



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:56 AM UTC

PDB ID : 9E11 / pdb_00009e11
EMDB ID : EMD-47380
Title : Dimeric motor domains from phi-like dynein-1 bound to a Lis1 dimer under Lis1 condition
Authors : Yang, J.; Zhang, K.
Deposited on : 2024-10-21
Resolution : 2.86 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

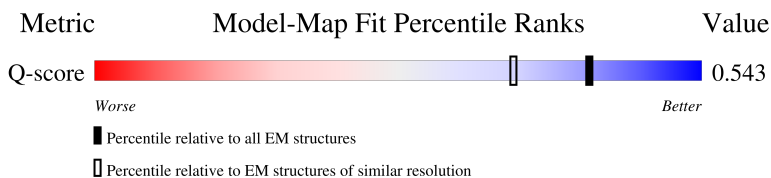
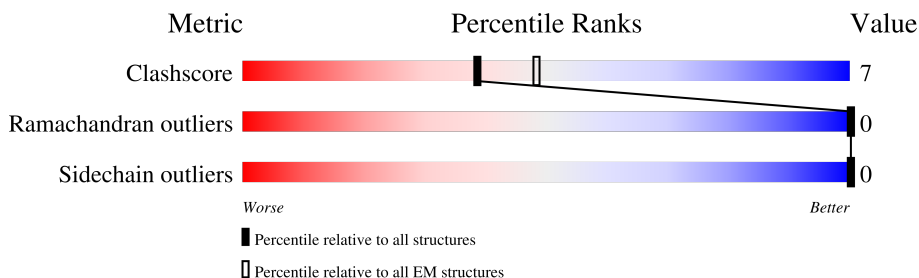
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

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	4646	 7% 51% 12% 30%
1	B	4646	 1% 52% 11% 36%
2	C	410	 1% 61% 18% 20%
2	D	410	 22% 52% 26% 22%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 52502 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.

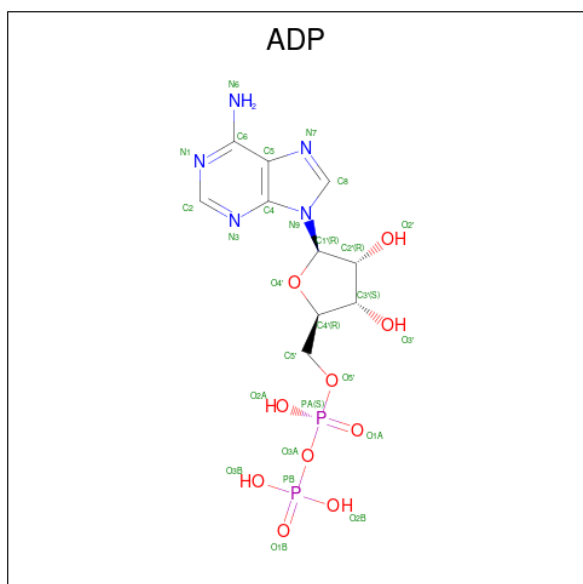
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2937	Total	C	N	O	S	0	0
			23593	15028	4070	4378	117		
1	B	2937	Total	C	N	O	S	0	0
			23593	15028	4070	4378	117		

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

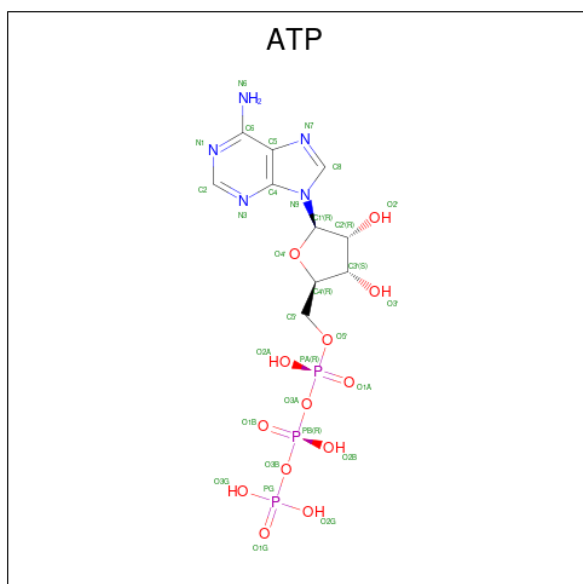
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
2	D	319	Total	C	N	O	S	0	0
			2531	1593	446	472	20		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Mg	0
			2	2	

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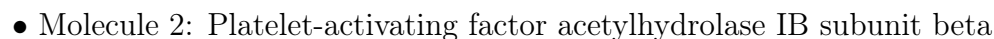
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	B	2	2	2	0

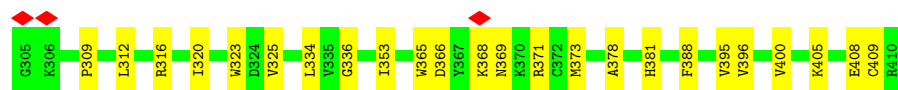
A2040	E1837	H1701	D1590	L1509	LYS	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
R2046	W1836	L1702	V1591	S1510	ASN	SER	ALA	GLU	PHE	PHE	GLN	LEU	LEU	LEU	PHE
Q2047	L1839	E1706	Q1595	K1514	GLU	THR	GLU	LYS	THR	THR	VAL	ASP	ILE	ARG	ASN
Q2051	R1843	K1707	G1596	V1515	ILE	PHE	VAL	LYS	PRO	GLN	ILE	MET	GLN	GLY	LYS
L2054	Q1850	E1708	V1597	F1516	VAL	GLN	LEU	VAL	PRO	SER	ARG	PRO	GLN	VAL	VAL
R2060	T1851	M1709	Q1598	E1517	LYS	ARG	GLN	ASP	TRP	SER	LYS	ASP	VAL	GLU	ASP
E2063	D1852	R1710	Q1599	E1518	ASP	THR	ASP	THR	TRP	TRP	LYS	GLY	ILE	ILE	ASP
A2066	T1852	V1711	R1599	D1519	VAL	LEU	GLY	ASN	TYR	TYR	ARG	PRO	TYR	LEU	LEU
I2069	Q1856	L1717	E1602	A1520	VAL	LYS	VAL	ARG	ASP	ILE	GLU	ASN	ASN	GLY	ILE
V2070	Y1872	V1721	D1606	L1521	THR	MET	TRP	PRO	ASN	ILE	LEU	LEU	PRO	VAL	VAL
P2071	D1877	W1724	L1607	S1522	GLN	LYS	SER	GLU	GLU	GLU	GLN	GLU	ARG	ARG	GLU
F2072	K1878	E1725	L1608	W1523	GLY	ILE	GLU	ALA	GLY	GLY	ASN	GLU	ILE	LEU	LYS
V2073	L1879	D1726	G1609	E1524	ASN	LEU	SER	LEU	LEU	SER	GLU	TYR	GLU	ALA	ILE
K2074	K1879	I1726	K1610	D1525	THR	GLN	LYS	GLN	TRP	THR	VAL	ALA	CYS	GLY	ASP
L2080	Q1881	F1727	I1611	K1526	LEU	VAL	VAL	ALA	GLY	ASP	THR	LYS	ARG	LEU	LEU
L2090	Q1888	G1728	Q1612	L1533	VAL	ILE	TRP	LEU	ALA	VAL	THR	LYS	TYR	ARG	GLU
R2091	C1895	A1729	E1617	F1534	ILE	GLU	GLU	THR	PHE	GLU	ALA	GLU	LEU	ALA	VAL
V2096	L1896	L1730	R1623	W1537	LYS	SER	GLN	GLY	ILE	ILE	SER	VAL	GLN	THR	SER
L2097	E1897	D1734	P1627	D1539	GLU	GLU	MET	LYS	ARG	ARG	VAL	VAL	LEU	LEU	THR
E2106	A1898	P1735	V1632	R1543	ALA	ALA	LYS	PHE	LYS	LYS	ILE	ILE	VAL	GLY	CYS
R2110	R1918	H1736	G1633	Y1546	ASP	ASP	PRO	ARG	SER	ILE	THR	VAL	GLY	GLY	ALA
R2113	N1931	I1739	D1634	L1547	TRP	HIS	TRP	LYS	ALA	ALA	THR	VAL	VAL	VAL	ASP
E2114	V1946	I1740	E1635	E1548	TRP	TRP	VAL	ASP	ILE	ILE	VAL	GLN	VAL	ALA	ASP
E2116	Q1950	V1750	D1636	E1548	LYS	GLN	GLN	ARG	GLN	GLN	GLN	TRP	VAL	LEU	LEU
R2117	R1962	I1756	I1640	D1554	ARG	LEU	PRO	CYS	VAL	VAL	LEU	ASN	VAL	PRO	ARG
E2118	E1984	E1760	K1649	T1557	LEU	LYS	ARG	ALA	ILE	ASN	ARG	GLN	GLN	ARG	MET
G2119	N1987	G1770	H1653	K1558	GLN	HIS	GLN	LYS	LYS	LYS	TRP	ASP	ASP	ASP	ASP
E2120	P1988	G1771	F1654	L1560	VAL	ASN	ASN	GLU	GLU	GLU	SER	ALA	ALA	ALA	VAL
A2121	N1989	G1772	K1655	E1564	TRP	TRP	LEU	ALA	ILE	PHE	GLN	ARG	GLN	GLN	LYS
V2122	Y1990	G1773	K1656	T1565	VAL	VAL	ASP	ASP	VAL	TRP	GLU	MET	GLN	VAL	VAL
D2123	D1991	D1774	I1665	Q1569	VAL	VAL	ALA	GLU	VAL	GLU	LYS	ALA	ALA	VAL	VAL
E2124	K1992	A1775	E1668	S1572	SER	SER	LEU	THR	GLU	GLU	GLU	GLY	GLY	VAL	SER
G2125	T1993	S1795	D1669	T1573	LEU	GLY	LEU	GLY	VAL	VAL	VAL	ILE	ILE	ILE	GLY
E2126	S1994	Q1800	N1670	L1576	THR	THR	LEU	THR	GLU	GLU	GLU	ASN	ASN	ASN	ASN
E2129	A1995	L1811	S1671	A1577	LEU	GLY	LYS	LEU	GLU	ARG	THR	ASN	GLY	GLY	GLY
R2130	E2000	E1814	R1679	L1578	LEU	ILE	THR	LEU	SER	ASN	GLY	ARG	GLY	GLY	LEU
L2131	V2006	E1814	E1683	M1579	GLN	THR	PHE	THR	ARG	GLY	GLN	GLY	THR	PRO	THR
E2133	V2006	H1817	K1687	K1580	ASP	ASP	ALA	SER	THR	LEU	GLY	LEU	GLY	LYS	LYS
Q2134	M2012	D1831	T1693	K1581	VAL	VAL	ARG	GLU	THR	ASP	LEU	ASP	GLY	ILE	ILE
I2138	R2037	S1835	T1698	S1583	GLN	GLN	ARG	GLU	LEU	LEU	LEU	ASN	GLY	LYS	LYS
L2149	L2039	F1836	E1700	L1587	GLN	GLN	THR	VAL	ASP	THR	GLY	TRP	THR	VAL	VAL
															HIS



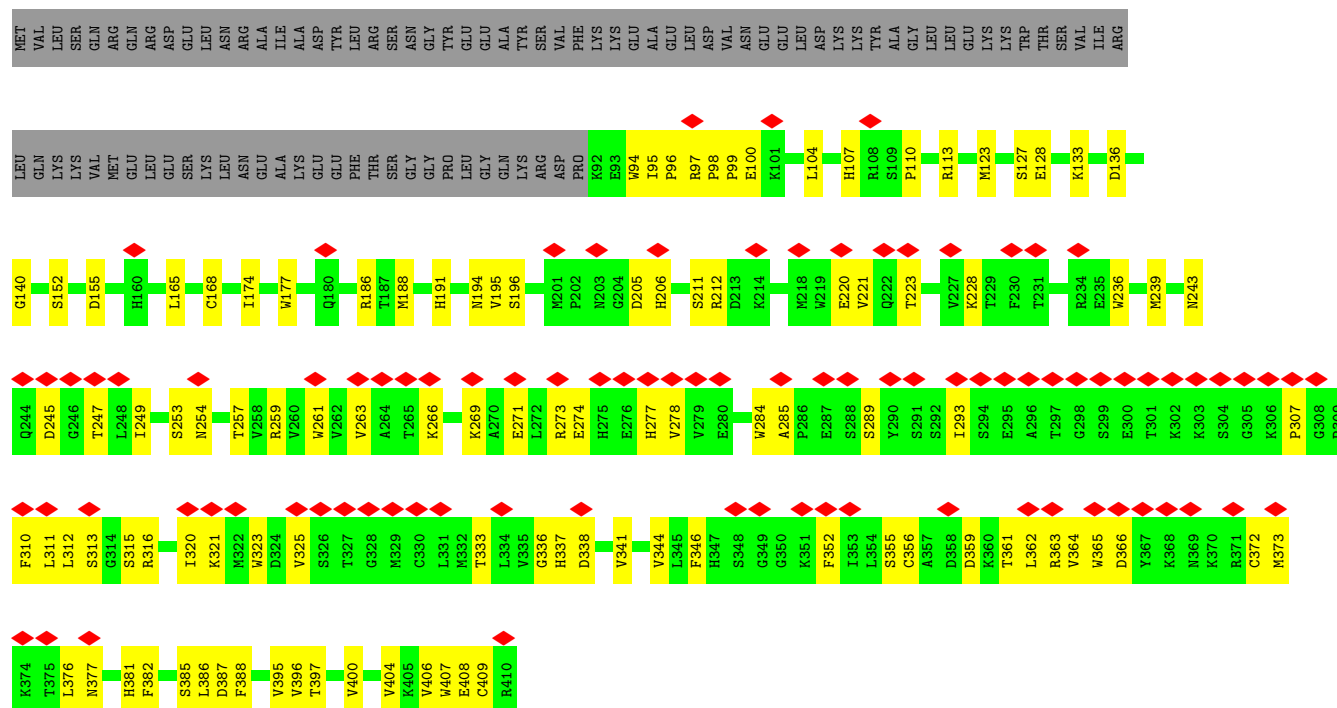








• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215049	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.214	Depositor
Minimum map value	-1.179	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	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: ATP, ADP, 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	0.11	0/24093	0.27	0/32651
1	B	0.12	0/24093	0.27	0/32651
2	C	0.13	0/2624	0.31	0/3555
2	D	0.13	0/2597	0.34	0/3518
All	All	0.12	0/53407	0.28	0/72375

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	23593	0	23659	340	0
1	B	23593	0	23657	305	0
2	C	2557	0	2487	48	0
2	D	2531	0	2463	77	0
3	A	81	0	36	0	0
3	B	81	0	36	2	0
4	A	31	0	12	2	0
4	B	31	0	12	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
All	All	52502	0	52362	767	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 7.

