:1689:GLU:HG3	1.82	0.43
1:C:1701:PRO:HG2	1:C:1704:PHE:HB2	1.99	0.43
1:A:1748:CYS:SG	1:A:1749:LEU:N	2.91	0.43
1:C:1956:ASP:OD1	1:C:1956:ASP:N	2.50	0.43
1:A:729:LEU:HD23	1:A:733:ALA:HB3	1.99	0.43
1:A:1377:PRO:HA	1:A:1389:VAL:HA	1.99	0.43
1:C:736:ASN:OD1	1:C:767:ARG:N	2.50	0.43
1:C:2125:SER:HA	1:C:2128:VAL:HG12	2.01	0.43
1:C:2435:LEU:HD13	1:C:2447:VAL:HG22	2.00	0.43
1:A:809:CYS:HA	1:A:992:ASN:HA	2.00	0.43
1:C:429:ASN:OD1	1:C:430:VAL:N	2.51	0.43
1:C:1333:ASN:ND2	1:C:1519:VAL:O	2.43	0.43
1:C:2491:SER:O	1:C:2491:SER:OG	2.35	0.43
1:A:150:LEU:HA	1:A:153:LEU:HD12	1.99	0.43
1:A:1286:ASN:HA	1:A:1322:LEU:HD12	2.00	0.43
1:C:744:LEU:HD12	1:C:744:LEU:HA	1.89	0.43
1:C:803:ILE:N	1:C:986:SER:OG	2.45	0.43
1:C:1286:ASN:HA	1:C:1322:LEU:HD12	2.00	0.43
1:A:201:GLU:HG3	1:A:202:ASN:H	1.83	0.43
1:A:998:ASP:O	1:A:1001:SER:OG	2.27	0.43
1:A:1388:LEU:HD21	1:A:1390:LEU:HD23	1.99	0.43
1:C:408:HIS:HB2	1:C:414:VAL:HG11	2.01	0.43
1:C:1748:CYS:SG	1:C:1749:LEU:N	2.91	0.43
1:C:1873:ASP:OD1	1:C:1873:ASP:N	2.52	0.43
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.85	0.43
1:A:295:VAL:O	1:A:299:VAL:HG23	2.18	0.43
1:A:667:VAL:HA	1:A:671:PHE:H	1.83	0.43
1:A:1147:ASN:OD1	1:A:1147:ASN:N	2.50	0.43
1:A:2291:LEU:HD21	1:A:2331:THR:HA	2.01	0.43
1:C:1251:HIS:HA	1:C:1274:ASP:HB3	2.00	0.43
1:C:2204:LEU:HA	1:C:2215:ILE:HA	2.01	0.43
2:D:42:LYS:HA	2:D:92:ARG:HB3	2.01	0.43
2:B:127:LYS:O	2:B:131:ASP:N	2.48	0.43
1:C:1378:ILE:HG12	1:C:1505:ILE:HD11	2.01	0.43
1:C:2372:VAL:HA	1:C:2388:ASP:HA	2.00	0.43
1:A:408:HIS:HB2	1:A:414:VAL:HG11	2.01	0.43
1:A:1237:LEU:HD12	1:A:1237:LEU:HA	1.93	0.43
1:A:2204:LEU:HA	1:A:2215:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1833:LYS:HA	1:C:1833:LYS:HD2	1.94	0.43
1:C:2272:LEU:HD23	1:C:2291:LEU:HD12	2.00	0.43
1:A:1747:TYR:CZ	1:A:1768:PRO:HD3	2.54	0.42
1:C:1092:TYR:CD1	1:C:1116:GLY:HA3	2.54	0.42
1:C:206:MET:O	1:C:207:ILE:C	2.62	0.42
1:C:1747:TYR:CZ	1:C:1768:PRO:HD3	2.54	0.42
1:A:212:LEU:HD13	1:A:251:ASN:HD22	1.83	0.42
1:A:2125:SER:HA	1:A:2128:VAL:HG12	2.01	0.42
2:B:42:LYS:HA	2:B:92:ARG:HB3	2.01	0.42
1:A:578:GLU:O	1:A:582:LEU:N	2.52	0.42
1:A:736:ASN:OD1	1:A:767:ARG:N	2.50	0.42
1:A:1026:PHE:O	1:A:1053:TYR:OH	2.28	0.42
1:A:2302:CYS:SG	1:A:2304:SER:OG	2.73	0.42
1:C:1912:THR:O	1:C:1943:ARG:NH2	2.43	0.42
1:A:1092:TYR:CD1	1:A:1116:GLY:HA3	2.54	0.42
1:A:2040:ALA:HB3	1:A:2043:VAL:HG23	2.02	0.42
1:C:2476:ASN:N	1:C:2490:GLN:O	2.52	0.42
1:A:1007:SER:HA	1:A:1010:LEU:HB2	2.01	0.42
1:A:1491:THR:OG1	1:A:1492:GLU:OE1	2.38	0.42
1:A:2476:ASN:N	1:A:2490:GLN:O	2.52	0.42
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.85	0.42
2:D:124:ILE:O	2:D:164:GLU:N	2.46	0.42
1:A:207:ILE:O	1:A:208:LEU:C	2.62	0.42
1:A:585:ALA:O	1:A:588:SER:OG	2.34	0.42
1:A:713:LEU:CD1	1:A:725:VAL:HG13	2.49	0.42
1:A:1251:HIS:HA	1:A:1274:ASP:HB3	2.00	0.42
1:C:1998:HIS:NE2	4:C:2602:ANP:O2B	2.42	0.42
1:C:2291:LEU:HD21	1:C:2331:THR:HA	2.01	0.42
1:A:212:LEU:HG	1:A:225:VAL:HG11	2.02	0.42
1:A:1601:LYS:HE3	1:A:1601:LYS:HB2	1.76	0.42
1:A:1755:LEU:HD12	1:A:1755:LEU:HA	1.83	0.42
1:C:1010:LEU:HD23	1:C:1010:LEU:HA	1.89	0.42
1:A:2429:THR:HG21	1:A:2433:HIS:HB2	2.02	0.42
1:A:220:GLU:O	1:A:224:HIS:ND1	2.38	0.42
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.85	0.42
2:B:124:ILE:O	2:B:164:GLU:N	2.46	0.42
1:C:713:LEU:CD1	1:C:725:VAL:HG13	2.49	0.42
1:C:1128:LEU:HD23	1:C:1128:LEU:HA	1.94	0.42
1:C:1843:PRO:HD2	1:C:1848:LEU:O	2.20	0.42
1:C:1931:SER:H	1:C:1931:SER:HG	1.65	0.42
1:C:2040:ALA:HB3	1:C:2043:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2146:LEU:HD23	1:A:2146:LEU:HA	1.85	0.41
1:A:2169:LEU:O	1:A:2180:SER:N	2.42	0.41
2:B:169:GLN:HA	2:B:172:LYS:HB2	2.02	0.41
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.87	0.41
1:A:1843:PRO:HD2	1:A:1848:LEU:O	2.20	0.41
1:A:2251:ASN:OD1	1:A:2251:ASN:N	2.52	0.41
1:A:2269:ASP:HA	1:A:2296:VAL:HA	2.02	0.41
1:C:171:PRO:HA	1:C:177:GLN:HE21	1.84	0.41
1:C:1007:SER:HA	1:C:1010:LEU:HB2	2.01	0.41
1:C:2167:ILE:HG13	1:C:2184:LEU:HD11	2.02	0.41
1:A:773:LYS:O	1:A:776:THR:OG1	2.37	0.41
1:A:1393:TRP:CZ3	1:A:1408:PHE:HB3	2.55	0.41
1:A:2311:GLU:OE1	1:A:2311:GLU:N	2.53	0.41
1:C:707:TYR:HA	1:C:710:ASN:HD22	1.85	0.41
1:C:1564:LEU:HD23	1:C:1564:LEU:HA	1.96	0.41
1:C:1712:LEU:HD12	1:C:1712:LEU:HA	1.89	0.41
1:C:1548:ILE:HD13	1:C:1548:ILE:HA	1.89	0.41
1:C:2251:ASN:OD1	1:C:2251:ASN:N	2.52	0.41
1:C:2269:ASP:HA	1:C:2296:VAL:HA	2.02	0.41
1:A:1378:ILE:HG12	1:A:1505:ILE:HD11	2.00	0.41
1:A:1526:CYS:HB2	1:A:1564:LEU:HG	2.02	0.41
1:A:1912:THR:O	1:A:1943:ARG:NH2	2.43	0.41
1:C:578:GLU:O	1:C:582:LEU:N	2.52	0.41
1:C:2429:THR:HG21	1:C:2433:HIS:HB2	2.02	0.41
1:A:801:ASN:C	1:A:984:ILE:HG13	2.45	0.41
1:A:1626:ILE:O	1:A:1668:LEU:N	2.53	0.41
1:A:1707:ARG:HB3	1:A:1787:LEU:HD11	2.02	0.41
1:C:252:ILE:H	1:C:252:ILE:HG13	1.69	0.41
1:A:63:PRO:HA	1:A:66:ILE:HG12	2.03	0.41
1:A:2415:LYS:HB3	1:A:2415:LYS:HE2	1.90	0.41
1:C:772:ARG:HH21	1:C:808:PHE:HE1	1.67	0.41
1:C:1491:THR:OG1	1:C:1492:GLU:OE1	2.38	0.41
1:C:2177:GLY:N	1:C:2195:ALA:O	2.54	0.41
1:C:2511:ILE:HD13	1:C:2511:ILE:HA	1.89	0.41
1:A:1015:LYS:HE3	1:A:1015:LYS:HB2	1.87	0.41
1:A:1342:ASN:HB3	1:A:1434:TRP:HE1	1.86	0.41
1:C:274:LEU:HA	1:C:274:LEU:HD23	1.85	0.41
1:A:568:SER:HB3	1:A:609:LEU:HG	2.03	0.41
1:A:1010:LEU:HD23	1:A:1010:LEU:HA	1.89	0.41
1:A:1709:ILE:HG12	1:A:1738:ILE:HD11	2.02	0.41
1:A:1894:TYR:HB2	1:A:1905:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1968:ARG:HH22	1:A:2101:CYS:HB2	1.86	0.41
1:A:2156:VAL:HG12	1:A:2168:TRP:HB2	2.02	0.41
1:A:2177:GLY:N	1:A:2195:ALA:O	2.54	0.41
2:B:152:LEU:HD12	2:B:152:LEU:HA	1.90	0.41
1:C:361:ARG:HA	1:C:367:GLN:HE22	1.86	0.41
1:C:801:ASN:C	1:C:984:ILE:HG13	2.45	0.41
1:C:815:PRO:HG3	1:C:1000:LEU:HD23	2.02	0.41
1:C:1342:ASN:HB3	1:C:1434:TRP:HE1	1.86	0.41
1:C:1526:CYS:HB2	1:C:1564:LEU:HG	2.02	0.41
1:C:1583:LEU:HD12	1:C:1600:PRO:HB3	2.03	0.41
1:C:1709:ILE:HG12	1:C:1738:ILE:HD11	2.02	0.41
1:C:2156:VAL:HG12	1:C:2168:TRP:HB2	2.02	0.41
1:C:2424:ALA:HB2	1:C:2501:PRO:HG3	2.02	0.41
1:A:422:LEU:HA	1:A:422:LEU:HD23	1.88	0.41
1:A:815:PRO:HG3	1:A:1000:LEU:HD23	2.02	0.41
1:A:2424:ALA:HB2	1:A:2501:PRO:HG3	2.02	0.41
1:C:63:PRO:HA	1:C:66:ILE:HG12	2.03	0.41
1:C:1626:ILE:O	1:C:1668:LEU:N	2.53	0.41
2:D:169:GLN:HA	2:D:172:LYS:HB2	2.02	0.41
1:A:744:LEU:HD12	1:A:744:LEU:HA	1.89	0.40
1:A:2222:GLY:HA2	1:A:2245:VAL:HG23	2.03	0.40
1:C:2311:GLU:OE1	1:C:2311:GLU:N	2.54	0.40
1:A:92:CYS:SG	1:A:95:THR:N	2.94	0.40
1:A:437:LEU:HD12	1:A:437:LEU:HA	1.88	0.40
1:A:699:PHE:HD2	1:A:843:VAL:HG21	1.87	0.40
1:A:361:ARG:HA	1:A:367:GLN:HE22	1.86	0.40
1:A:1189:PRO:O	1:A:1192:ILE:HG22	2.21	0.40
1:A:2167:ILE:HG13	1:A:2184:LEU:HD11	2.02	0.40
1:C:56:GLN:HA	1:C:61:HIS:H	1.86	0.40
1:C:92:CYS:SG	1:C:95:THR:N	2.94	0.40
1:C:135:GLY:O	1:C:138:THR:OG1	2.35	0.40
1:C:1707:ARG:HB3	1:C:1787:LEU:HD11	2.02	0.40
1:C:2151:ILE:N	1:C:2173:HIS:HB3	2.36	0.40
2:D:61:ARG:HA	2:D:61:ARG:HD2	1.92	0.40
1:A:985:THR:O	1:A:985:THR:OG1	2.28	0.40
1:A:1994:ASP:OD1	1:A:1994:ASP:N	2.53	0.40
2:B:61:ARG:HA	2:B:61:ARG:HD2	1.92	0.40
1:C:568:SER:HB3	1:C:609:LEU:HG	2.03	0.40
1:C:1189:PRO:O	1:C:1192:ILE:HG22	2.21	0.40
2:D:121:VAL:HG13	2:D:153:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2177/2527 (86%)	1966 (90%)	211 (10%)	0	100	100
1	C	2177/2527 (86%)	1968 (90%)	209 (10%)	0	100	100
2	B	169/176 (96%)	154 (91%)	15 (9%)	0	100	100
2	D	169/176 (96%)	154 (91%)	15 (9%)	0	100	100
All	All	4692/5406 (87%)	4242 (90%)	450 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1423/2281 (62%)	1422 (100%)	1 (0%)	88	89
1	C	1428/2281 (63%)	1428 (100%)	0	100	100
2	B	104/156 (67%)	104 (100%)	0	100	100
2	D	104/156 (67%)	104 (100%)	0	100	100
All	All	3059/4874 (63%)	3058 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1349	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	185	HIS
1	A	227	HIS
1	A	309	GLN
1	A	408	HIS
1	A	551	ASN
1	A	560	GLN
1	A	645	GLN
1	A	710	ASN
1	A	737	GLN
1	A	800	ASN
1	A	847	GLN
1	A	1021	ASN
1	A	1094	GLN
1	A	1139	ASN
1	A	1194	ASN
1	A	1278	ASN
1	A	1305	ASN
1	A	1510	ASN
1	A	1758	HIS
1	A	1871	ASN
1	A	1872	ASN
1	A	2008	ASN
1	A	2053	GLN
1	A	2220	GLN
1	A	2333	GLN
1	A	2353	ASN
1	A	2369	ASN
2	B	192	ASN
1	C	173	ASN
1	C	185	HIS
1	C	227	HIS
1	C	309	GLN
1	C	385	HIS
1	C	408	HIS
1	C	551	ASN
1	C	560	GLN
1	C	645	GLN
1	C	710	ASN
1	C	737	GLN
1	C	847	GLN
1	C	1021	ASN

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Mol	Chain	Res	Type
1	C	1094	GLN
1	C	1139	ASN
1	C	1194	ASN
1	C	1216	HIS
1	C	1251	HIS
1	C	1278	ASN
1	C	1305	ASN
1	C	1510	ASN
1	C	1574	HIS
1	C	1871	ASN
1	C	1872	ASN
1	C	2008	ASN
1	C	2053	GLN
1	C	2220	GLN
1	C	2333	GLN
1	C	2353	ASN
2	D	192	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDP	A	2601	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	5 (11%)
6	GNP	D	302	5	34,34,34	1.16	5 (14%)	47,54,54	0.68	1 (2%)
6	GNP	B	302	5	34,34,34	1.16	5 (14%)	47,54,54	0.68	2 (4%)
3	GDP	C	2601	-	29,30,30	1.19	3 (10%)	45,47,47	1.75	5 (11%)
4	ANP	A	2602	-	33,33,33	0.95	4 (12%)	45,52,52	0.53	0
4	ANP	C	2602	-	33,33,33	0.94	4 (12%)	45,52,52	0.53	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
3	GDP	A	2601	-	-	4/16/32/32	0/3/3/3
6	GNP	D	302	5	-	7/18/38/38	0/3/3/3
6	GNP	B	302	5	-	7/18/38/38	0/3/3/3
3	GDP	C	2601	-	-	4/16/32/32	0/3/3/3
4	ANP	A	2602	-	-	8/18/38/38	0/3/3/3
4	ANP	C	2602	-	-	8/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	302	GNP	PB-O3A	3.49	1.63	1.59
6	B	302	GNP	PB-O3A	3.44	1.63	1.59
3	C	2601	GDP	C6-N1	-2.95	1.33	1.38
3	A	2601	GDP	C5-C4	2.95	1.46	1.38
3	C	2601	GDP	C5-C4	2.93	1.46	1.38
3	A	2601	GDP	C6-N1	-2.91	1.33	1.38
6	B	302	GNP	PB-O1B	2.69	1.50	1.46
6	D	302	GNP	PB-O1B	2.67	1.50	1.46
4	A	2602	ANP	PB-O3A	-2.63	1.55	1.59
6	D	302	GNP	PG-N3B	2.59	1.70	1.63
6	B	302	GNP	PG-N3B	2.59	1.70	1.63
4	C	2602	ANP	PB-O3A	-2.57	1.55	1.59
4	A	2602	ANP	PG-O1G	2.49	1.49	1.46
4	C	2602	ANP	PG-O1G	2.47	1.49	1.46
6	B	302	GNP	PG-O1G	2.46	1.49	1.46
6	D	302	GNP	PG-O1G	2.43	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2602	ANP	PG-N3B	2.43	1.69	1.63
4	A	2602	ANP	PG-N3B	2.42	1.69	1.63
3	C	2601	GDP	C5-N7	-2.40	1.34	1.39
3	A	2601	GDP	C5-N7	-2.33	1.34	1.39
6	B	302	GNP	PB-O2B	-2.30	1.50	1.56
6	D	302	GNP	PB-O2B	-2.30	1.50	1.56
4	C	2602	ANP	PB-O1B	2.23	1.49	1.46
4	A	2602	ANP	PB-O1B	2.23	1.49	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	GDP	C5-C4-N3	-6.31	118.34	128.39
3	C	2601	GDP	C5-C4-N3	-6.24	118.46	128.39
3	A	2601	GDP	C2-N3-C4	4.97	120.85	112.30
3	C	2601	GDP	C2-N3-C4	4.92	120.78	112.30
3	A	2601	GDP	N9-C4-N3	4.46	134.86	125.95
3	C	2601	GDP	N9-C4-N3	4.42	134.78	125.95
3	C	2601	GDP	C6-C5-N7	3.22	136.15	130.29
3	A	2601	GDP	C6-C5-N7	3.20	136.12	130.29
3	A	2601	GDP	C4-C5-N7	-2.75	106.31	110.67
3	C	2601	GDP	C4-C5-N7	-2.72	106.36	110.67
6	B	302	GNP	O3G-PG-O1G	-2.28	107.74	113.45
6	D	302	GNP	O3G-PG-O1G	-2.25	107.81	113.45
6	B	302	GNP	O1B-PB-N3B	-2.01	108.82	111.77

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	GDP	C5'-O5'-PA-O3A
3	A	2601	GDP	C5'-O5'-PA-O1A
3	A	2601	GDP	C5'-O5'-PA-O2A
3	C	2601	GDP	C5'-O5'-PA-O3A
3	C	2601	GDP	C5'-O5'-PA-O1A
3	C	2601	GDP	C5'-O5'-PA-O2A
4	A	2602	ANP	PB-N3B-PG-O1G
4	A	2602	ANP	PG-N3B-PB-O1B
4	A	2602	ANP	PG-N3B-PB-O3A
4	A	2602	ANP	C5'-O5'-PA-O1A
4	A	2602	ANP	C5'-O5'-PA-O2A
4	A	2602	ANP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	C	2602	ANP	PB-N3B-PG-O1G
4	C	2602	ANP	PG-N3B-PB-O1B
4	C	2602	ANP	PG-N3B-PB-O3A
4	C	2602	ANP	C5'-O5'-PA-O1A
4	C	2602	ANP	C5'-O5'-PA-O2A
4	C	2602	ANP	C5'-O5'-PA-O3A
6	B	302	GNP	PB-N3B-PG-O1G
6	B	302	GNP	PG-N3B-PB-O1B
6	D	302	GNP	PB-N3B-PG-O1G
6	D	302	GNP	PG-N3B-PB-O1B
6	B	302	GNP	O4'-C4'-C5'-O5'
6	B	302	GNP	C3'-C4'-C5'-O5'
6	D	302	GNP	O4'-C4'-C5'-O5'
6	D	302	GNP	C3'-C4'-C5'-O5'
3	A	2601	GDP	C3'-C4'-C5'-O5'
3	C	2601	GDP	C3'-C4'-C5'-O5'
6	B	302	GNP	C5'-O5'-PA-O3A
6	B	302	GNP	C5'-O5'-PA-O1A
6	B	302	GNP	C5'-O5'-PA-O2A
6	D	302	GNP	C5'-O5'-PA-O3A
6	D	302	GNP	C5'-O5'-PA-O1A
6	D	302	GNP	C5'-O5'-PA-O2A
4	A	2602	ANP	PB-O3A-PA-O1A
4	C	2602	ANP	PB-O3A-PA-O1A
4	A	2602	ANP	PB-O3A-PA-O2A
4	C	2602	ANP	PB-O3A-PA-O2A