All (767) 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:A:4296:MET:HE3	1:A:4297:PRO:HD2	1.53	0.91
1:B:1490:TRP:HH2	1:B:1537:TRP:HD1	1.24	0.86
1:A:1565:THR:HG22	1:A:1569:GLN:HE22	1.43	0.84
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.59	0.84
1:B:2495:VAL:HG21	1:B:2524:VAL:HG21	1.65	0.79
1:A:2644:THR:HG22	1:A:2646:ASN:H	1.49	0.78
1:A:2633:LYS:HD2	1:A:3019:GLY:HA3	1.65	0.78
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.66	0.77
1:A:4055:VAL:HB	1:A:4095:MET:HE1	1.68	0.76
1:B:3989:ARG:HG3	1:B:4004:MET:HE2	1.68	0.74
2:D:257:THR:HG22	2:D:273:ARG:HB3	1.68	0.74
1:A:2452:LEU:HD13	1:A:2729:ARG:HH21	1.52	0.74
1:B:3242:LYS:NZ	1:B:3451:TYR:OH	2.20	0.73
1:B:2221:MET:HG2	1:B:2343:PHE:HB2	1.72	0.71
1:B:2257:LYS:NZ	1:B:2308:ASP:OD2	2.24	0.70
1:B:2671:MET:HE3	1:B:2675:GLY:HA2	1.74	0.69
1:A:1565:THR:O	1:A:1569:GLN:NE2	2.25	0.69
2:C:91:PRO:HA	2:C:94:TRP:HZ3	1.57	0.69
1:B:4398:LEU:HG	1:B:4417:VAL:HG11	1.73	0.69
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.72	0.69
1:B:4505:LYS:NZ	1:B:4554:ASP:O	2.21	0.69
1:A:3873:ARG:HD3	1:A:4021:MET:HE1	1.75	0.69
1:B:1490:TRP:CH2	1:B:1537:TRP:HD1	2.10	0.68
1:B:2047:GLN:NE2	1:B:2067:ASN:OD1	2.26	0.68
1:B:3178:ASP:OD2	1:B:3585:ARG:NE	2.27	0.68
1:A:3584:ASN:O	1:A:3651:ARG:NH1	2.26	0.67
2:D:396:VAL:HG12	2:D:406:VAL:HG22	1.75	0.67
1:B:2078:GLU:O	1:B:4415:ARG:NH1	2.27	0.67
1:B:2181:GLU:HG3	1:B:2244:LEU:HB2	1.77	0.67
2:D:95:ILE:HD11	2:D:352:PHE:HD2	1.60	0.67
1:A:2304:ASP:OD1	1:A:2726:ARG:NH1	2.25	0.66
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2976:LEU:HD21	1:B:3008:MET:HE1	1.76	0.66
1:B:1623:ARG:NH2	1:B:1634:ASP:OD1	2.29	0.66
1:B:4178:ARG:NH2	1:B:4297:PRO:O	2.29	0.66
1:B:1769:MET:HE3	1:B:1777:PRO:HD2	1.77	0.66
1:B:2573:ASP:OD1	1:B:2576:ARG:NH2	2.28	0.65
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.79	0.65
1:B:1965:GLU:HG2	1:B:2026:SER:HB3	1.79	0.65
1:B:4150:PRO:O	1:B:4195:ARG:NH2	2.29	0.65
1:A:4081:ASP:OD1	1:A:4112:LYS:NZ	2.26	0.65
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.29	0.65
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.30	0.65
2:D:243:ASN:HB3	2:D:284:TRP:HZ3	1.61	0.65
1:A:1612:GLN:NE2	1:A:1635:GLU:OE1	2.26	0.65
1:B:3638:VAL:HG12	1:B:3681:THR:HB	1.78	0.64
2:D:243:ASN:ND2	2:D:245:ASP:OD1	2.30	0.64
1:A:2126:GLU:OE1	1:A:2126:GLU:N	2.29	0.64
1:A:2607:SER:HA	1:A:2610:ARG:HE	1.62	0.64
1:B:2444:GLU:HG2	1:B:2510:MET:HE3	1.79	0.64
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.29	0.64
1:B:3914:ILE:O	1:B:3937:ARG:NH1	2.31	0.64
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.30	0.64
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.80	0.64
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.81	0.63
2:D:243:ASN:ND2	2:D:247:THR:OG1	2.31	0.63
1:A:1554:SER:O	1:A:1558:LYS:NZ	2.30	0.63
1:B:2452:LEU:HD13	1:B:2729:ARG:HH21	1.64	0.63
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.31	0.63
2:C:90:ASP:HB3	2:C:93:GLU:HB3	1.80	0.63
2:C:91:PRO:HA	2:C:94:TRP:CZ3	2.32	0.63
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	1.80	0.63
2:C:278:VAL:HB	2:C:316:ARG:HD2	1.80	0.63
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.80	0.63
1:A:1636:ASP:OD2	1:A:1656:LYS:NZ	2.32	0.62
1:A:4492:ILE:HG22	1:A:4507:ILE:HD13	1.82	0.62
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.80	0.62
1:B:3229:LEU:O	1:B:3233:ASN:ND2	2.31	0.62
1:B:4326:ASN:ND2	1:B:4579:ASN:O	2.31	0.62
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.81	0.62
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.65	0.62
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.33	0.62
1:A:3661:LEU:HD12	1:A:3668:ASP:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:ASP:O	1:A:1495:ASN:ND2	2.33	0.62
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.80	0.62
1:B:3481:SER:HB3	1:B:3774:LYS:HE2	1.82	0.62
1:A:3946:ASP:OD2	1:A:3950:LYS:NZ	2.33	0.61
2:C:295:GLU:OE2	2:C:368:LYS:NZ	2.33	0.61
2:D:123:MET:HG3	2:D:396:VAL:HG11	1.81	0.61
1:A:4049:TYR:OH	1:A:4191:GLN:OE1	2.18	0.61
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.33	0.61
1:B:3230:GLU:HA	1:B:3233:ASN:HD21	1.65	0.61
2:D:174:ILE:HD11	2:D:195:VAL:HG11	1.81	0.61
1:B:4492:ILE:HG13	1:B:4507:ILE:HD13	1.82	0.61
1:A:1558:LYS:HG3	1:A:1565:THR:HG21	1.83	0.60
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.82	0.60
2:D:277:HIS:CG	2:D:278:VAL:H	2.18	0.60
1:B:3983:ILE:O	1:B:3987:ILE:HD12	2.01	0.60
1:B:4037:PRO:HB2	1:B:4118:PRO:HG2	1.82	0.60
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.65	0.60
1:A:3972:TYR:OH	1:A:3976:GLU:OE2	2.18	0.60
1:B:3561:ARG:NH1	1:B:3603:GLU:OE2	2.34	0.60
1:A:4075:GLU:O	1:A:4079:GLN:HG3	2.02	0.60
2:C:101:LYS:NZ	2:C:408:GLU:OE2	2.26	0.60
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.83	0.60
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.35	0.60
1:B:2457:SER:HB3	1:B:2732:PRO:HB3	1.83	0.60
1:B:3219:ARG:HH21	1:B:3472:VAL:HG22	1.65	0.60
2:C:312:LEU:HD21	2:C:353:ILE:HD13	1.83	0.60
1:B:2592:VAL:HG23	1:B:2731:VAL:HG11	1.85	0.59
1:B:4611:LEU:HB2	1:B:4619:ILE:HD11	1.84	0.59
1:B:2138:ILE:HD12	1:B:2161:LEU:HD22	1.83	0.59
2:D:336:GLY:O	2:D:363:ARG:NH1	2.36	0.59
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.84	0.59
1:B:1537:TRP:CE3	1:B:1601:LEU:HD21	2.38	0.59
1:B:4496:ALA:HB2	1:B:4504:LEU:HD21	1.83	0.59
1:A:1897:GLU:O	1:A:1899:ARG:NH1	2.36	0.59
1:B:2987:ASN:OD1	1:B:3060:ARG:NH2	2.35	0.59
2:D:228:LYS:NZ	2:D:263:VAL:O	2.36	0.59
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.85	0.59
1:A:2386:PRO:HG3	1:A:2413:LEU:HD12	1.85	0.59
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.85	0.58
1:B:1959:GLU:HB3	1:B:1962:ARG:HD3	1.85	0.58
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.85	0.58
1:A:3892:LEU:HD11	1:A:3983:ILE:HG21	1.85	0.58
1:B:1537:TRP:HE3	1:B:1601:LEU:HD11	1.68	0.58
1:B:1484:CYS:SG	1:B:1579:MET:HG2	2.43	0.58
1:A:4110:GLU:OE1	1:A:4137:ASN:ND2	2.36	0.58
1:B:3779:GLU:OE2	1:B:3782:ARG:NH2	2.35	0.58
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	1.85	0.58
1:B:2905:LEU:HD11	1:B:3652:GLU:HB3	1.85	0.58
1:B:2925:ILE:HG21	1:B:2933:LEU:HG	1.86	0.58
1:A:2987:ASN:OD1	1:A:3060:ARG:NH2	2.31	0.58
1:B:3839:VAL:HG21	1:B:3863:LEU:HA	1.85	0.58
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.37	0.57
1:B:3219:ARG:NH2	1:B:3472:VAL:HG13	2.18	0.57
2:D:277:HIS:HD2	2:D:316:ARG:HB2	1.70	0.57
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.38	0.57
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.68	0.57
1:B:3789:ILE:HA	1:B:3792:GLN:OE1	2.05	0.57
2:D:269:LYS:NZ	2:D:325:VAL:O	2.37	0.57
1:A:1709:MET:HE3	1:A:1872:TYR:H	1.69	0.57
1:B:2488:ARG:O	1:B:2492:ARG:HG2	2.05	0.57
1:B:4176:ARG:NH1	1:B:4220:ASP:OD1	2.36	0.57
1:B:4226:THR:HG21	1:B:4239:PRO:HD3	1.86	0.57
2:C:123:MET:SD	2:C:396:VAL:HG21	2.44	0.57
1:A:1494:PHE:O	1:A:1498:LYS:HG2	2.04	0.57
1:A:1888:CYS:HA	1:A:2039:LEU:HD22	1.87	0.57
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	1.86	0.57
1:B:1620:GLU:OE2	1:B:1943:ARG:NH1	2.37	0.57
1:B:2449:LEU:HA	1:B:2453:ARG:HH21	1.69	0.57
2:C:265:THR:HG23	2:C:267:GLU:HG2	1.86	0.57
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.86	0.57
1:A:1879:LEU:HD13	1:A:1918:ALA:HB2	1.86	0.57
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.37	0.57
1:B:4096:LEU:HD13	1:B:4105:TRP:HH2	1.69	0.57
1:B:1897:GLU:O	1:B:1899:ARG:NH1	2.38	0.56
2:D:196:SER:OG	2:D:236:TRP:NE1	2.34	0.56
2:D:366:ASP:HB2	2:D:372:CYS:HB2	1.86	0.56
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.37	0.56
1:A:2472:TYR:HD2	1:A:2481:MET:HE3	1.70	0.56
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.39	0.56
1:B:1490:TRP:HH2	1:B:1537:TRP:CD1	2.14	0.56
2:D:236:TRP:HB3	2:D:254:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2581:LEU:HD21	1:B:2593:LEU:HD21	1.88	0.56
1:A:1492:ASP:OD1	1:A:1493:LEU:N	2.39	0.56
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.88	0.56
1:B:2430:ASN:O	1:B:2435:LYS:NZ	2.39	0.56
1:B:3782:ARG:NH1	1:B:3786:GLU:OE2	2.39	0.56
1:B:4387:TRP:HE3	1:B:4431:LEU:HD11	1.70	0.56
2:C:110:PRO:HB3	2:C:400:VAL:HA	1.86	0.56
2:C:388:PHE:HD1	2:C:395:VAL:HG22	1.70	0.56
1:A:2934:LEU:HD11	1:A:3068:MET:HE2	1.87	0.56
1:A:1487:ILE:HD12	1:A:1537:TRP:HE1	1.70	0.56
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.87	0.56
1:A:2538:GLU:OE2	1:A:2551:LYS:NZ	2.29	0.56
1:A:3940:CYS:O	1:A:3945:LYS:NZ	2.39	0.56
1:B:4190:ILE:HD12	1:B:4201:TRP:HZ2	1.71	0.56
2:C:353:ILE:HB	2:C:365:TRP:HB2	1.88	0.56
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.39	0.56
2:D:362:LEU:HD11	2:D:397:THR:HG21	1.88	0.56
1:A:4021:MET:HE3	1:A:4021:MET:HA	1.89	0.55
1:B:3708:LEU:HD23	1:B:3809:SER:HA	1.88	0.55
1:B:4413:PHE:CD2	1:B:4492:ILE:HG21	2.41	0.55
2:D:212:ARG:HD3	2:D:236:TRP:CG	2.41	0.55
1:B:3601:MET:HE2	1:B:3601:MET:HA	1.87	0.55
1:A:2371:THR:HG22	1:A:2451:ARG:HD2	1.89	0.55
1:A:2324:LEU:HD22	1:A:2332:ARG:HB3	1.87	0.55
1:A:4100:HIS:HB3	1:A:4128:MET:HB2	1.87	0.55
1:B:2372:ASP:OD2	1:B:2429:SER:OG	2.24	0.55
1:B:2778:THR:O	1:B:2782:GLU:HG3	2.06	0.55
1:B:2356:VAL:HG13	1:B:2361:MET:HE3	1.89	0.55
1:B:4502:LYS:H	1:B:4502:LYS:HD2	1.71	0.55
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.42	0.55
2:D:359:ASP:OD1	2:D:361:THR:OG1	2.17	0.55
1:B:3096:ASP:OD1	1:B:3097:TRP:N	2.40	0.55
2:C:320:ILE:HB	2:C:334:LEU:HB2	1.89	0.55
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	1.88	0.54
1:B:1839:LEU:O	1:B:1843:ARG:NH1	2.40	0.54
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.88	0.54
2:D:94:TRP:HB3	2:D:409:CYS:HB3	1.89	0.54
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.37	0.54
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.89	0.54
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.42	0.54
1:B:3715:GLU:HB3	1:B:3836:TYR:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3845:ASN:ND2	1:A:3862:ASP:OD2	2.33	0.54
2:C:128:GLU:HA	2:C:152:SER:HB2	1.90	0.54
1:B:2066:ALA:HA	1:B:2069:ILE:HG22	1.90	0.54
2:C:186:ARG:HD3	2:C:224:GLY:HA3	1.90	0.54
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.90	0.54
1:B:4549:GLN:HG3	1:B:4587:LEU:HB2	1.90	0.54
1:B:3099:THR:HG23	1:B:3148:VAL:HG11	1.90	0.53
2:C:216:ILE:HB	2:C:230:PHE:HB2	1.90	0.53
1:B:3214:GLN:OE1	1:B:3759:ARG:HD2	2.08	0.53
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.43	0.53
1:A:2051:GLN:HE21	1:A:2063:GLU:HG2	1.74	0.53
1:B:2684:ARG:NH1	1:B:2688:GLU:OE1	2.42	0.53
1:B:3584:ASN:O	1:B:3651:ARG:NH2	2.41	0.53
2:D:356:CYS:SG	2:D:386:LEU:HD22	2.48	0.53
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.90	0.53
1:B:2855:LEU:HD21	1:B:2863:ARG:HG3	1.88	0.53
2:D:311:LEU:HB3	2:D:323:TRP:HB2	1.91	0.53
2:C:211:SER:OG	2:C:213:ASP:OD1	2.27	0.53
2:D:110:PRO:HB3	2:D:400:VAL:HA	1.90	0.53
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.91	0.53
2:C:280:GLU:OE2	2:C:316:ARG:NE	2.37	0.53
2:D:104:LEU:N	2:D:404:VAL:O	2.41	0.53
1:A:3731:LEU:HD21	1:A:3790:VAL:HG13	1.91	0.53
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	1.91	0.53
1:B:1914:GLU:HG3	3:B:4701:ADP:H2'	1.91	0.53
1:B:3001:ASP:OD1	1:B:3002:SER:N	2.41	0.53
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.42	0.52
1:B:3174:ARG:NH1	1:B:3650:ASN:OD1	2.42	0.52
1:A:1487:ILE:HD12	1:A:1537:TRP:NE1	2.25	0.52
1:A:4153:VAL:O	1:A:4157:MET:HG3	2.09	0.52
1:B:4413:PHE:HZ	1:B:4509:VAL:HG11	1.74	0.52
1:B:4488:GLN:O	1:B:4492:ILE:HD12	2.09	0.52
2:C:123:MET:N	2:C:135:TRP:O	2.37	0.52
1:A:1470:TRP:HE1	1:A:1527:LEU:HD21	1.73	0.52
2:D:205:ASP:O	2:D:206:HIS:ND1	2.40	0.52
1:A:1467:ARG:HE	1:A:1523:TRP:HZ2	1.58	0.52
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.09	0.52
2:D:278:VAL:HB	2:D:316:ARG:HD2	1.92	0.52
1:B:1667:ASN:ND2	1:B:1672:VAL:HG12	2.24	0.52
1:B:3114:ASP:O	1:B:3140:ARG:NH2	2.43	0.52
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3008:MET:HA	1:A:3008:MET:HE2	1.92	0.52
1:B:2943:LYS:N	3:B:4704:ADP:O1B	2.41	0.52
1:B:3154:LEU:HG	1:B:3516:TYR:CD1	2.45	0.52
1:A:4039:THR:HG23	1:A:4142:GLY:HA2	1.90	0.52
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.92	0.52
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.74	0.52
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.50	0.52
1:B:3835:ILE:HG12	1:B:3870:ARG:HD2	1.92	0.52
1:A:2768:PRO:HB2	1:A:2858:PHE:HE1	1.74	0.52
1:A:4213:ARG:HB2	1:A:4213:ARG:NH1	2.24	0.52
1:B:3735:GLN:HG3	1:B:3787:THR:HG21	1.92	0.52
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.92	0.51
1:B:2433:VAL:HG22	1:B:2498:ILE:HD11	1.91	0.51
1:B:2797:ARG:O	1:B:2801:ARG:HG3	2.10	0.51
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.92	0.51
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.46	0.51
1:B:3492:THR:HA	1:B:3495:THR:HG22	1.91	0.51
1:B:3560:LEU:HD11	1:B:3743:ARG:HH22	1.75	0.51
1:B:1946:VAL:HG22	1:B:2006:VAL:HG21	1.92	0.51
2:D:95:ILE:HD11	2:D:352:PHE:CD2	2.44	0.51
1:B:2481:MET:HE3	1:B:2485:GLN:HG2	1.92	0.51
1:A:1709:MET:CE	1:A:1872:TYR:H	2.24	0.51
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.92	0.51
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.93	0.51
1:B:1561:LEU:HB3	1:B:1564:GLU:HB2	1.92	0.51
1:B:3548:ALA:HB3	1:B:3551:GLU:HG2	1.93	0.51
1:B:3623:LEU:O	1:B:3627:LEU:HG	2.10	0.51
1:A:2626:THR:HB	1:A:2669:PRO:HG3	1.92	0.51
1:A:3459:GLN:O	1:A:3462:LYS:HG2	2.10	0.51
2:D:361:THR:HA	2:D:377:ASN:HA	1.92	0.51
2:C:220:GLU:OE1	2:C:223:THR:OG1	2.27	0.51
1:B:1958:ASP:HA	1:B:2017:THR:HB	1.92	0.51
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.19	0.51
1:A:4463:SER:HG	1:A:4464:TRP:CD1	2.29	0.51
2:D:127:SER:OG	2:D:128:GLU:N	2.44	0.51
1:A:2172:ARG:HH22	1:A:2205:GLU:HG3	1.75	0.50
1:B:2231:SER:HA	1:B:2234:TRP:CD1	2.46	0.50
1:B:2967:TYR:OH	1:B:2975:ASP:OD2	2.28	0.50
1:B:3876:LEU:HD23	1:B:4146:VAL:HG11	1.93	0.50
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.93	0.50
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3970:VAL:HB	1:B:3989:ARG:HH11	1.76	0.50
1:B:3072:SER:O	1:B:3076:LYS:HG3	2.12	0.50
1:B:4039:THR:HG23	1:B:4142:GLY:HA2	1.93	0.50
1:B:3817:SER:OG	1:B:4346:MET:HB3	2.11	0.50
2:D:274:GLU:HG3	2:D:323:TRP:CH2	2.47	0.50
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.93	0.50
1:B:4544:ASN:HB2	1:B:4573:ASN:HD21	1.77	0.50
2:D:257:THR:OG1	2:D:259:ARG:NH1	2.44	0.50
1:B:1460:GLU:OE2	1:B:1460:GLU:N	2.30	0.50
1:B:4318:PRO:HG2	1:B:4325:ASN:HA	1.94	0.50
2:C:274:GLU:HB2	2:C:323:TRP:HH2	1.77	0.50
1:A:2964:HIS:HA	1:A:3643:PRO:HD2	1.93	0.50
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.93	0.50
1:B:2290:SER:HB2	1:B:2295:LEU:HG	1.93	0.50
1:B:2879:LYS:HE2	2:C:336:GLY:HA2	1.94	0.50
1:A:1533:LEU:HD11	1:A:1597:VAL:HG22	1.94	0.49
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.47	0.49
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.94	0.49
2:C:90:ASP:OD1	2:C:91:PRO:HD2	2.12	0.49
1:A:1565:THR:HG22	1:A:1569:GLN:NE2	2.20	0.49
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.94	0.49
1:B:4387:TRP:HE1	1:B:4476:ILE:HD12	1.77	0.49
2:D:277:HIS:CD2	2:D:278:VAL:H	2.30	0.49
1:B:1569:GLN:O	1:B:1573:THR:HG23	2.12	0.49
2:C:254:ASN:HD22	2:C:278:VAL:HG21	1.77	0.49
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.95	0.49
1:A:2877:LEU:HD11	1:A:2884:VAL:HG23	1.93	0.49
2:D:165:LEU:HB3	2:D:177:TRP:HB2	1.94	0.49
1:A:2051:GLN:NE2	1:A:2063:GLU:HG2	2.28	0.49
1:B:4187:HIS:ND1	1:B:4252:TYR:OH	2.41	0.49
1:B:1508:LYS:HG2	1:B:1513:TYR:CZ	2.47	0.49
1:B:3110:THR:O	1:B:3140:ARG:NH1	2.45	0.49
1:B:3551:GLU:HA	1:B:3559:ARG:HH12	1.77	0.49
1:B:3981:THR:HG23	1:B:3984:GLY:H	1.76	0.49
2:C:112:THR:HG21	2:C:154:GLN:HA	1.94	0.49
2:D:321:LYS:HG2	2:D:333:THR:HG22	1.94	0.49
1:B:1543:ARG:HA	1:B:1546:TYR:CE1	2.47	0.49
1:B:1619:LEU:HD11	1:B:1638:LEU:HG	1.94	0.49
1:B:4297:PRO:HG3	1:B:4308:TRP:CD2	2.47	0.49
1:B:4381:HIS:HB2	1:B:4438:CYS:HB3	1.94	0.49
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1533:LEU:HD11	1:B:1597:VAL:HG22	1.93	0.49
1:B:3228:GLU:HA	1:B:3231:VAL:HG12	1.94	0.49
1:B:3985:GLN:O	1:B:3989:ARG:HG2	2.12	0.49
2:C:193:HIS:HD1	2:C:194:ASN:H	1.59	0.49
1:A:2822:ILE:HD11	1:A:2858:PHE:CD2	2.48	0.49
1:B:2257:LYS:HE3	1:B:2676:THR:HG21	1.94	0.49
1:B:1850:GLN:HB3	1:B:1856:GLN:HG2	1.94	0.49
2:D:206:HIS:CE1	2:D:220:GLU:HG2	2.48	0.49
2:D:243:ASN:HD21	2:D:247:THR:H	1.61	0.49
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.46	0.48
1:A:1547:LEU:HD12	1:A:1608:LEU:HD22	1.95	0.48
1:A:1795:SER:O	1:A:1800:GLN:NE2	2.30	0.48
1:A:1706:GLU:O	1:A:1710:ARG:HG3	2.14	0.48
1:A:1949:CYS:SG	1:A:2012:MET:HE3	2.53	0.48
2:C:277:HIS:ND1	2:C:316:ARG:HB2	2.28	0.48
1:A:1462:PHE:O	1:A:1466:ILE:HG12	2.13	0.48
1:A:2073:PHE:HZ	1:A:2096:VAL:HG21	1.79	0.48
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.48	0.48
1:A:2186:CYS:HA	1:A:2191:LEU:HB2	1.96	0.48
1:A:2483:ILE:O	1:A:2486:LEU:N	2.46	0.48
1:B:1627:PRO:HB3	1:B:1950:GLN:HB3	1.94	0.48
1:B:3013:ALA:HA	1:B:3088:ARG:HG3	1.94	0.48
1:B:4027:LEU:HB3	1:B:4058:LEU:HD22	1.96	0.48
1:B:4045:SER:HB3	1:B:4147:PHE:HB2	1.96	0.48
2:C:123:MET:HE2	2:C:137:TYR:HB3	1.95	0.48
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.96	0.48
1:A:2592:VAL:HG23	1:A:2731:VAL:HG11	1.96	0.48
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.96	0.48
1:A:2227:GLY:HA3	1:A:2452:LEU:HD12	1.95	0.48
1:B:3551:GLU:HA	1:B:3559:ARG:NH1	2.29	0.48
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.95	0.48
1:A:4409:LEU:HD11	1:A:4558:PHE:HE2	1.77	0.48
1:B:4543:VAL:HG11	1:B:4622:VAL:HB	1.94	0.48
1:B:2564:ALA:HB3	1:B:2567:VAL:HG23	1.95	0.48
1:B:4517:PRO:HG2	1:B:4619:ILE:HD12	1.95	0.48
1:A:2046:ARG:HG2	1:A:2090:LEU:HD13	1.96	0.47
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.46	0.47
1:B:3835:ILE:HG23	1:B:3866:VAL:HG12	1.96	0.47
1:B:3967:GLU:OE1	1:B:4000:ARG:NE	2.41	0.47
2:D:95:ILE:HG22	2:D:97:ARG:HH12	1.79	0.47
1:B:1708:GLU:HA	1:B:1711:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2943:LYS:HG2	1:B:3094:PHE:CD2	2.48	0.47
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.95	0.47
1:B:2863:ARG:HH11	1:B:2863:ARG:HG2	1.78	0.47
1:B:3129:VAL:HG21	1:B:3149:PHE:HB2	1.96	0.47
1:A:1480:TYR:OH	1:A:1548:GLU:OE2	2.23	0.47
1:A:1507:MET:O	1:A:1510:SER:OG	2.25	0.47
1:A:1582:VAL:HG13	1:A:1591:VAL:HG11	1.96	0.47
1:A:2232:MET:HG3	4:A:4702:ATP:C8	2.48	0.47
1:B:2454:CYS:HB3	1:B:2502:LEU:HD12	1.97	0.47
1:B:4052:SER:O	1:B:4056:GLU:HG2	2.14	0.47
1:B:4088:VAL:HG11	1:B:4116:LEU:HD23	1.97	0.47
1:B:4412:PHE:CZ	1:B:4520:TYR:HB2	2.50	0.47
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.80	0.47
1:B:4554:ASP:OD2	1:B:4557:SER:OG	2.29	0.47
1:A:2837:LEU:HD13	1:A:2842:GLU:HB3	1.97	0.47
1:A:2943:LYS:HE2	1:A:3067:THR:HB	1.97	0.47
1:B:2507:ARG:HH21	1:B:2509:LYS:HE3	1.79	0.47
1:B:3135:GLN:O	1:B:3137:PRO:HD3	2.14	0.47
2:D:277:HIS:CG	2:D:278:VAL:N	2.83	0.47
2:D:338:ASP:HB3	2:D:359:ASP:HB3	1.96	0.47
1:A:2423:MET:HE2	1:A:2462:LEU:HD22	1.96	0.47
1:A:2508:LEU:HD11	1:A:2576:ARG:HH22	1.79	0.47
1:A:3597:THR:HG21	1:A:3611:ARG:HH12	1.80	0.47
1:B:1459:LEU:HG	1:B:1507:MET:HG3	1.95	0.47
1:B:1475:LEU:HD13	1:B:1487:ILE:HD13	1.97	0.47
1:B:2529:ALA:HB1	1:B:2532:ILE:HD12	1.97	0.47
1:B:3738:PHE:CE1	1:B:3783:LYS:HB3	2.50	0.47
2:D:243:ASN:HB3	2:D:284:TRP:CZ3	2.47	0.47
1:A:1476:ASP:O	1:A:1487:ILE:HA	2.15	0.47
1:A:2179:ARG:HH11	1:A:2208:LEU:HD11	1.80	0.47
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.95	0.47
2:C:369:ASN:HB2	2:C:371:ARG:HG2	1.96	0.47
1:A:2759:ILE:HD12	1:A:2815:THR:HA	1.97	0.47
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.79	0.47
1:B:2538:GLU:HB3	1:B:2548:TRP:CE2	2.49	0.47
1:B:2964:HIS:H	1:B:2967:TYR:HB2	1.80	0.47
1:A:2211:TYR:O	1:A:2215:GLN:HG3	2.15	0.46
1:A:3214:GLN:O	1:A:3217:GLU:HG3	2.15	0.46
1:B:3230:GLU:HA	1:B:3233:ASN:ND2	2.30	0.46
1:A:1687:LYS:HD3	1:A:1712:THR:HG23	1.96	0.46
1:B:3753:LEU:HD21	1:B:3770:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2285:ARG:NH1	1:A:2331:GLU:OE2	2.39	0.46
1:A:4156:ASN:ND2	1:A:4188:ALA:HA	2.30	0.46
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.98	0.46
1:B:3211:THR:HG22	1:B:3479:LEU:HD21	1.97	0.46
1:B:4160:THR:HG23	1:B:4212:LEU:HD21	1.97	0.46
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.45	0.46
1:B:2784:PHE:HB2	1:B:2794:TYR:HE2	1.81	0.46
1:B:3175:HIS:HB3	1:B:3516:TYR:CE1	2.50	0.46
2:C:169:SER:HB3	2:C:171:ASP:OD1	2.15	0.46
1:A:2074:LYS:HE3	1:A:2074:LYS:HB3	1.77	0.46
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.98	0.46
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.50	0.46
1:A:4247:MET:HE1	1:A:4273:PHE:CZ	2.50	0.46
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	1.96	0.46
1:B:3214:GLN:HG2	1:B:3761:LEU:HD12	1.98	0.46
2:C:274:GLU:HB2	2:C:323:TRP:CH2	2.51	0.46
1:A:1476:ASP:HB3	1:A:1488:ARG:CZ	2.46	0.46
1:A:2897:LEU:HD11	1:A:2911:LEU:HD21	1.98	0.46
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.49	0.46
1:B:2665:GLU:HB3	1:B:2668:LEU:HD12	1.98	0.46
2:D:312:LEU:HD23	2:D:313:SER:N	2.31	0.46
1:A:3211:THR:HG22	1:A:3479:LEU:HD11	1.98	0.46
1:B:3759:ARG:NH2	1:B:3762:ASP:OD1	2.30	0.46
2:C:366:ASP:HB2	2:C:373:MET:HG3	1.97	0.46
2:D:381:HIS:CD2	2:D:382:PHE:CD2	3.04	0.46
1:B:3135:GLN:HB2	1:B:3136:PRO:HD3	1.97	0.46
2:D:136:ASP:O	2:D:140:GLY:N	2.49	0.46
2:D:289:SER:O	2:D:293:ILE:HG12	2.15	0.46
1:A:1708:GLU:HA	1:A:1711:VAL:HG22	1.98	0.46
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.81	0.46
1:A:3615:LEU:HD11	1:A:4111:LYS:HD3	1.97	0.46
1:A:4489:LEU:HD23	1:A:4492:ILE:HD11	1.98	0.46
1:B:1728:GLY:O	1:B:1729:LYS:HG3	2.16	0.46
2:D:315:SER:O	2:D:341:VAL:HG22	2.16	0.46
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.98	0.45
1:A:2091:ARG:NH1	1:A:2320:ASP:OD1	2.49	0.45
1:A:1665:ILE:HD11	1:A:1683:GLU:HB2	1.98	0.45
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.98	0.45
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.52	0.45
1:A:2190:TYR:CE2	1:A:2385:ILE:HD11	2.51	0.45
1:B:1601:LEU:HA	1:B:1601:LEU:HD23	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4544:ASN:OD1	1:B:4589:GLN:HB2	2.17	0.45
1:A:1459:LEU:HG	1:A:1507:MET:SD	2.57	0.45
1:B:2308:ASP:O	1:B:2312:VAL:HG12	2.16	0.45
1:B:2211:TYR:O	1:B:2214:THR:OG1	2.32	0.45
1:B:2270:PRO:HA	1:B:2273:ARG:HH11	1.82	0.45
1:B:3475:SER:O	1:B:3479:LEU:HD23	2.16	0.45
1:A:3787:THR:HA	1:A:3790:VAL:HG12	1.99	0.45
1:A:4052:SER:O	1:A:4056:GLU:HG3	2.17	0.45
1:B:1505:SER:HA	1:B:1508:LYS:HZ3	1.82	0.45
1:B:3662:ILE:HG23	1:B:3669:ILE:HB	1.97	0.45
1:B:4487:LYS:O	1:B:4490:GLN:HG2	2.16	0.45
2:C:252:CYS:HB2	2:C:279:VAL:HB	1.98	0.45
1:A:2189:MET:HB2	1:A:2191:LEU:HD23	1.99	0.45
1:A:4414:GLU:HA	1:A:4417:VAL:HG22	1.98	0.45
1:B:2969:GLY:HA2	1:B:3004:PHE:HE1	1.82	0.45
2:D:113:ARG:HA	2:D:385:SER:HB3	1.99	0.45
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.48	0.45
1:A:3452:ALA:HA	1:A:3455:ILE:HG12	1.98	0.45
1:A:3790:VAL:O	1:A:3793:GLU:HG2	2.17	0.45
1:A:3904:GLU:HG3	1:A:3941:LEU:HD21	1.99	0.45
2:C:200:ILE:HG12	2:C:207:ILE:HG12	1.99	0.45
1:B:2562:VAL:O	1:B:2804:ARG:NH1	2.40	0.45
1:A:2060:ARG:NH2	1:A:2129:GLU:HA	2.32	0.45
1:A:2793:ILE:O	1:A:2836:ARG:NH1	2.50	0.45
1:B:1508:LYS:NZ	1:B:1524:GLU:OE2	2.50	0.45
2:D:220:GLU:OE1	2:D:223:THR:OG1	2.25	0.45
2:D:249:ILE:O	2:D:261:TRP:N	2.34	0.45
2:D:320:ILE:HD11	2:D:337:HIS:CD2	2.52	0.45
1:A:2222:MET:HE1	1:A:2234:TRP:HB3	1.98	0.44
1:A:3194:LEU:HD12	1:A:3194:LEU:HA	1.85	0.44
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.52	0.44
1:B:1526:LYS:HE2	1:B:1589:MET:HE1	1.98	0.44
1:B:2138:ILE:HG22	1:B:2170:TYR:HB2	1.99	0.44
1:B:3881:ILE:O	1:B:3885:MET:HG2	2.16	0.44
1:A:2507:ARG:NH2	1:A:2509:LYS:HD2	2.32	0.44
1:B:2304:ASP:OD1	1:B:2684:ARG:NH2	2.51	0.44
2:D:253:SER:OG	2:D:254:ASN:N	2.49	0.44
2:D:344:VAL:HG23	2:D:355:SER:OG	2.17	0.44
1:A:3012:LEU:HD11	1:A:3066:PHE:HE2	1.82	0.44
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.99	0.44
1:B:1550:ILE:HG13	1:B:1641:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3741:ARG:NH2	1:A:3776:GLU:OE1	2.50	0.44
1:B:2906:ASP:HB2	1:B:3654:ARG:HA	1.99	0.44
1:B:3716:VAL:HB	1:B:3836:TYR:OH	2.17	0.44
2:C:309:PRO:HG2	2:C:325:VAL:HB	1.98	0.44
2:C:381:HIS:ND1	2:C:400:VAL:HB	2.32	0.44
2:D:381:HIS:CD2	2:D:382:PHE:HD2	2.35	0.44
1:A:1756:ILE:O	1:A:1760:GLU:HG2	2.18	0.44
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.53	0.44
1:A:2899:VAL:O	1:A:2903:GLU:HG3	2.17	0.44
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.99	0.44
1:B:3929:VAL:O	1:B:3932:ALA:N	2.51	0.44
1:B:4534:TRP:CD2	1:B:4594:LYS:HD3	2.52	0.44
1:B:2756:LEU:HD13	1:B:2762:LEU:O	2.18	0.44
1:B:3158:ASN:ND2	1:B:3169:MET:O	2.50	0.44
1:B:3751:GLN:O	1:B:3754:ASN:N	2.50	0.44
1:B:4401:THR:HB	1:B:4404:ASN:HB2	1.98	0.44
2:D:307:PRO:HB2	2:D:310:PHE:CZ	2.52	0.44
1:A:1476:ASP:HB3	1:A:1488:ARG:NH1	2.32	0.44
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.53	0.44
1:A:1637:LEU:O	1:A:1641:ILE:HG12	2.18	0.44
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.18	0.44
1:A:2792:TYR:OH	1:A:2842:GLU:OE1	2.32	0.44
1:A:2894:LYS:HG2	1:A:2911:LEU:HD12	2.00	0.44
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.99	0.44
1:B:2446:ILE:HD11	1:B:2714:PRO:HB3	1.99	0.44
1:A:1478:VAL:HG23	1:A:1488:ARG:NH1	2.32	0.44
1:A:1543:ARG:HB3	1:A:1608:LEU:HD13	1.99	0.44
1:A:1895:ALA:HB2	1:A:2037:ARG:HB2	1.99	0.44
1:A:3204:GLY:O	1:A:3208:ILE:HG12	2.18	0.44
1:A:3211:THR:O	1:A:3215:VAL:HG23	2.18	0.44
1:B:1606:ASP:O	1:B:1610:LYS:HG2	2.17	0.44
1:B:4179:LEU:HD12	1:B:4223:LEU:HD22	1.98	0.44
2:C:155:ASP:HB3	2:C:198:VAL:HG12	1.99	0.44
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.33	0.44
1:A:3194:LEU:HD23	1:A:3500:MET:SD	2.58	0.44
1:A:4058:LEU:HD11	1:A:4062:GLN:HE21	1.83	0.44
1:A:4168:ARG:HH21	1:A:4216:CYS:HB3	1.81	0.44
1:B:2138:ILE:HD11	1:B:2165:PHE:CG	2.53	0.44
1:B:2802:TRP:CZ2	1:B:2829:ALA:HB2	2.52	0.44
2:D:186:ARG:NH1	2:D:221:VAL:O	2.51	0.44
1:A:1814:GLU:HB2	1:A:1878:LYS:HE2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1817:HIS:CE1	1:A:1881:GLN:HG2	2.53	0.43
1:A:4423:LEU:HD12	1:A:4466:HIS:ND1	2.33	0.43
1:B:1558:LYS:HD2	1:B:1565:THR:HG21	2.00	0.43
1:B:2257:LYS:CE	1:B:2676:THR:HG21	2.48	0.43
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.18	0.43
1:A:3923:ARG:NH1	1:A:3924:ILE:O	2.51	0.43
1:B:1665:ILE:HD11	1:B:1683:GLU:HG2	2.00	0.43
1:B:1969:SER:OG	1:B:4098:ASN:ND2	2.47	0.43
1:B:2605:LEU:HD13	1:B:2709:VAL:HG11	2.00	0.43
1:A:1497:VAL:O	1:A:1501:ILE:HG12	2.18	0.43
1:A:2191:LEU:HD12	4:A:4702:ATP:C6	2.53	0.43
1:A:2654:GLN:NE2	1:A:3048:GLU:HG2	2.33	0.43
1:A:2495:VAL:HG11	1:A:2526:LEU:HD21	2.00	0.43
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.01	0.43
1:A:3948:ILE:HA	1:A:3951:VAL:HG12	2.00	0.43
1:B:1879:LEU:HD21	1:B:1914:GLU:HB3	2.01	0.43
1:B:2063:GLU:O	1:B:2067:ASN:ND2	2.51	0.43
1:B:2134:GLN:O	1:B:2138:ILE:HG12	2.18	0.43
1:B:3172:THR:HG21	1:B:3694:SER:HB3	2.00	0.43
1:B:3521:ASP:N	1:B:3521:ASP:OD1	2.49	0.43
2:D:191:HIS:CD2	2:D:211:SER:HB3	2.54	0.43
1:A:3764:ASP:O	1:A:3768:THR:HG23	2.18	0.43
1:B:2755:MET:HE2	1:B:2807:PHE:HB2	2.00	0.43
1:B:2825:TRP:CZ3	1:B:2854:ALA:HB2	2.54	0.43
1:B:3163:LYS:HE2	1:B:3163:LYS:HB3	1.92	0.43
1:B:4485:ARG:HG2	1:B:4513:GLY:HA2	2.01	0.43
1:A:1654:PHE:HE1	1:A:1702:LEU:HD21	1.84	0.43
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	2.01	0.43
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	2.00	0.43
1:B:1687:LYS:HG3	1:B:1715:LYS:HD2	2.00	0.43
1:B:2972:PHE:HZ	1:B:3008:MET:HE3	1.83	0.43
1:B:4002:LEU:O	1:B:4006:HIS:ND1	2.34	0.43
1:B:4387:TRP:HE1	1:B:4476:ILE:CD1	2.32	0.43
1:A:2980:LEU:HD21	1:A:3011:LEU:HD11	2.01	0.43
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.36	0.43
1:B:2943:LYS:HE2	1:B:3067:THR:HB	2.01	0.43
1:B:4395:LEU:HD12	1:B:4486:ILE:HG23	1.99	0.43
1:B:4516:VAL:HG12	1:B:4519:ALA:H	1.84	0.43
2:C:378:ALA:O	2:C:405:LYS:NZ	2.35	0.43
1:A:1565:THR:C	1:A:1569:GLN:HE22	2.26	0.43
1:A:3753:LEU:HD21	1:A:3770:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4098:ASN:N	1:A:4127:THR:O	2.51	0.43
1:B:1470:TRP:NE1	1:B:1527:LEU:HD21	2.34	0.43
1:B:1492:ASP:OD1	1:B:1493:LEU:N	2.51	0.43
2:C:214:LYS:HG2	2:C:235:GLU:C	2.43	0.43
2:D:98:PRO:N	2:D:99:PRO:HD2	2.34	0.43
2:D:259:ARG:HG2	2:D:271:GLU:HG3	2.01	0.43
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.37	0.43
1:A:3482:LEU:HD11	1:A:3770:LEU:HD23	2.00	0.43
1:B:3790:VAL:HA	1:B:3793:GLU:HG3	2.00	0.43
1:A:2773:MET:HG2	1:A:2825:TRP:NE1	2.29	0.43
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.53	0.43
1:A:3491:LYS:O	1:A:3495:THR:HG23	2.19	0.43
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	2.00	0.43
1:B:1741:TRP:CH2	1:B:1750:VAL:HG13	2.54	0.43
1:B:2273:ARG:HA	1:B:2273:ARG:HD2	1.81	0.43
1:B:2469:VAL:HG13	1:B:2481:MET:SD	2.59	0.43
1:B:3849:VAL:HG12	1:B:3855:ARG:HG2	2.01	0.43
2:C:236:TRP:HB3	2:C:254:ASN:OD1	2.19	0.43
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	2.00	0.42
1:A:3049:GLU:H	1:A:3049:GLU:CD	2.26	0.42
1:B:1518:GLU:HG2	1:B:1519:ASP:N	2.34	0.42
1:B:2413:LEU:O	1:B:2417:ARG:HG3	2.19	0.42
1:B:2623:SER:OG	1:B:3006:GLU:OE1	2.36	0.42
1:B:2956:LEU:HD22	1:B:2989:LYS:HB3	2.00	0.42
1:B:3114:ASP:O	1:B:3116:GLU:HG2	2.19	0.42
1:B:4246:LEU:HD23	1:B:4246:LEU:HA	1.82	0.42
1:A:2584:TRP:HZ3	1:A:2734:VAL:HB	1.84	0.42
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	2.01	0.42
1:B:2190:TYR:CE2	1:B:2385:ILE:HD11	2.53	0.42
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.34	0.42
1:A:2823:ARG:HH22	1:A:2868:SER:HB3	1.84	0.42
1:A:3973:LEU:HD23	1:A:3973:LEU:O	2.19	0.42
2:C:176:LEU:HD13	2:C:207:ILE:HD11	2.01	0.42
2:D:387:ASP:OD1	2:D:388:PHE:N	2.52	0.42
1:A:2040:ALA:HB1	1:A:4257:ASP:HB3	2.02	0.42
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.83	0.42
1:A:3451:TYR:HA	1:A:3454:LEU:HG	2.02	0.42
1:A:3627:LEU:HD12	1:A:3664:LEU:HD22	2.01	0.42
1:B:2043:LYS:HE2	1:B:2043:LYS:HB2	1.71	0.42
1:B:2837:LEU:HD13	1:B:2842:GLU:HB3	2.00	0.42
1:B:3148:VAL:O	1:B:3152:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:212:ARG:HG3	2:C:236:TRP:CG	2.55	0.42
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.92	0.42
1:A:2387:LEU:HD23	1:A:2467:ARG:CZ	2.49	0.42
1:B:1888:CYS:HA	1:B:2039:LEU:HD22	2.01	0.42
1:B:2643:ARG:HH11	1:B:2648:VAL:HG23	1.84	0.42
1:B:3483:SER:O	1:B:3486:ARG:HG2	2.18	0.42
1:B:3877:HIS:CE1	1:B:4151:PRO:HB3	2.55	0.42
2:C:193:HIS:HB3	2:C:212:ARG:HB3	2.01	0.42
1:A:1490:TRP:HH2	1:A:1537:TRP:CD1	2.38	0.42
1:A:2221:MET:SD	1:A:2361:MET:HE1	2.60	0.42
1:A:2607:SER:HA	1:A:2610:ARG:NE	2.32	0.42
1:A:3216:GLU:HA	1:A:3219:ARG:NH1	2.35	0.42
1:B:3567:LEU:HD12	1:B:3568:PRO:HD2	2.02	0.42
2:D:100:GLU:HB3	2:D:407:TRP:CZ3	2.55	0.42
2:D:243:ASN:ND2	2:D:247:THR:H	2.17	0.42
1:A:1534:PHE:HA	1:A:1537:TRP:HB3	2.02	0.42
1:A:3727:LYS:O	1:A:3731:LEU:HD13	2.19	0.42
1:B:1581:LYS:HA	1:B:1584:LYS:HE3	2.01	0.42
1:B:2224:GLY:O	1:B:2346:GLN:HA	2.20	0.42
1:B:3222:LEU:HD22	1:B:3472:VAL:HG21	2.01	0.42
1:A:1572:SER:O	1:A:1576:LEU:HG	2.20	0.42
1:B:2073:PHE:HZ	1:B:2096:VAL:HG21	1.85	0.42
1:B:2319:LEU:HD13	1:B:2359:CYS:SG	2.60	0.42
1:B:2324:LEU:HD22	1:B:2332:ARG:HB3	2.01	0.42
1:B:2989:LYS:NZ	2:C:276:GLU:O	2.42	0.42
1:B:4097:LYS:HA	1:B:4127:THR:HB	2.01	0.42
1:B:4099:VAL:HB	1:B:4106:LEU:HD21	2.01	0.42
2:D:365:TRP:HD1	2:D:373:MET:HA	1.84	0.42
1:B:1514:LYS:H	1:B:1514:LYS:HG2	1.62	0.42
1:B:2517:TYR:CE2	1:B:2521:ILE:HD13	2.55	0.42
1:B:4115:SER:O	1:B:4116:LEU:HD12	2.20	0.42
2:D:228:LYS:HB2	2:D:266:LYS:HE2	2.02	0.42
1:A:1931:ASN:HD21	1:A:2316:ASN:HB2	1.84	0.42
1:A:3161:LEU:HD23	1:A:3168:THR:HG22	2.01	0.42
1:A:4187:HIS:ND1	1:A:4252:TYR:OH	2.49	0.42
1:B:2437:LEU:HD21	1:B:2451:ARG:HG3	2.01	0.42
1:B:2999:VAL:HG11	1:B:3005:LEU:HG	2.02	0.42
1:B:3970:VAL:HB	1:B:3989:ARG:NH1	2.35	0.42
2:C:109:SER:HB3	2:C:128:GLU:HB2	2.01	0.42
1:A:2221:MET:HE1	1:A:2355:THR:HG22	2.02	0.41
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4285:ALA:O	1:A:4293:ASP:HB2	2.20	0.41
1:B:1469:VAL:O	1:B:1473:TYR:HB2	2.20	0.41
1:B:2590:PRO:O	1:B:2732:PRO:HD2	2.20	0.41
2:D:155:ASP:HB3	2:D:168:CYS:SG	2.60	0.41
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	2.01	0.41
1:A:2060:ARG:HH21	1:A:2129:GLU:HA	1.84	0.41
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	2.00	0.41
1:A:2662:PHE:HD1	1:A:2709:VAL:HG13	1.85	0.41
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.92	0.41
1:A:4444:GLN:HG2	1:A:4449:ARG:HG3	2.01	0.41
1:B:2756:LEU:HD23	1:B:2756:LEU:HA	1.85	0.41
1:B:2848:GLU:O	1:B:2852:THR:HG23	2.21	0.41
1:B:3846:LEU:HD22	1:B:3855:ARG:HD2	2.01	0.41
1:B:3973:LEU:O	1:B:3973:LEU:HD23	2.20	0.41
1:B:4185:TRP:O	1:B:4189:ILE:HG12	2.20	0.41
1:B:4339:MET:HE2	1:B:4339:MET:HB3	1.87	0.41
1:B:4453:ASN:O	1:B:4457:LYS:HG3	2.20	0.41
2:D:95:ILE:HD12	2:D:364:VAL:HG11	2.03	0.41
2:D:128:GLU:HA	2:D:152:SER:HB2	2.02	0.41
2:D:285:ALA:HA	2:D:346:PHE:CD2	2.54	0.41
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.54	0.41
1:A:3659:ARG:NH2	1:B:3629:PHE:O	2.52	0.41
1:B:2172:ARG:HH22	1:B:2209:GLN:HG3	1.85	0.41
1:B:2265:TYR:OH	1:B:2311:TRP:O	2.24	0.41
1:B:3036:GLY:O	1:B:3040:GLU:HG2	2.20	0.41
2:D:194:ASN:C	2:D:211:SER:HG	2.24	0.41
2:D:381:HIS:CD2	2:D:382:PHE:H	2.39	0.41
1:A:1522:SER:O	1:A:1526:LYS:HG2	2.19	0.41
1:A:1962:ARG:NH2	1:A:2314:ASN:OD1	2.54	0.41
1:A:2172:ARG:NH2	1:A:2205:GLU:HG3	2.35	0.41
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	2.01	0.41
1:A:4413:PHE:CD1	1:A:4492:ILE:HD12	2.55	0.41
1:B:2896:ARG:HA	1:B:2896:ARG:HD3	1.81	0.41
1:B:3214:GLN:O	1:B:3218:LEU:HD23	2.20	0.41
1:B:4480:SER:O	1:B:4484:GLU:HG3	2.20	0.41
2:D:96:PRO:HA	2:D:408:GLU:O	2.21	0.41
2:D:362:LEU:N	2:D:376:LEU:O	2.33	0.41
1:A:1724:VAL:HG23	1:A:1727:PHE:HD2	1.86	0.41
1:A:2054:LEU:HD21	1:A:2097:LEU:HD22	2.02	0.41
1:A:2769:LEU:O	1:A:2773:MET:HG3	2.20	0.41
1:A:3772:ASN:OD1	1:A:3775:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4190:ILE:HD12	1:A:4201:TRP:CZ2	2.55	0.41
1:B:1882:THR:HA	1:B:2048:LEU:HD23	2.01	0.41
2:C:233:HIS:CE1	2:C:259:ARG:HD2	2.55	0.41
2:D:211:SER:OG	2:D:212:ARG:N	2.54	0.41
1:A:2091:ARG:HD2	1:A:2357:SER:HB2	2.02	0.41
1:A:3044:LEU:HD22	1:A:3049:GLU:CG	2.51	0.41
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.20	0.41
1:A:3993:ILE:HD13	1:A:3993:ILE:HA	1.98	0.41
1:A:4069:ILE:HD13	1:A:4080:ALA:HA	2.02	0.41
1:B:2465:ALA:HB2	1:B:2493:TYR:CD1	2.56	0.41
1:B:3478:LEU:HD12	1:B:3767:ILE:HG23	2.00	0.41
2:C:395:VAL:HG23	2:C:409:CYS:SG	2.61	0.41
1:A:2176:THR:O	1:A:2180:GLU:HG2	2.21	0.41
1:A:2896:ARG:HA	1:A:2896:ARG:HD2	1.83	0.41
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.52	0.41
1:A:4106:LEU:HD13	1:A:4138:LEU:HD22	2.02	0.41
1:B:1487:ILE:HD12	1:B:1537:TRP:NE1	2.36	0.41
1:B:1836:PHE:HA	1:B:1839:LEU:HB2	2.03	0.41
2:C:113:ARG:HD2	2:C:155:ASP:HA	2.01	0.41
2:D:395:VAL:HG23	2:D:407:TRP:HD1	1.86	0.41
1:A:1556:ASP:O	1:A:1560:LEU:HG	2.21	0.41
1:A:1735:PRO:O	1:A:1739:ILE:HG12	2.21	0.41
1:A:3709:GLN:HG3	1:A:3809:SER:HB3	2.03	0.41
1:A:3728:ARG:HG3	1:A:3791:MET:HE1	2.02	0.41
1:A:4549:GLN:HG3	1:A:4587:LEU:HB2	2.02	0.41
1:B:2183:LYS:O	1:B:2187:GLN:HG2	2.21	0.41
1:B:2452:LEU:HD23	1:B:2452:LEU:HA	1.93	0.41
1:B:4433:ASP:HB3	1:B:4448:LEU:HD21	2.02	0.41
2:D:107:HIS:CE1	2:D:133:LYS:HG3	2.56	0.41
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	2.02	0.41
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	2.02	0.41
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.20	0.41
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.21	0.41
1:A:4424:LEU:HA	1:A:4482:PHE:HZ	1.86	0.41
1:A:4503:GLU:H	1:A:4503:GLU:HG2	1.73	0.41
1:B:1721:VAL:HA	1:B:1724:VAL:HG12	2.03	0.41
1:B:1733:ILE:HB	1:B:1791:VAL:HG21	2.03	0.41
1:B:2818:VAL:O	1:B:2822:ILE:HG12	2.21	0.41
1:B:3214:GLN:HE22	1:B:3759:ARG:NH1	2.19	0.41
1:B:3779:GLU:HG3	1:B:3783:LYS:HE3	2.03	0.41
1:B:3790:VAL:O	1:B:3793:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4172:SER:HB2	1:B:4173:PRO:HD3	2.02	0.41
2:D:239:MET:HE3	2:D:239:MET:HB2	1.90	0.41
2:D:269:LYS:NZ	2:D:325:VAL:HG12	2.36	0.41
1:A:1470:TRP:CE3	1:A:1470:TRP:HA	2.55	0.41
1:A:1519:ASP:OD1	1:A:1520:ALA:N	2.54	0.41
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.21	0.41
1:A:2387:LEU:HD21	1:A:2463:HIS:HB3	2.03	0.41
1:A:3941:LEU:HD23	1:A:3944:PHE:CD2	2.56	0.41
1:A:4437:VAL:HG21	1:A:4448:LEU:HD13	2.03	0.41
1:B:1547:LEU:HD12	1:B:1608:LEU:HD22	2.03	0.41
1:B:2018:MET:HE3	1:B:2018:MET:HB2	1.80	0.41
1:A:1473:TYR:OH	1:A:1493:LEU:HB2	2.21	0.40
1:A:4292:LYS:HG3	1:A:4293:ASP:N	2.35	0.40
1:B:1895:ALA:HB2	1:B:2037:ARG:HB2	2.03	0.40
1:B:2422:ILE:HD13	1:B:2487:GLU:HA	2.03	0.40
2:D:236:TRP:HB3	2:D:254:ASN:HD22	1.83	0.40
1:A:2619:GLY:O	1:A:3014:ASN:ND2	2.55	0.40
1:B:2937:GLY:C	1:B:3070:PRO:HD3	2.46	0.40
1:B:3045:ASP:OD1	1:B:3045:ASP:N	2.53	0.40
1:A:2756:LEU:HD23	1:A:2756:LEU:HA	1.84	0.40
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.20	0.40
1:B:2220:LEU:HB2	1:B:2342:MET:HG2	2.03	0.40
1:B:2776:PHE:HZ	1:B:2846:THR:HG23	1.86	0.40
1:B:3692:LEU:O	1:B:3696:VAL:HG22	2.21	0.40
1:A:1547:LEU:HD23	1:A:1547:LEU:HA	1.90	0.40
1:A:2635:PHE:HB3	1:A:2650:LEU:HD21	2.03	0.40
1:A:3033:CYS:SG	1:A:3054:PHE:HB2	2.61	0.40
1:A:3783:LYS:O	1:A:3786:GLU:HG2	2.21	0.40
1:A:4172:SER:HB2	1:A:4173:PRO:HD3	2.02	0.40
1:B:1945:PHE:HB3	1:B:1978:ILE:HD11	2.03	0.40
1:B:2804:ARG:HA	1:B:2804:ARG:HD2	1.83	0.40
1:B:3107:LYS:HD2	1:B:3144:VAL:HG21	2.03	0.40
2:D:188:MET:HE3	2:D:188:MET:HB2	1.96	0.40
1:A:3474:ARG:HH22	1:A:3768:THR:HG22	1.86	0.40
1:B:2297:LYS:O	1:B:2338:ASN:ND2	2.39	0.40
1:B:2721:LYS:HE2	1:B:2721:LYS:HB2	1.94	0.40
1:B:3034:LYS:HE3	1:B:3050:LEU:HD11	2.04	0.40
1:B:3217:GLU:O	1:B:3220:ARG:HG2	2.21	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	2929/4646 (63%)	2879 (98%)	50 (2%)	0	100	100
1	B	2929/4646 (63%)	2868 (98%)	61 (2%)	0	100	100
2	C	320/410 (78%)	310 (97%)	10 (3%)	0	100	100
2	D	317/410 (77%)	305 (96%)	12 (4%)	0	100	100
All	All	6495/10112 (64%)	6362 (98%)	133 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2605/4125 (63%)	2605 (100%)	0	100	100
1	B	2605/4125 (63%)	2605 (100%)	0	100	100
2	C	287/364 (79%)	287 (100%)	0	100	100
2	D	284/364 (78%)	284 (100%)	0	100	100
All	All	5781/8978 (64%)	5781 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1495	ASN
1	A	1569	GLN
1	A	1779	HIS
1	A	1850	GLN
1	A	1950	GLN
1	A	1974	GLN
1	A	1979	GLN
1	A	2067	ASN
1	A	2212	GLN
1	A	2485	GLN
1	A	2549	GLN
1	A	2577	HIS
1	A	2588	HIS
1	A	2707	GLN
1	A	2781	GLN
1	A	2786	GLN
1	A	3061	ASN
1	A	3158	ASN
1	A	3198	GLN
1	A	3499	GLN
1	A	3526	GLN
1	A	3538	GLN
1	A	3709	GLN
1	A	3820	GLN
1	A	3952	GLN
1	A	4012	ASN
1	A	4062	GLN
1	A	4100	HIS
1	A	4114	HIS
1	A	4174	ASN
1	A	4490	GLN
1	A	4506	ASN
1	A	4530	GLN
1	A	4566	GLN
1	B	1495	ASN
1	B	1559	HIS
1	B	1569	GLN
1	B	1643	ASN
1	B	1755	GLN
1	B	1841	GLN
1	B	1950	GLN
1	B	1973	GLN
1	B	1976	GLN

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Mol	Chain	Res	Type
1	B	1979	GLN
1	B	2047	GLN
1	B	2067	ASN
1	B	2217	ASN
1	B	2263	HIS
1	B	2464	GLN
1	B	2485	GLN
1	B	2637	HIS
1	B	2654	GLN
1	B	2752	ASN
1	B	2960	GLN
1	B	3063	HIS
1	B	3119	ASN
1	B	3233	ASN
1	B	3526	GLN
1	B	3735	GLN
1	B	3744	GLN
1	B	3820	GLN
1	B	3877	HIS
1	B	4012	ASN
1	B	4098	ASN
1	B	4156	ASN
1	B	4191	GLN
1	B	4249	GLN
1	B	4258	ASN
2	C	206	HIS
2	D	222	GLN
2	D	277	HIS
2	D	381	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	B	4702	5	32,33,33	0.37	0	48,52,52	0.27	0
3	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
3	ADP	B	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.87	8 (18%)
3	ADP	B	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
3	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
4	ATP	A	4702	5	32,33,33	0.34	0	48,52,52	0.29	0
3	ADP	A	4701	5	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
3	ADP	B	4701	5	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	4702	5	-	4/22/38/38	0/3/3/3
3	ADP	A	4703	-	-	2/16/32/32	0/3/3/3
3	ADP	B	4703	-	-	1/16/32/32	0/3/3/3
3	ADP	B	4704	-	-	1/16/32/32	0/3/3/3
3	ADP	A	4704	-	-	3/16/32/32	0/3/3/3
4	ATP	A	4702	5	-	3/22/38/38	0/3/3/3
3	ADP	A	4701	5	-	2/16/32/32	0/3/3/3
3	ADP	B	4701	5	-	4/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4703	ADP	C5-C4	4.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4703	ADP	C5-C4	4.72	1.47	1.39
3	A	4704	ADP	C5-C4	4.69	1.47	1.39
3	A	4701	ADP	C5-C4	4.60	1.47	1.39
3	B	4701	ADP	C5-C4	4.60	1.47	1.39
3	B	4704	ADP	C5-C4	4.59	1.47	1.39
3	A	4703	ADP	C5-C6	2.68	1.48	1.41
3	B	4703	ADP	C5-C6	2.68	1.48	1.41
3	A	4704	ADP	C5-C6	2.68	1.48	1.41
3	A	4701	ADP	C5-C6	2.67	1.48	1.41
3	B	4701	ADP	C5-C6	2.62	1.48	1.41
3	B	4704	ADP	C5-C6	2.62	1.48	1.41
3	B	4704	ADP	C5-N7	-2.35	1.34	1.39
3	B	4703	ADP	C5-N7	-2.33	1.34	1.39
3	B	4701	ADP	C5-N7	-2.33	1.34	1.39
3	A	4704	ADP	C5-N7	-2.30	1.34	1.39
3	A	4701	ADP	C8-N7	2.30	1.36	1.31
3	A	4703	ADP	C8-N7	2.29	1.36	1.31
3	B	4704	ADP	C8-N7	2.29	1.36	1.31
3	B	4703	ADP	C8-N7	2.29	1.36	1.31
3	A	4703	ADP	C5-N7	-2.29	1.34	1.39
3	A	4701	ADP	C5-N7	-2.28	1.34	1.39
3	A	4704	ADP	C8-N7	2.26	1.36	1.31
3	B	4701	ADP	C8-N7	2.25	1.36	1.31