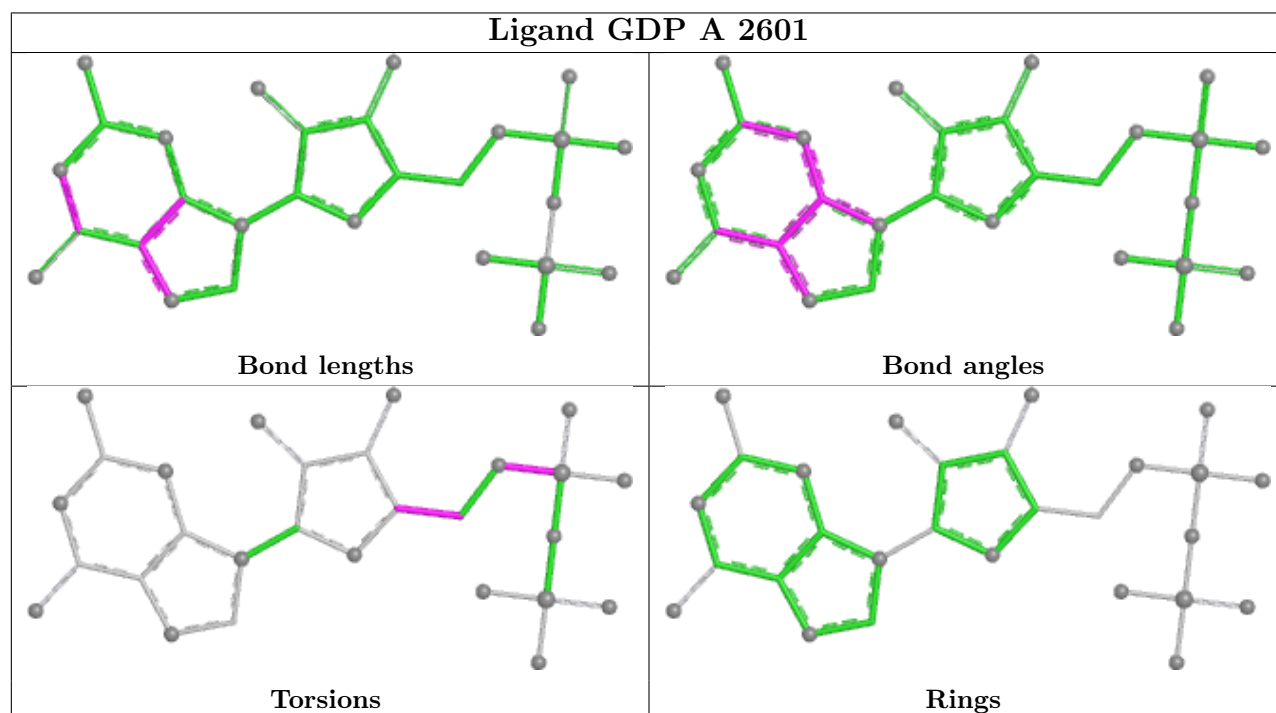
There are no ring outliers.

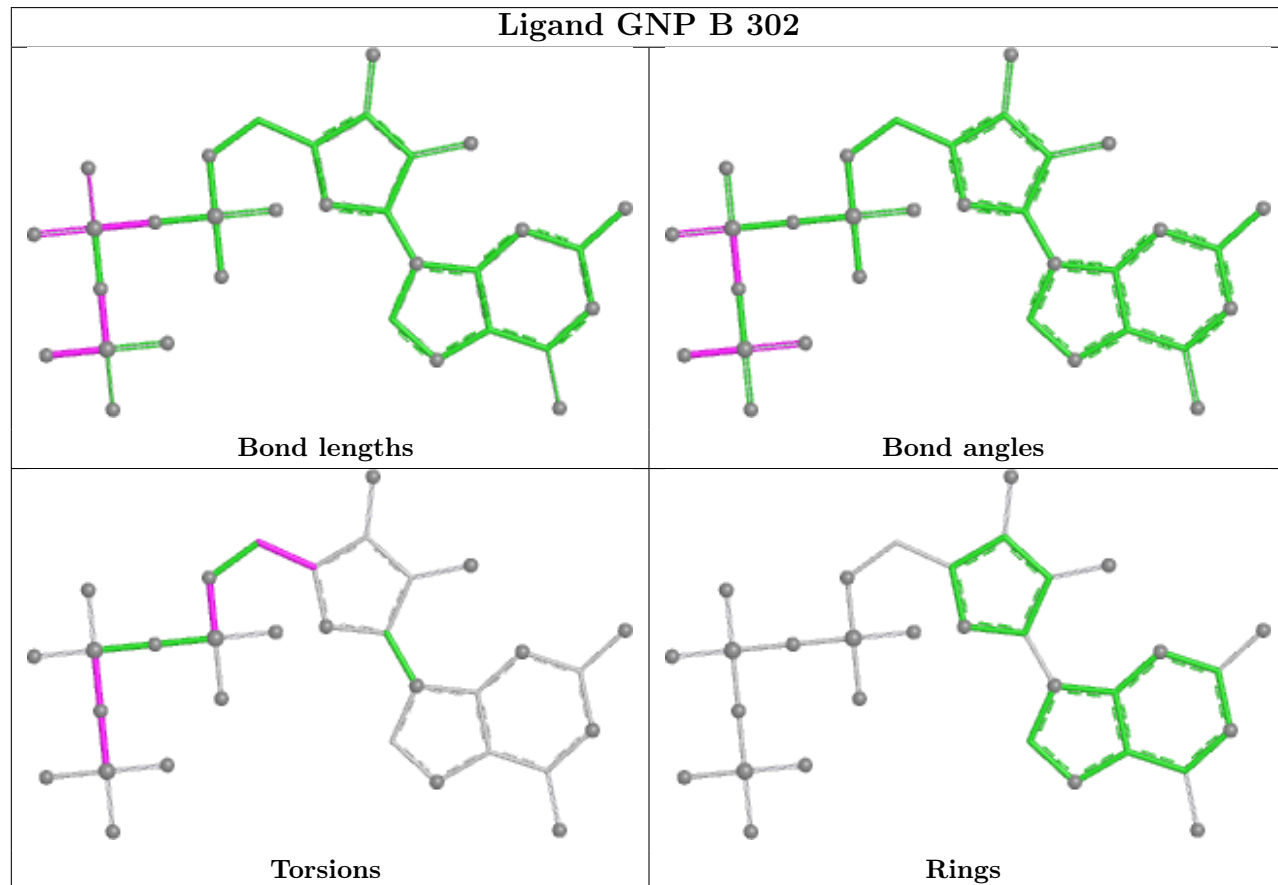
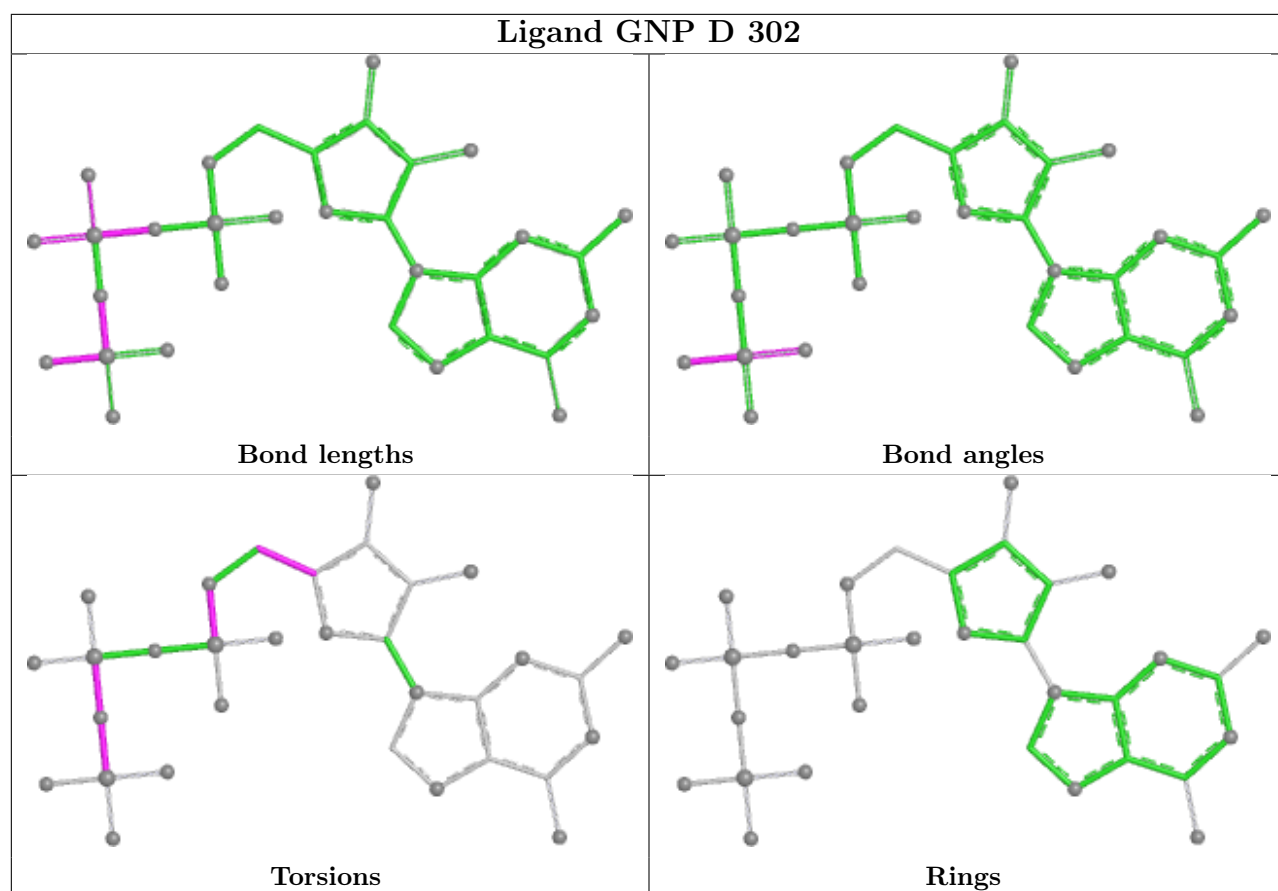
4 monomers are involved in 9 short contacts:

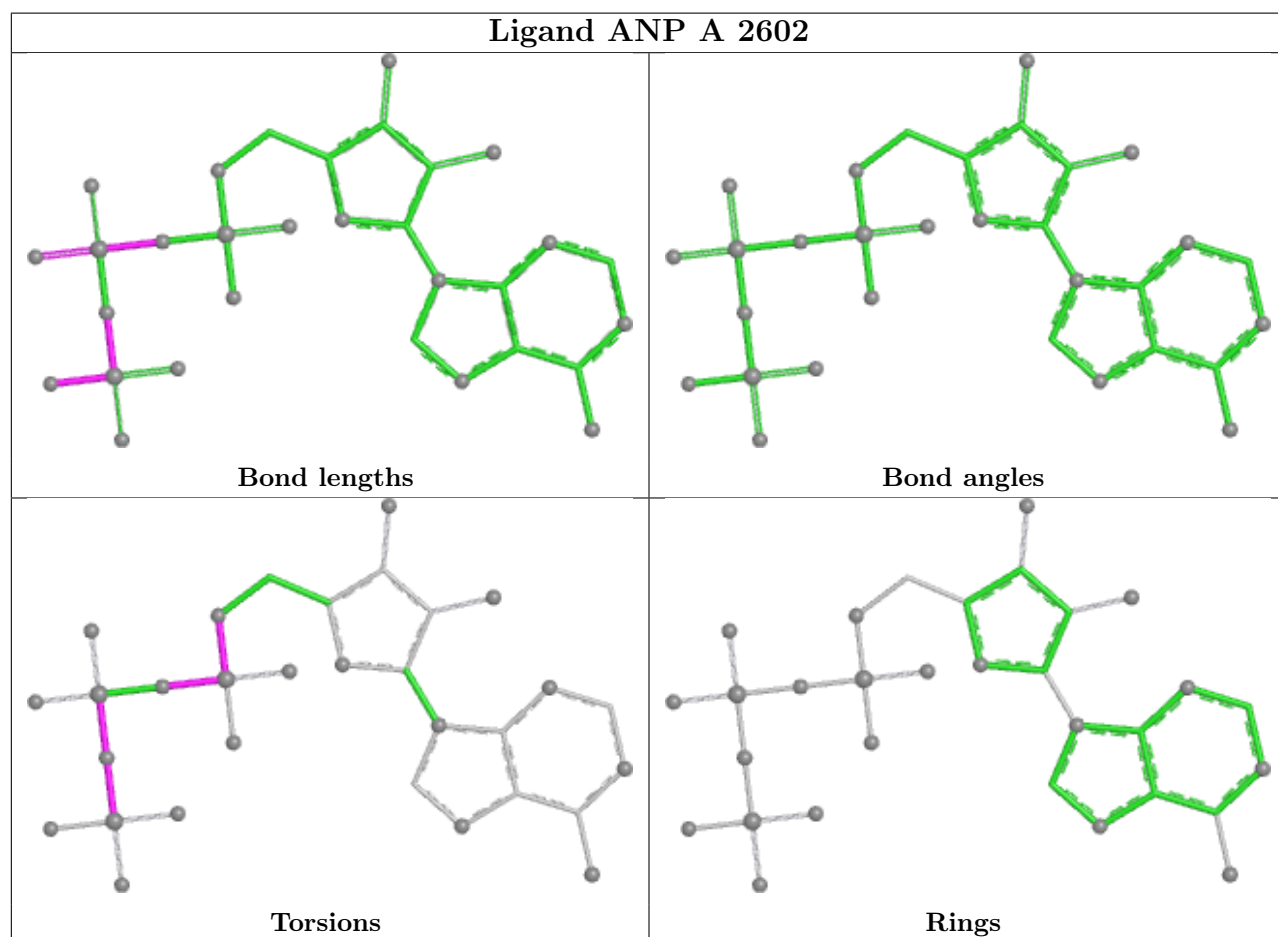
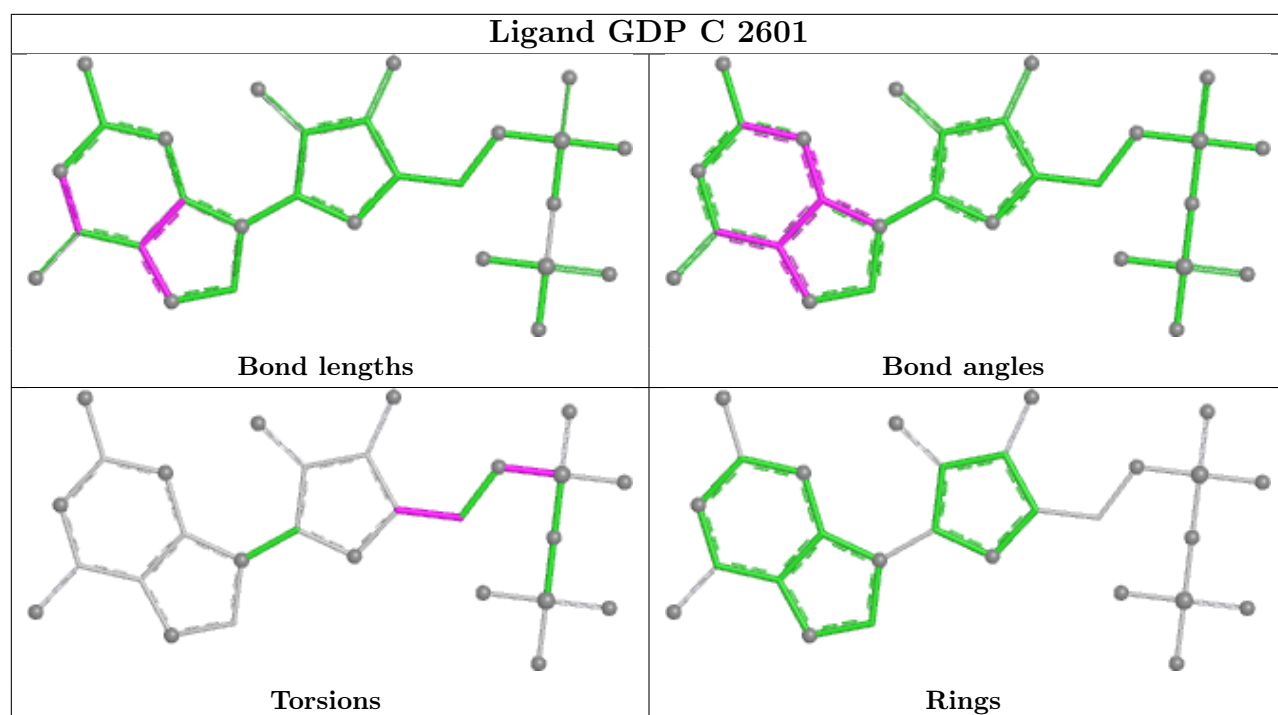
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	302	GNP	3	0
6	B	302	GNP	3	0
4	A	2602	ANP	1	0
4	C	2602	ANP	2	0

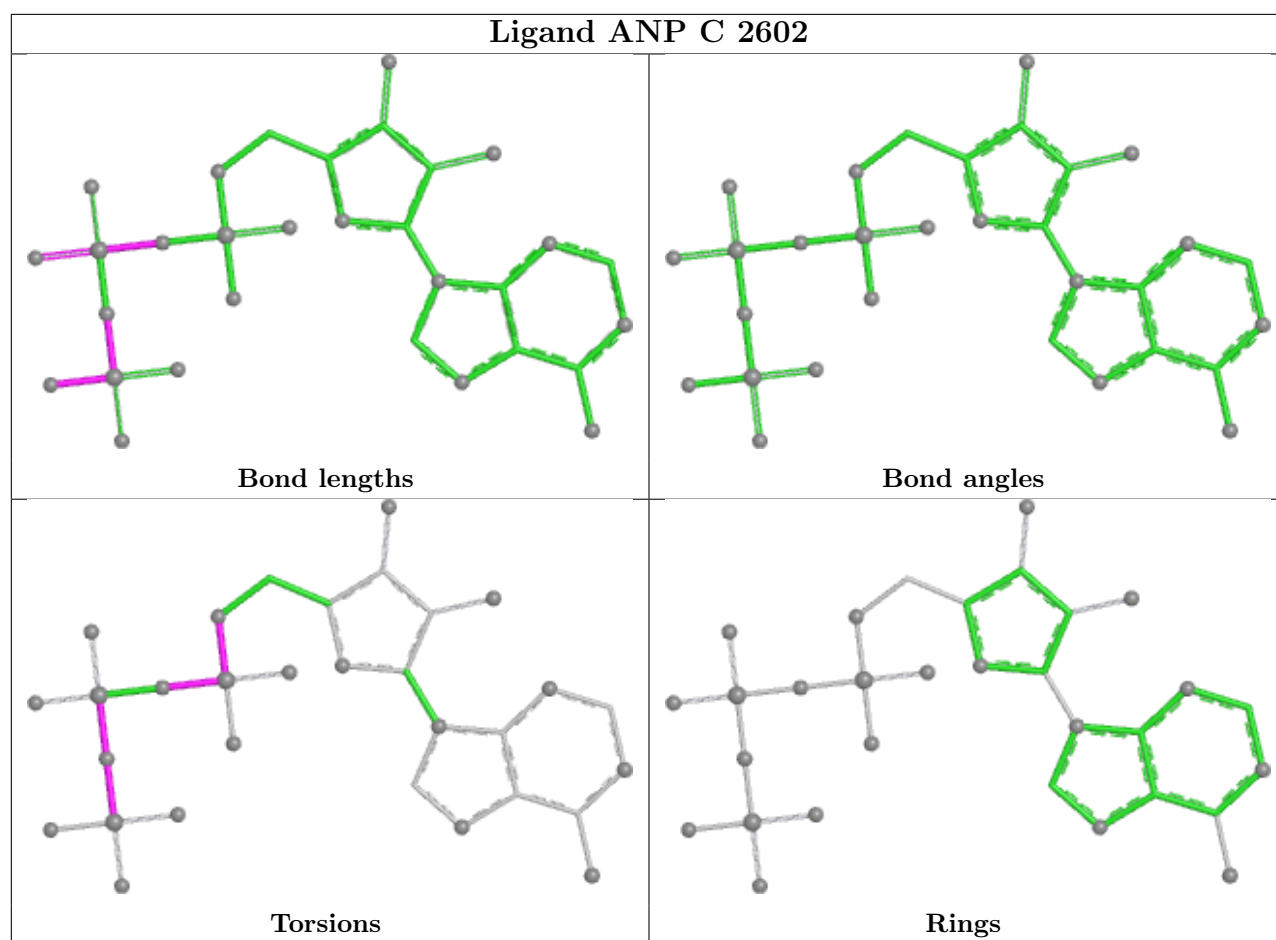
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

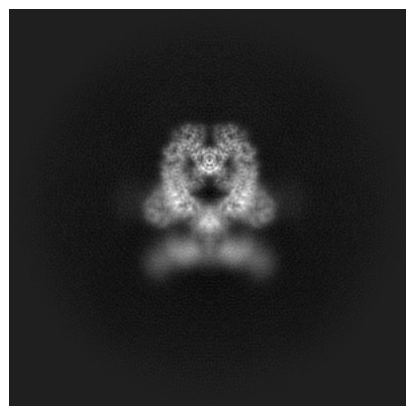
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43235. These allow visual inspection of the internal detail of the map and identification of artifacts.