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4703	ADP	C5-C4-N3	-6.12	118.29	126.72
3	A	4703	ADP	C5-C4-N3	-6.04	118.40	126.72
3	A	4704	ADP	C5-C4-N3	-5.86	118.65	126.72
3	B	4704	ADP	C5-C4-N3	-5.86	118.65	126.72
3	B	4701	ADP	C5-C4-N3	-5.79	118.74	126.72
3	A	4701	ADP	C5-C4-N3	-5.70	118.87	126.72
3	B	4703	ADP	N3-C4-N9	4.90	135.50	127.17
3	A	4703	ADP	N3-C4-N9	4.79	135.31	127.17
3	A	4704	ADP	N3-C4-N9	4.67	135.11	127.17
3	B	4704	ADP	N3-C4-N9	4.63	135.05	127.17
3	B	4701	ADP	N3-C4-N9	4.57	134.95	127.17
3	A	4701	ADP	N3-C4-N9	4.47	134.76	127.17
3	B	4703	ADP	C2-N3-C4	3.85	121.23	111.83
3	A	4703	ADP	C2-N3-C4	3.78	121.06	111.83
3	B	4704	ADP	C2-N3-C4	3.72	120.90	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4704	ADP	C2-N3-C4	3.71	120.89	111.83
3	A	4701	ADP	C2-N3-C4	3.69	120.83	111.83
3	B	4701	ADP	C2-N3-C4	3.68	120.82	111.83
3	A	4701	ADP	C4-C5-N7	-3.55	106.52	110.58
3	B	4701	ADP	C4-C5-N7	-3.46	106.63	110.58
3	B	4704	ADP	C4-C5-N7	-3.42	106.67	110.58
3	A	4704	ADP	C4-C5-N7	-3.41	106.68	110.58
3	A	4703	ADP	C4-C5-N7	-3.41	106.69	110.58
3	B	4703	ADP	C4-C5-N7	-3.38	106.71	110.58
3	B	4703	ADP	N3-C2-N1	-3.30	123.58	128.58
3	A	4701	ADP	N3-C2-N1	-3.30	123.58	128.58
3	B	4704	ADP	N3-C2-N1	-3.29	123.60	128.58
3	A	4703	ADP	N3-C2-N1	-3.27	123.64	128.58
3	B	4701	ADP	N3-C2-N1	-3.24	123.68	128.58
3	A	4704	ADP	N3-C2-N1	-3.24	123.68	128.58
3	A	4701	ADP	C4-N9-C8	2.72	108.60	105.74
3	B	4701	ADP	C4-N9-C8	2.64	108.50	105.74
3	B	4704	ADP	C4-N9-C8	2.59	108.46	105.74
3	A	4701	ADP	C5-N7-C8	2.58	107.51	103.45
3	A	4703	ADP	C3'-C2'-C1'	2.57	106.32	101.46
3	A	4704	ADP	C4-N9-C8	2.55	108.41	105.74
3	A	4704	ADP	C3'-C2'-C1'	2.54	106.27	101.46
3	B	4703	ADP	C3'-C2'-C1'	2.53	106.25	101.46
3	B	4703	ADP	C4-N9-C8	2.52	108.38	105.74
3	A	4703	ADP	C5-N7-C8	2.50	107.38	103.45
3	B	4703	ADP	C5-N7-C8	2.50	107.37	103.45
3	A	4704	ADP	C5-N7-C8	2.49	107.37	103.45
3	B	4701	ADP	C5-N7-C8	2.49	107.37	103.45
3	B	4704	ADP	C5-N7-C8	2.48	107.36	103.45
3	A	4703	ADP	C4-N9-C8	2.48	108.35	105.74
3	B	4704	ADP	C3'-C2'-C1'	2.44	106.07	101.46
3	A	4701	ADP	C6-C5-N7	2.22	136.37	132.09
3	B	4701	ADP	C6-C5-N7	2.08	136.10	132.09
3	A	4701	ADP	N9-C8-N7	-2.07	111.00	113.94
3	B	4704	ADP	C6-C5-N7	2.04	136.02	132.09
3	A	4704	ADP	C6-C5-N7	2.03	136.00	132.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4703	ADP	C5'-O5'-PA-O1A