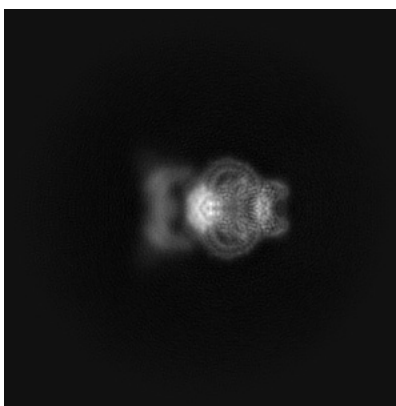
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

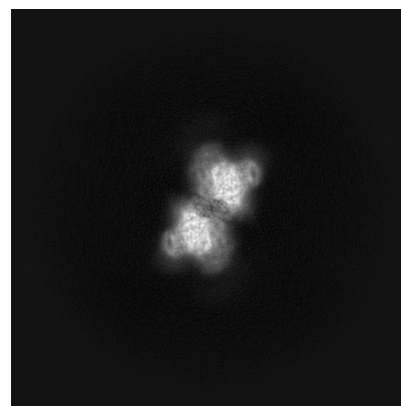
6.1.1 Primary map



X

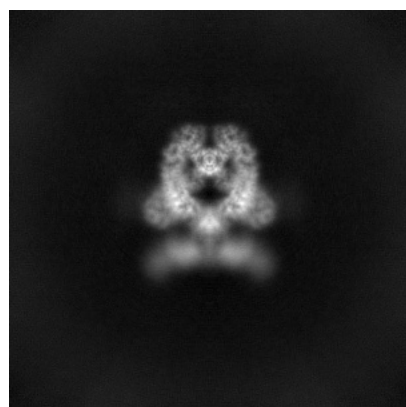


Y

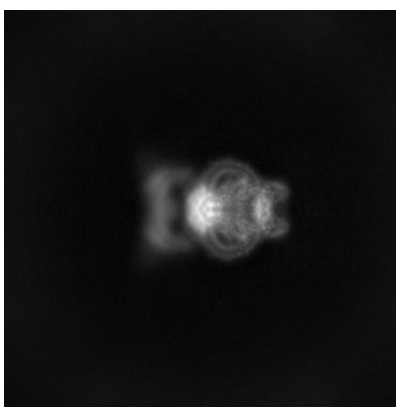


Z

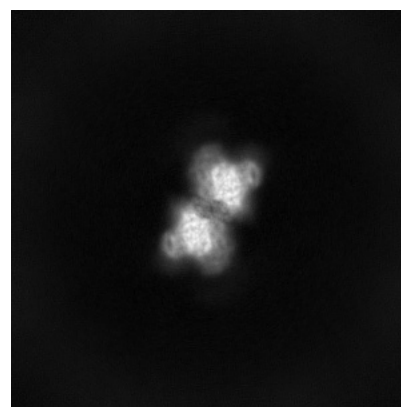
6.1.2 Raw map



X



Y

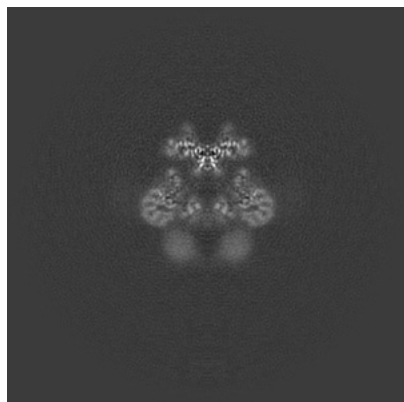


Z

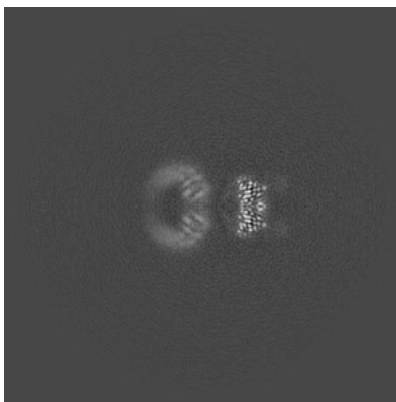
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

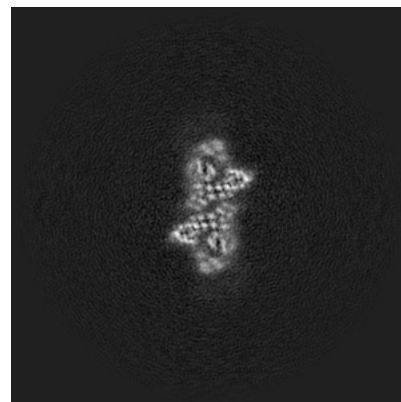
6.2.1 Primary map



X Index: 176

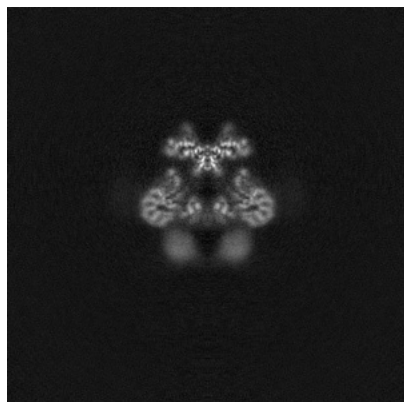


Y Index: 176

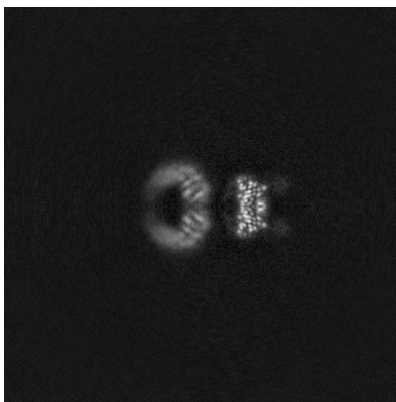


Z Index: 176

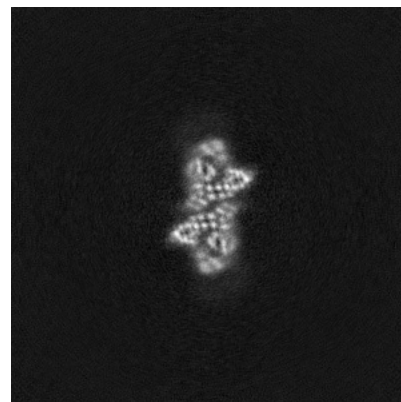
6.2.2 Raw map



X Index: 176



Y Index: 176

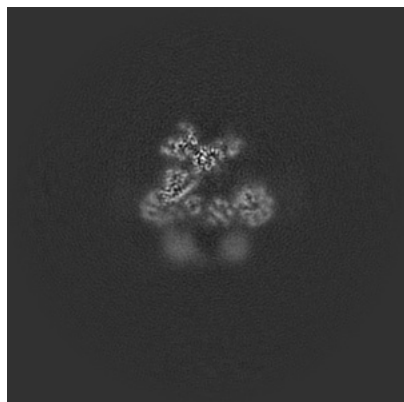


Z Index: 176

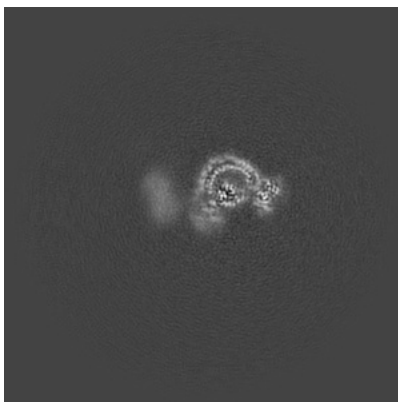
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

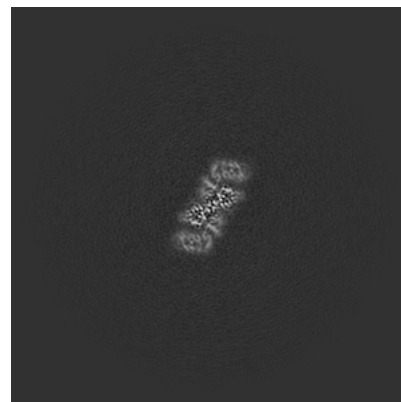
6.3.1 Primary map



X Index: 172

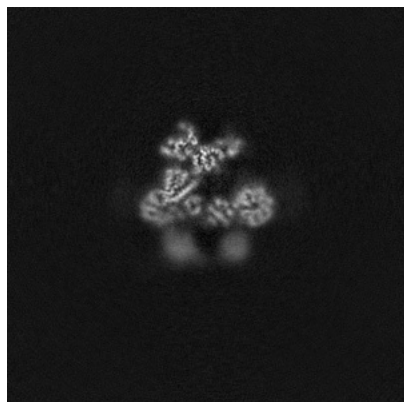


Y Index: 203

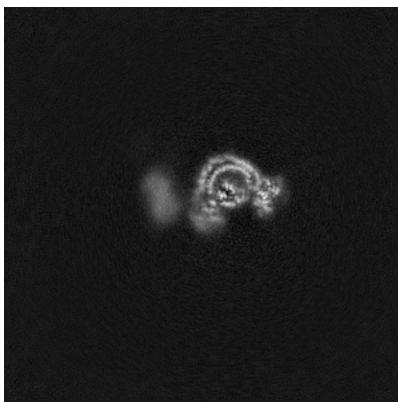


Z Index: 223

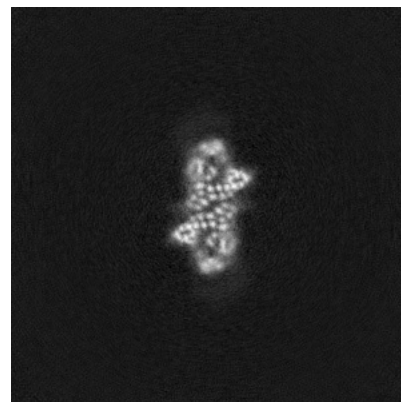
6.3.2 Raw map



X Index: 172



Y Index: 203

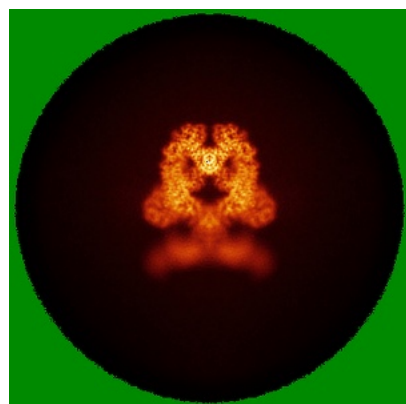


Z Index: 175

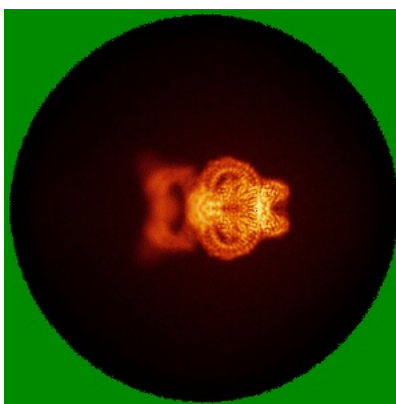
The images above show the largest variance slices of the map in three orthogonal directions.

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

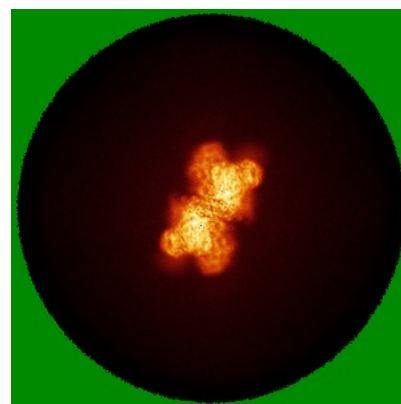
6.4.1 Primary map



X

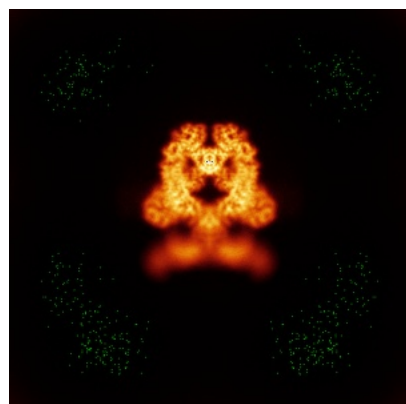


Y

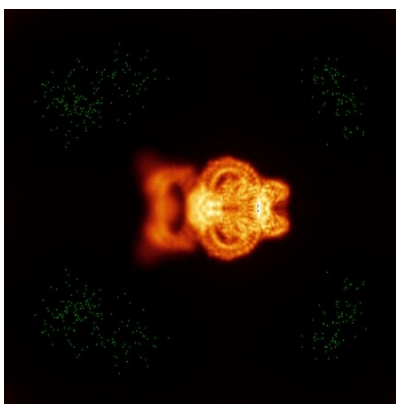


Z

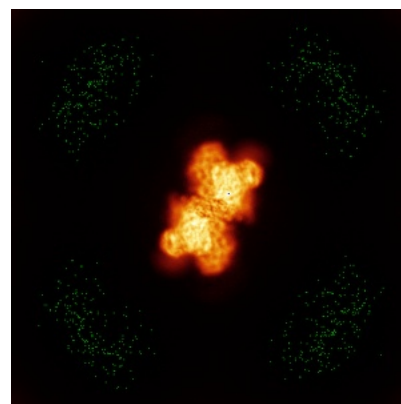
6.4.2 Raw map



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 0.5. 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.

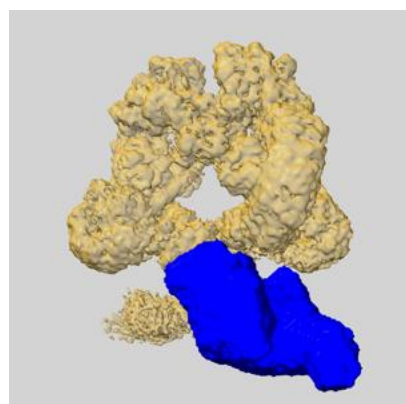
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

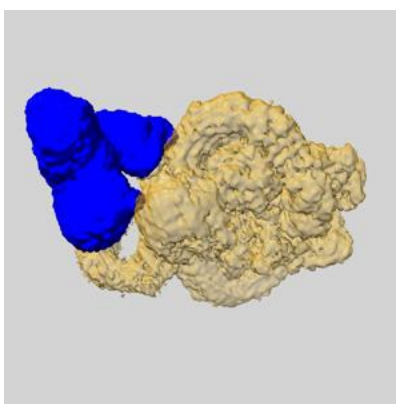
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

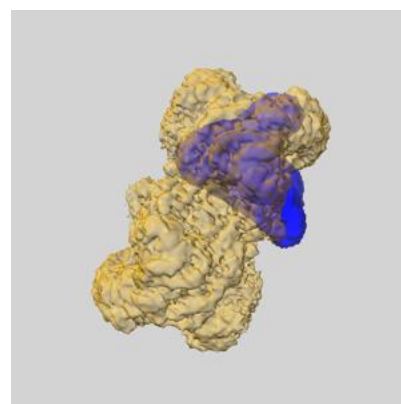
6.6.1 emd_43235_msk_1.map [i](#)



X

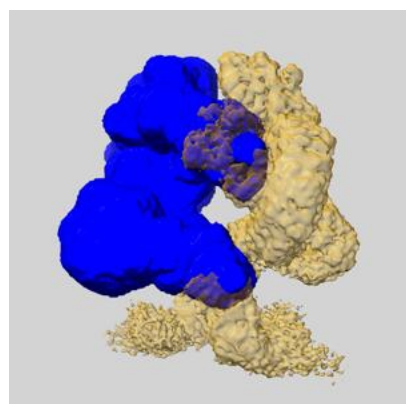


Y

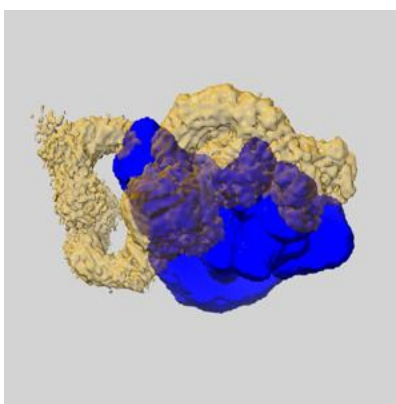


Z

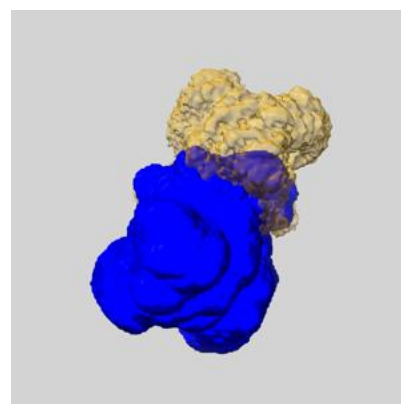
6.6.2 emd_43235_msk_2.map [i](#)