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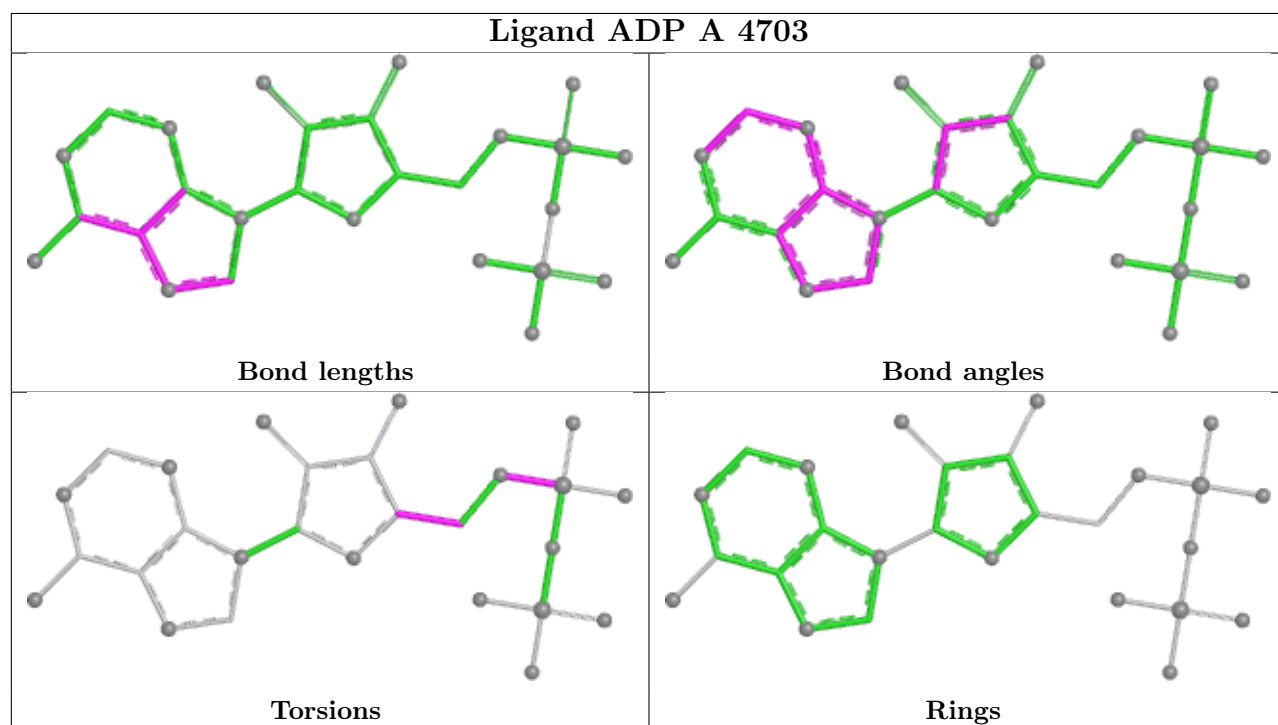
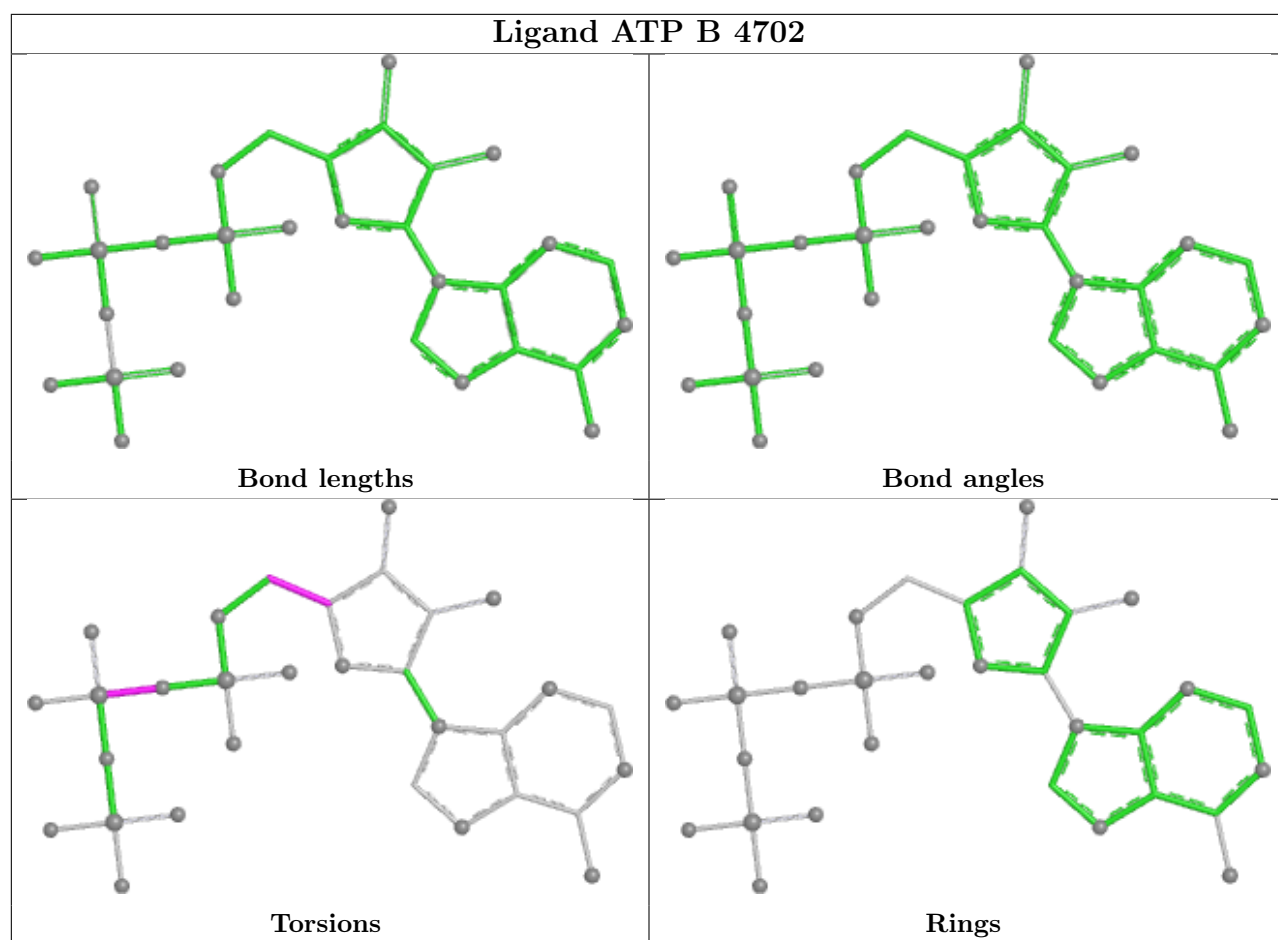
Mol	Chain	Res	Type	Atoms
3	A	4704	ADP	C5'-O5'-PA-O1A
3	B	4701	ADP	C5'-O5'-PA-O1A
3	B	4701	ADP	C5'-O5'-PA-O3A
4	B	4702	ATP	O4'-C4'-C5'-O5'
4	A	4702	ATP	O4'-C4'-C5'-O5'
4	A	4702	ATP	C3'-C4'-C5'-O5'
4	B	4702	ATP	C3'-C4'-C5'-O5'
3	B	4701	ADP	O4'-C4'-C5'-O5'
3	A	4701	ADP	PA-O3A-PB-O2B
3	A	4701	ADP	PA-O3A-PB-O3B
4	B	4702	ATP	PA-O3A-PB-O2B
3	B	4701	ADP	C5'-O5'-PA-O2A
3	B	4704	ADP	C5'-O5'-PA-O1A
4	A	4702	ATP	PA-O3A-PB-O2B
3	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4704	ADP	O4'-C4'-C5'-O5'
4	B	4702	ATP	PA-O3A-PB-O1B
3	A	4703	ADP	O4'-C4'-C5'-O5'
3	B	4703	ADP	O4'-C4'-C5'-O5'

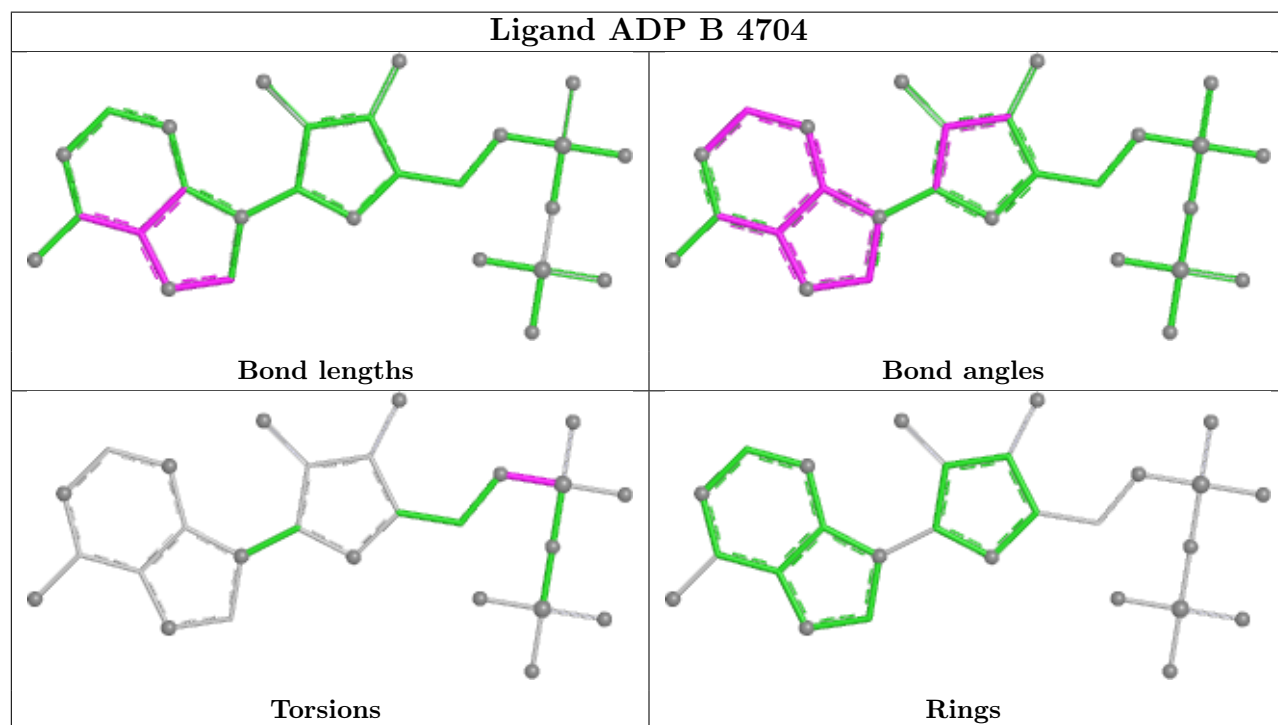
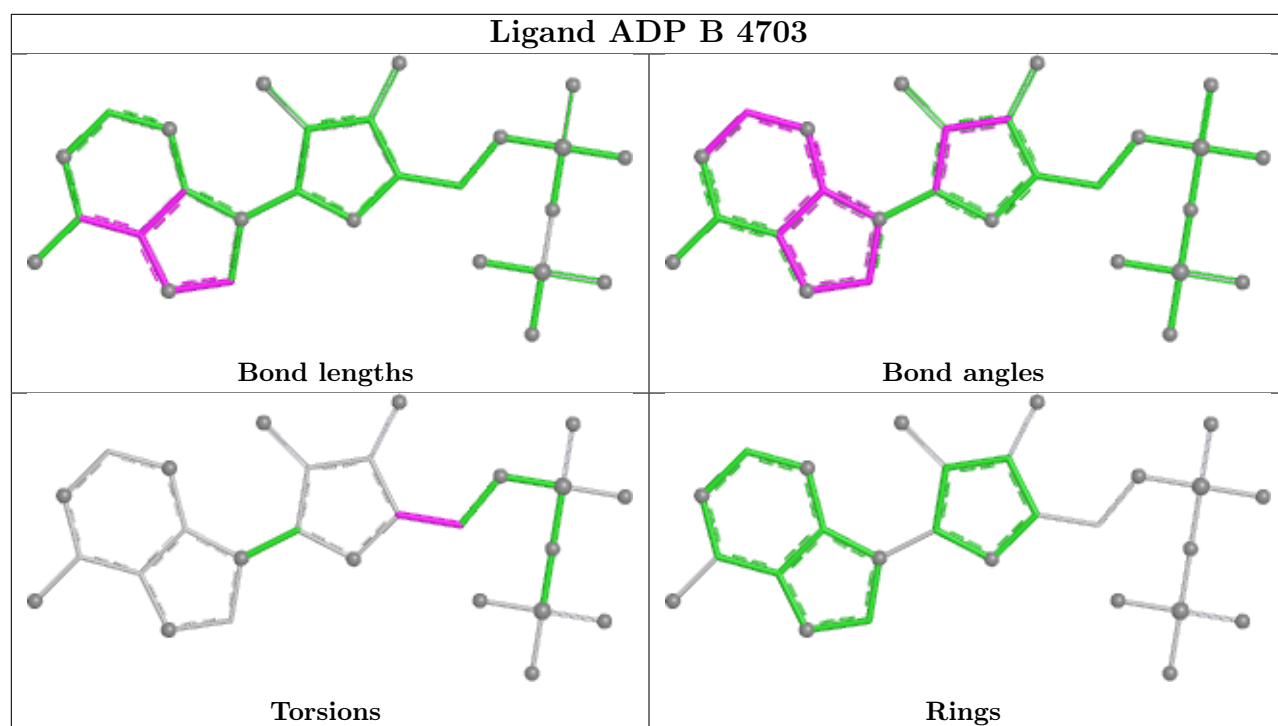
There are no ring outliers.