X



Y

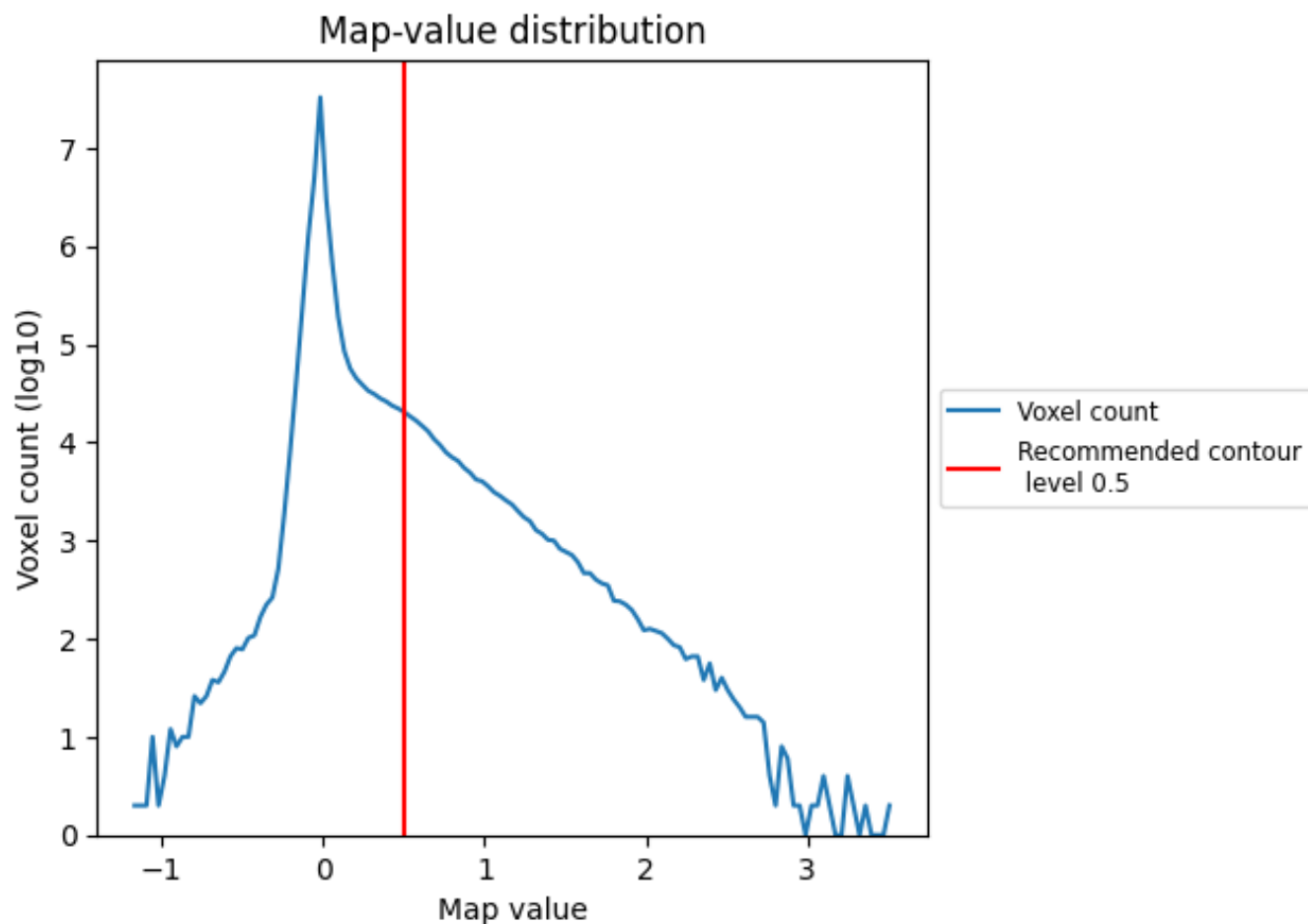


Z

7 Map analysis [i](#)

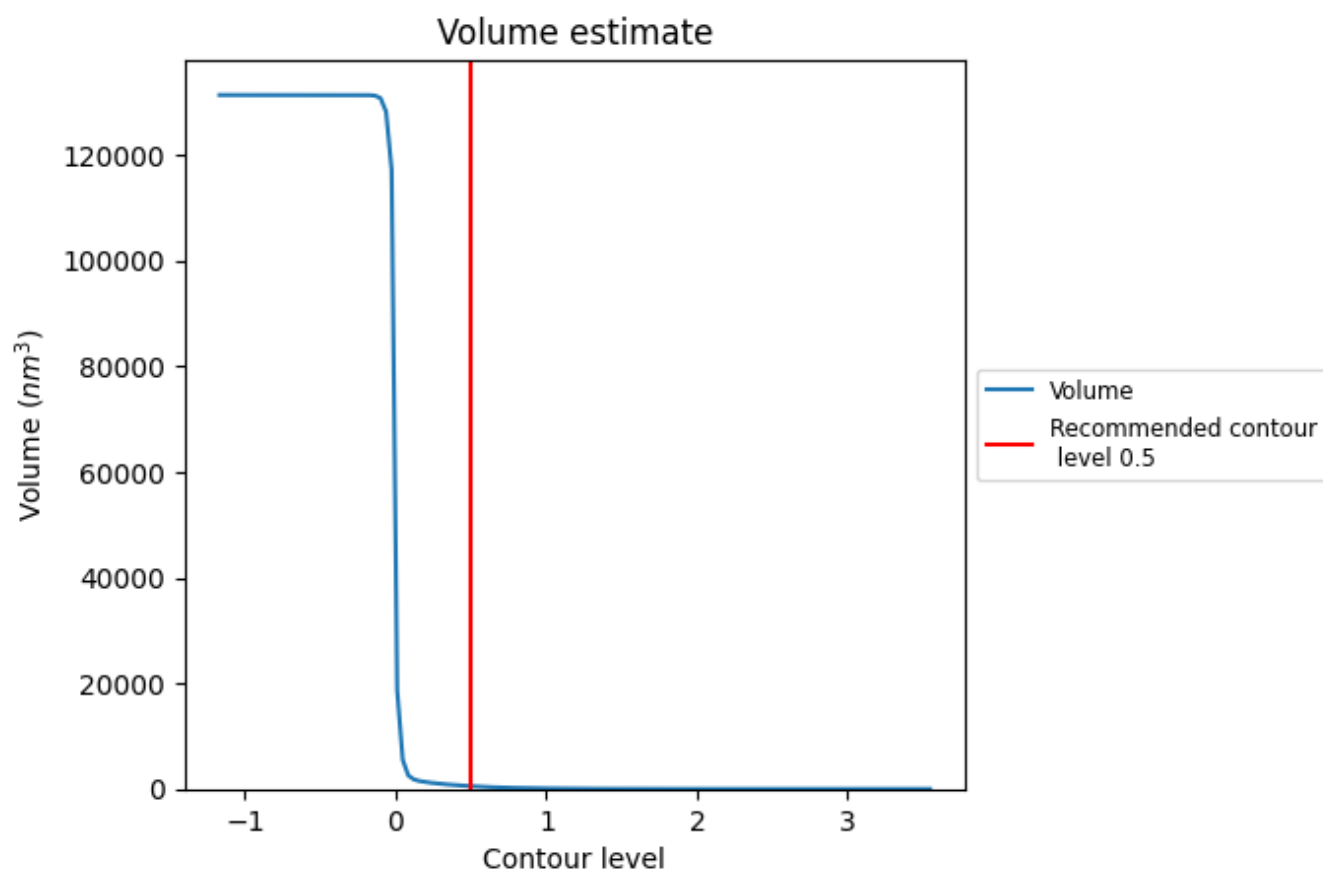
This section contains the results of statistical analysis of the map.

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.

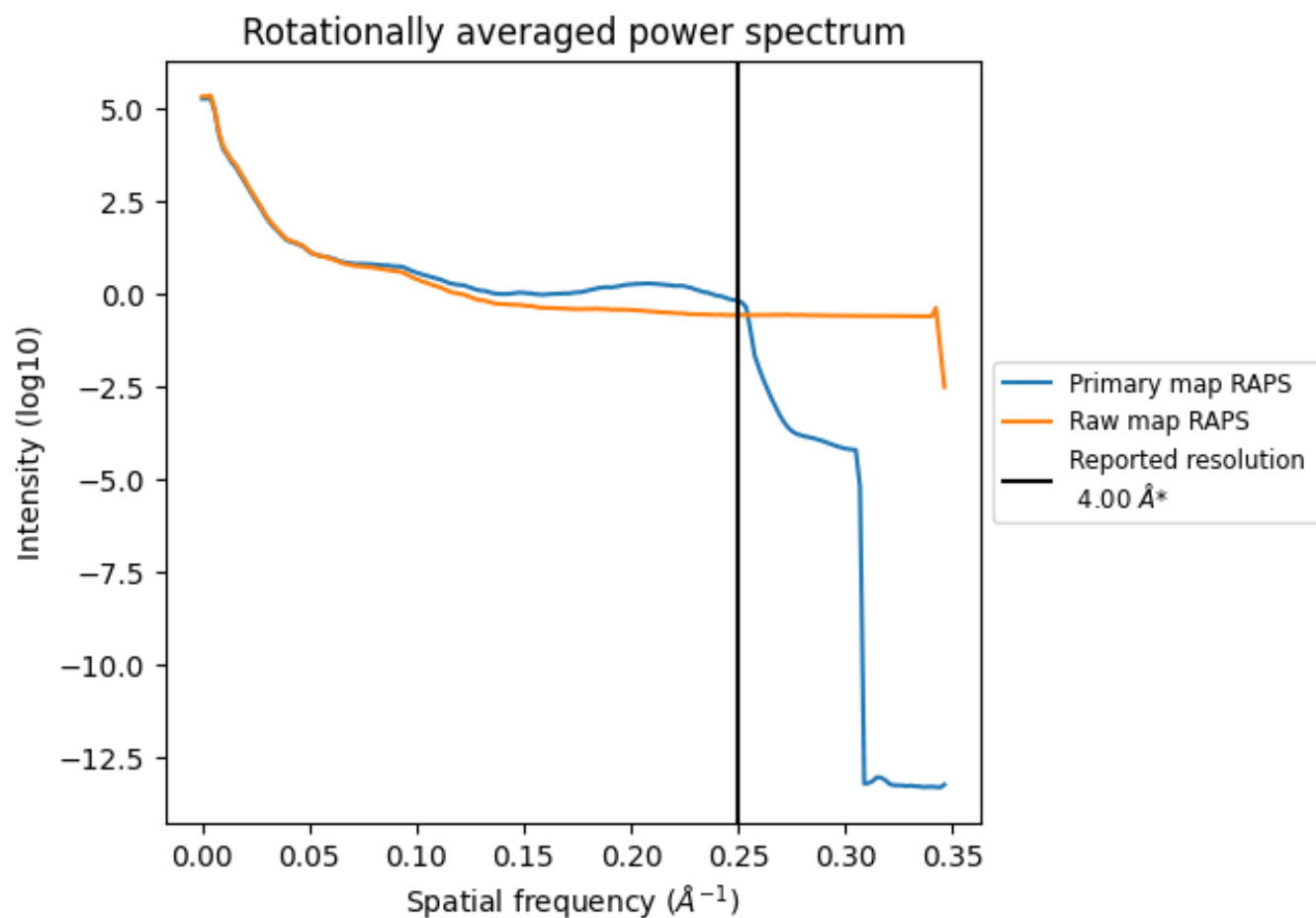
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 530 nm^3 ; this corresponds to an approximate mass of 479 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 ⓘ

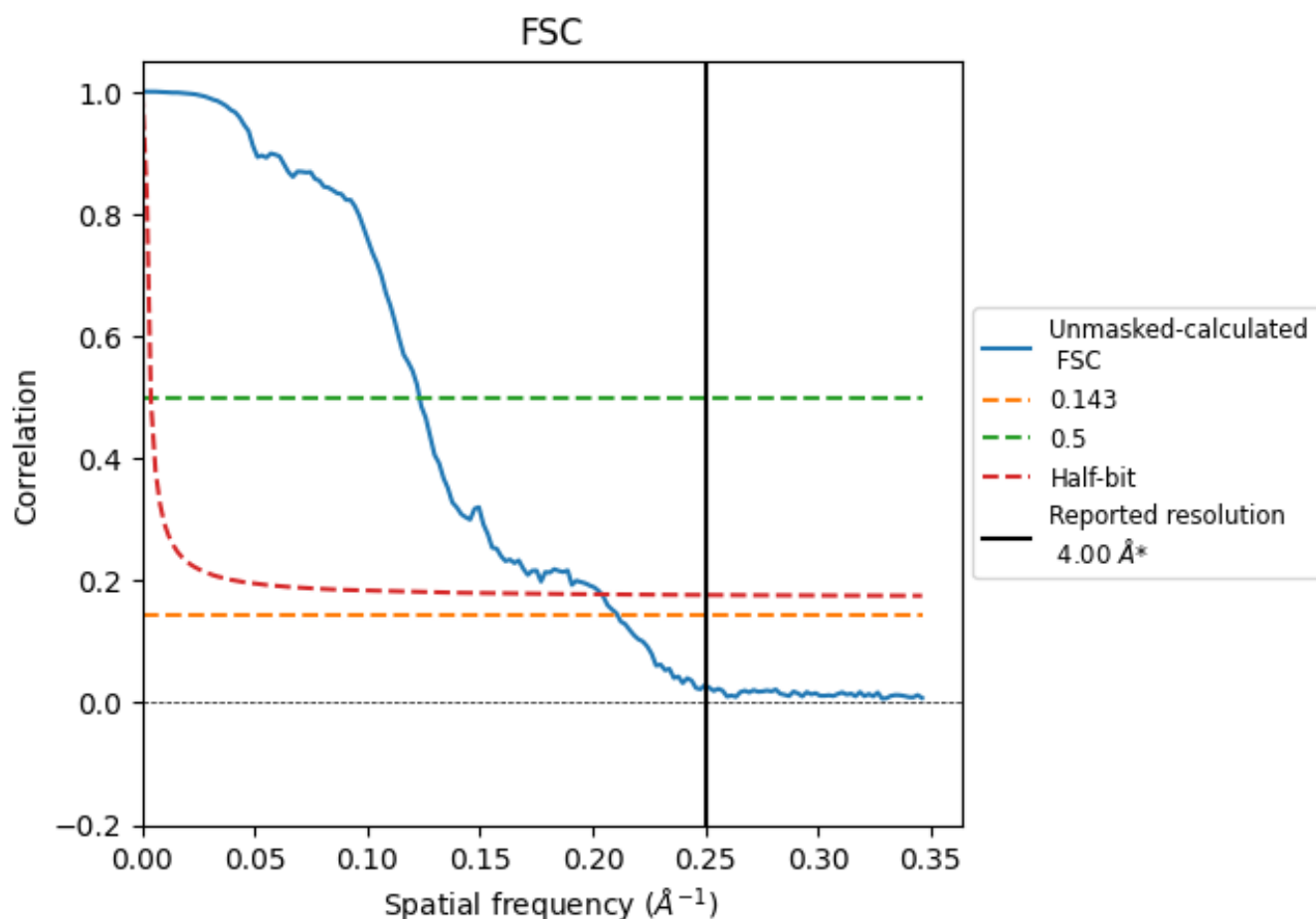


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

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 $0.250 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