3 monomers are involved in 4 short contacts:

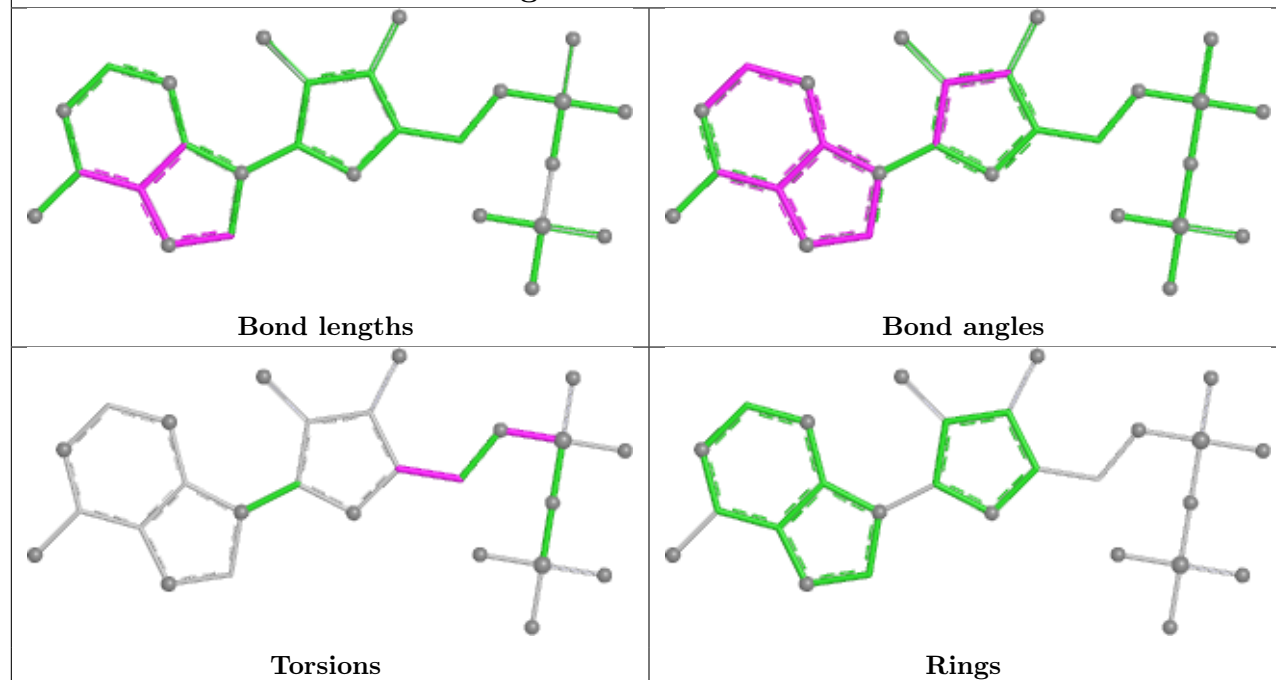
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4704	ADP	1	0
4	A	4702	ATP	2	0
3	B	4701	ADP	1	0