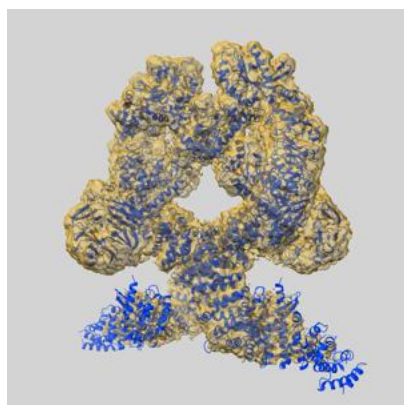
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.74	8.12	4.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.74 differs from the reported value 4.0 by more than 10 %

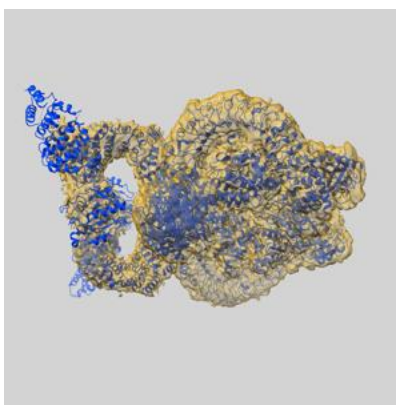
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43235 and PDB model 8VH5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

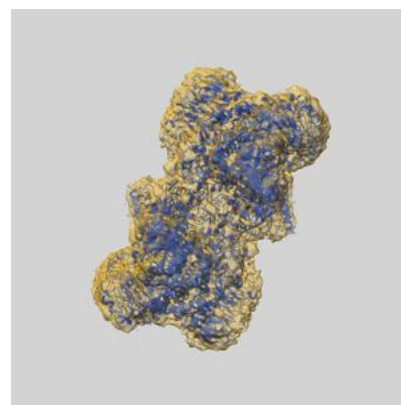
9.1 Map-model overlay [i](#)



X



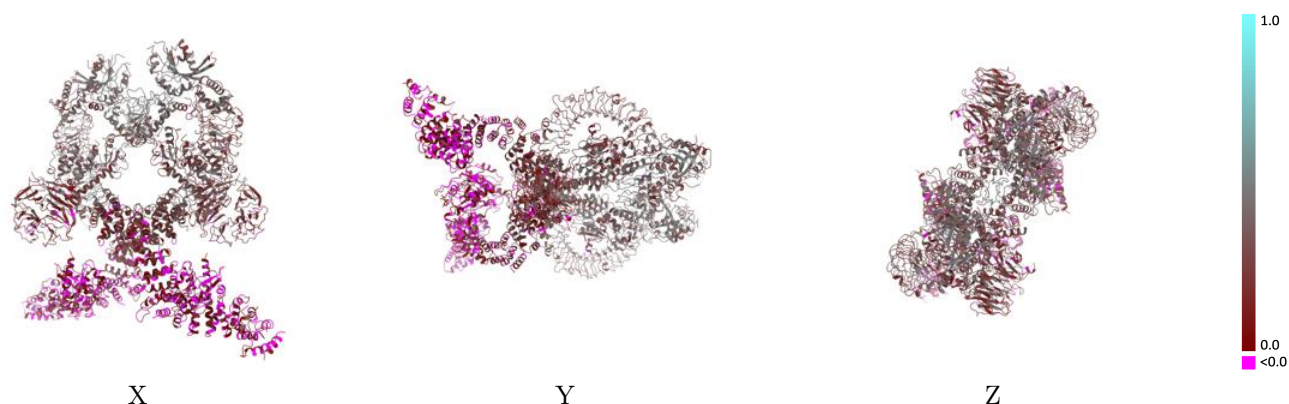
Y



Z

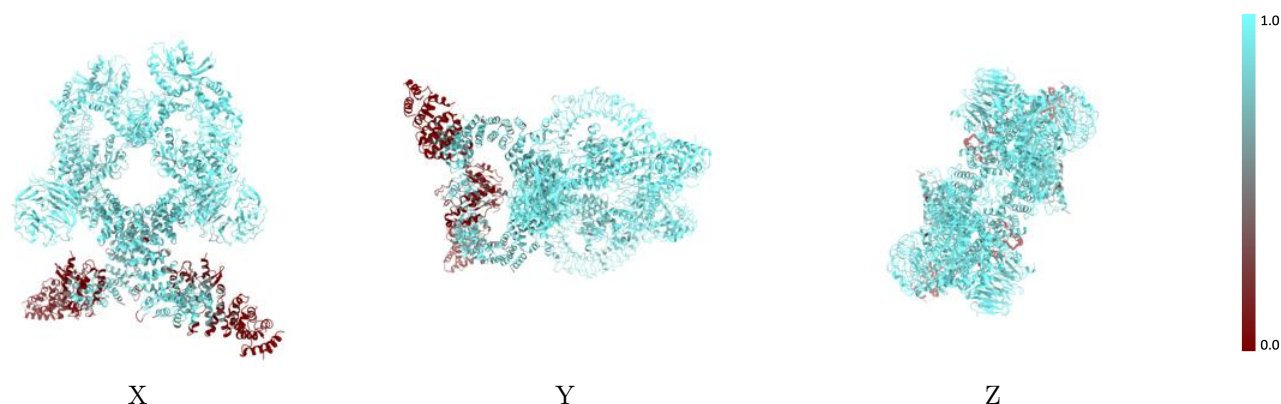
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



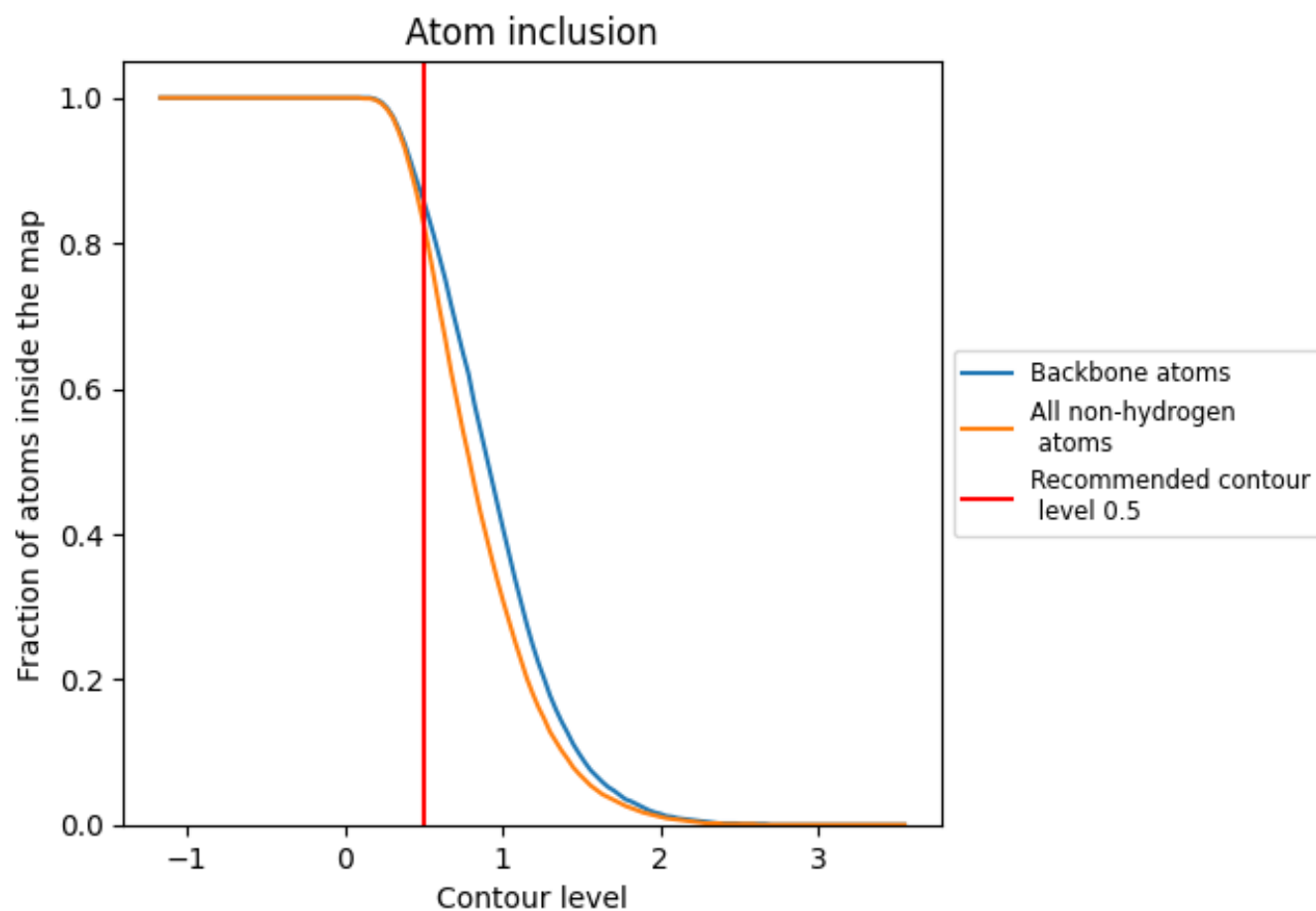
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.2480
A	0.8600	0.2600
B	0.3670	0.0350
C	0.8650	0.2690
D	0.3400	0.0440