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

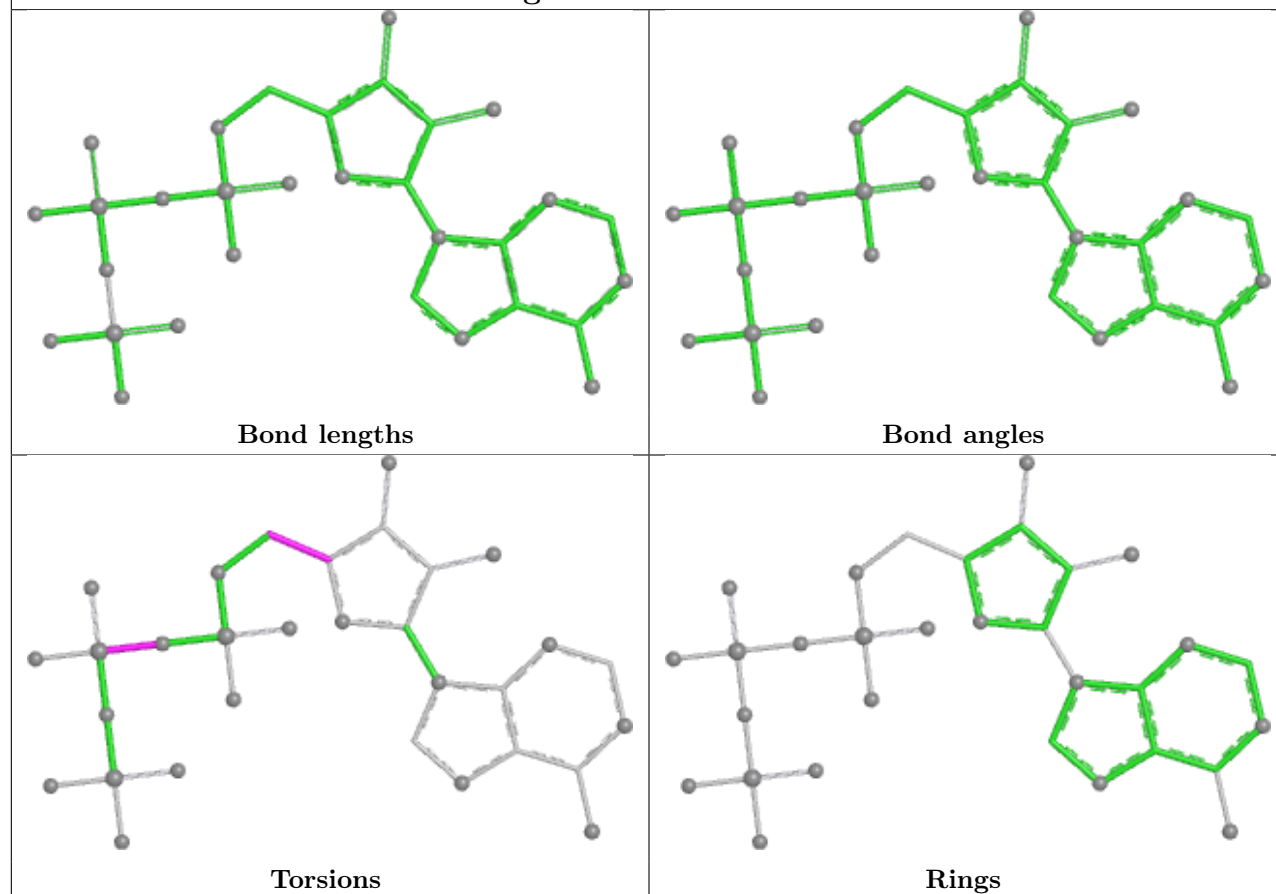


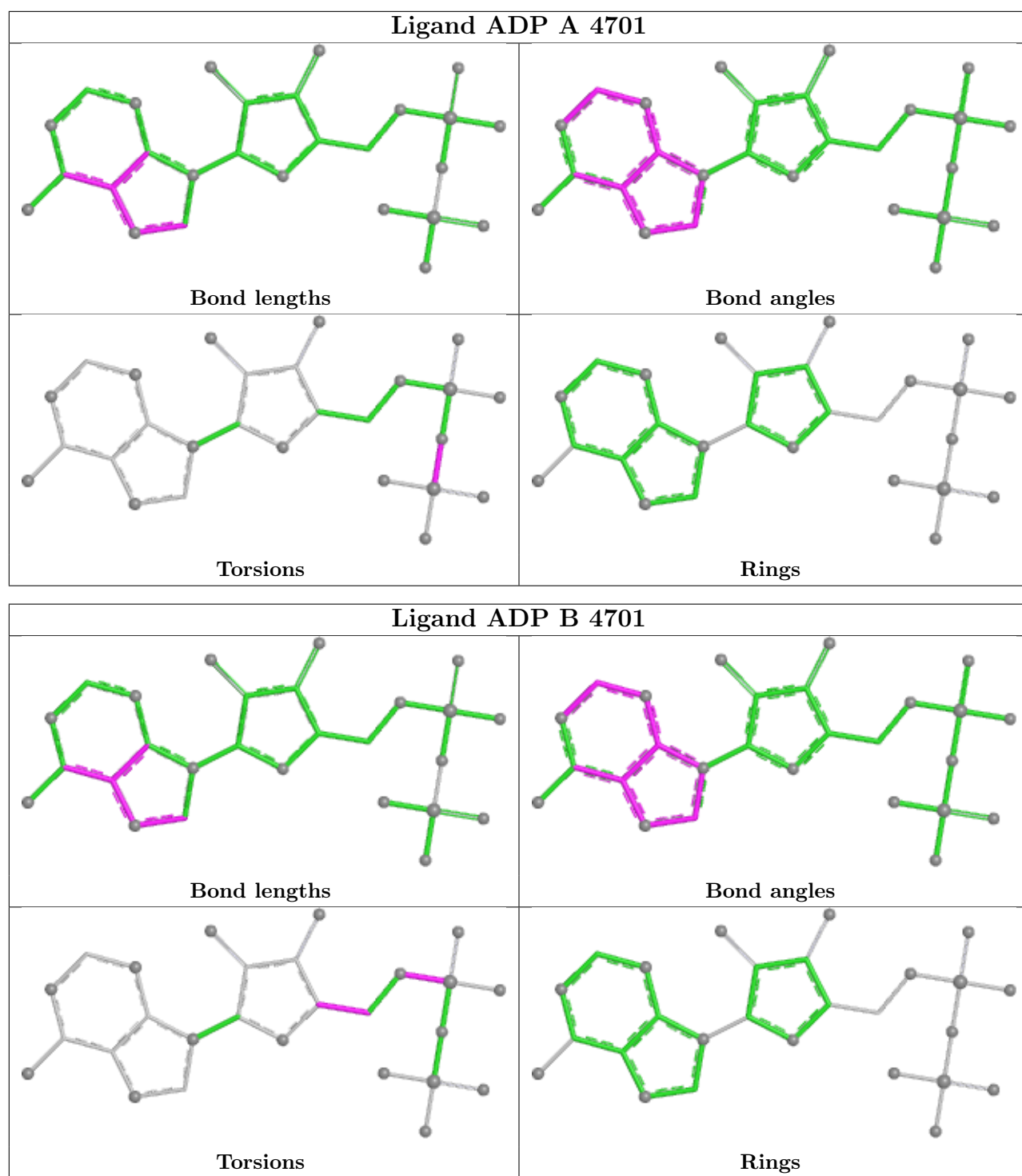


Ligand ADP A 4704



Ligand ATP A 4702





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

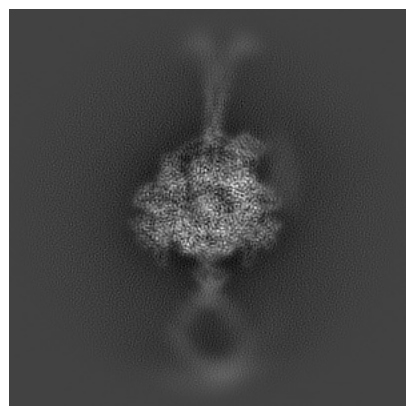
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47380. These allow visual inspection of the internal detail of the map and identification of artifacts.

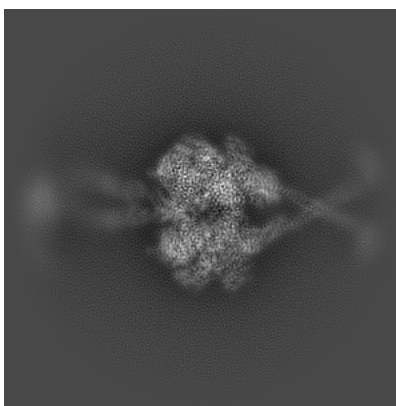
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

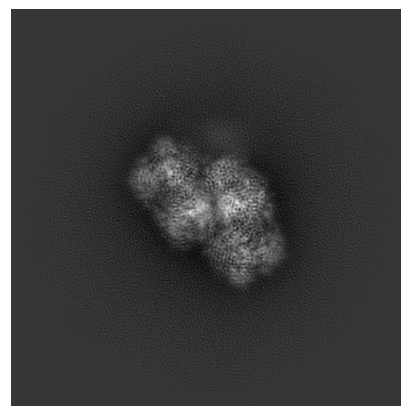
6.1.1 Primary map



X

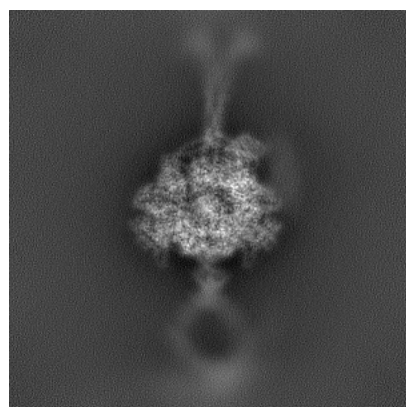


Y

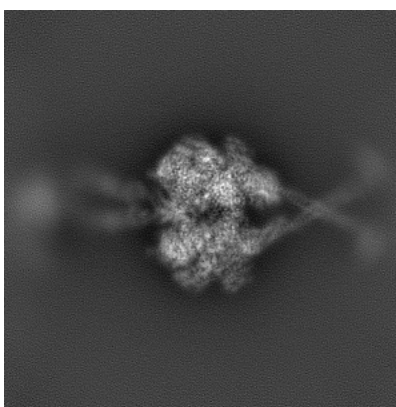


Z

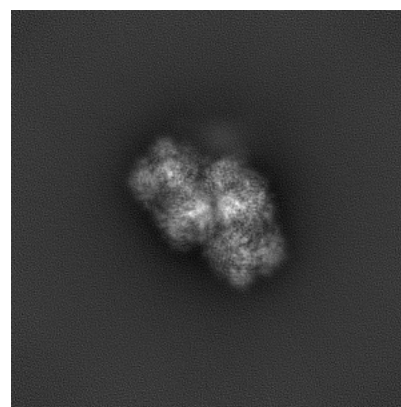
6.1.2 Raw map



X



Y



Z

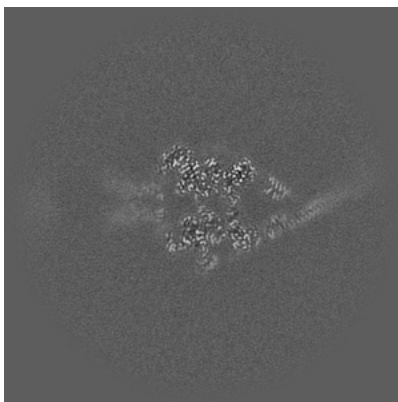
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

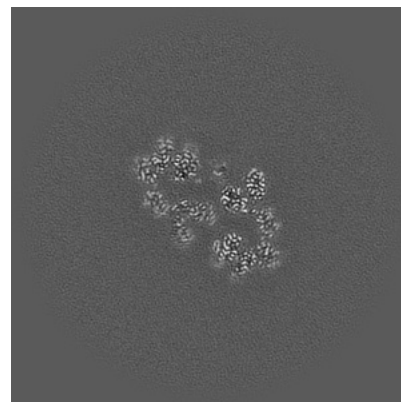
6.2.1 Primary map



X Index: 192



Y Index: 192

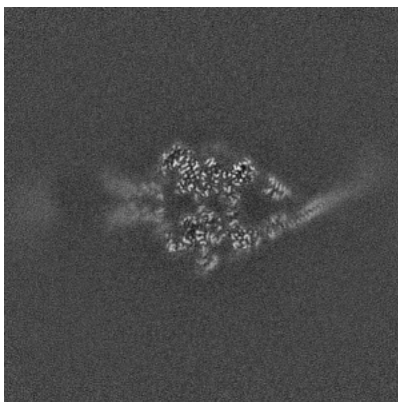


Z Index: 192

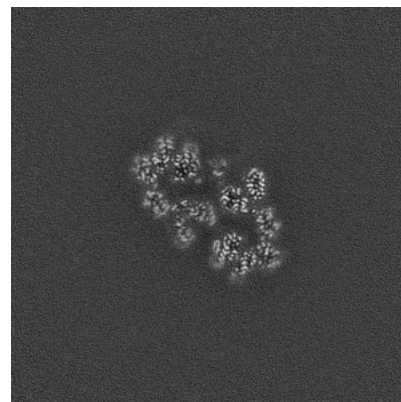
6.2.2 Raw map



X Index: 192



Y Index: 192

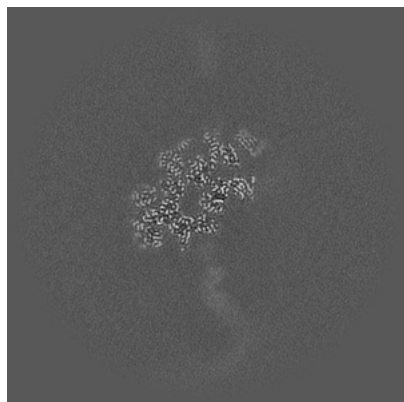


Z Index: 192

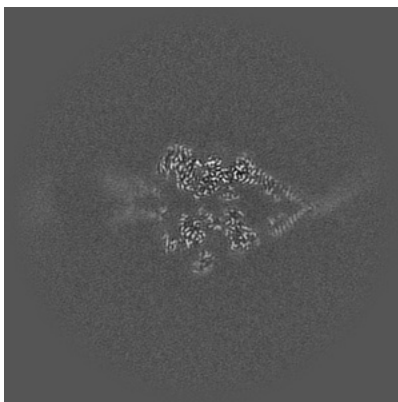
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

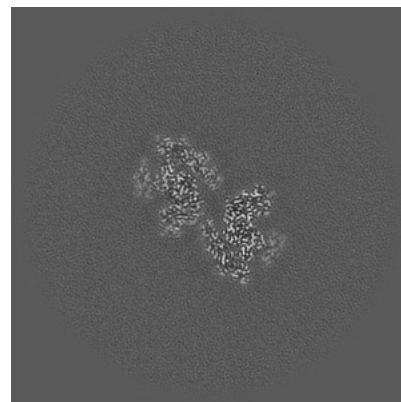
6.3.1 Primary map



X Index: 215

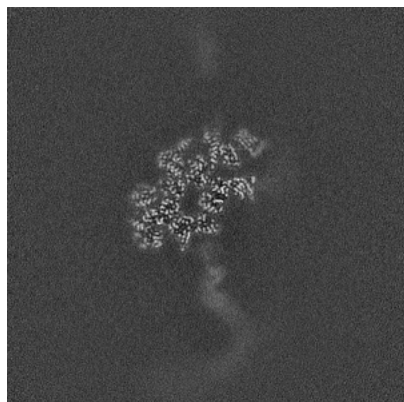


Y Index: 196

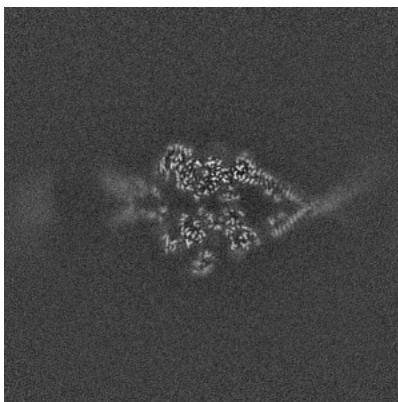


Z Index: 173

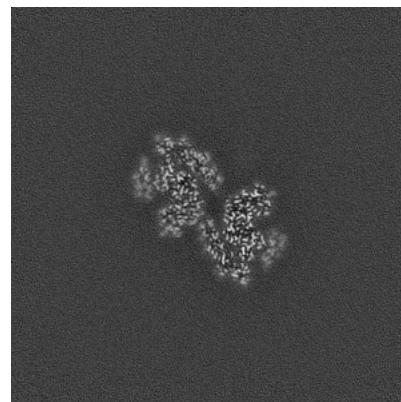
6.3.2 Raw map



X Index: 215



Y Index: 196

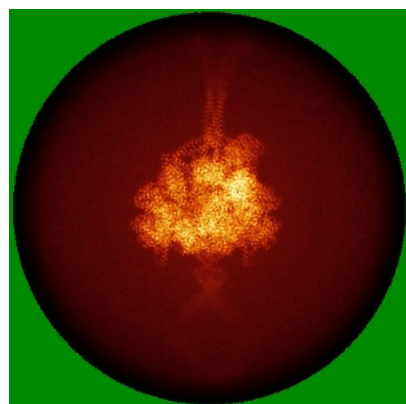


Z Index: 173

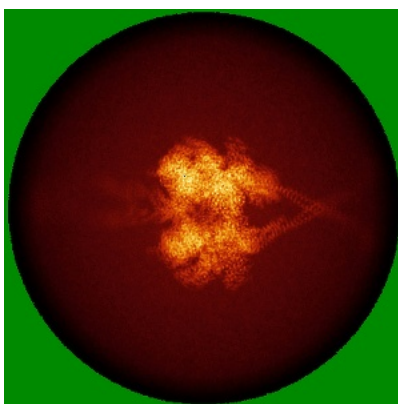
The images above show the largest variance slices of the map in three orthogonal directions.

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

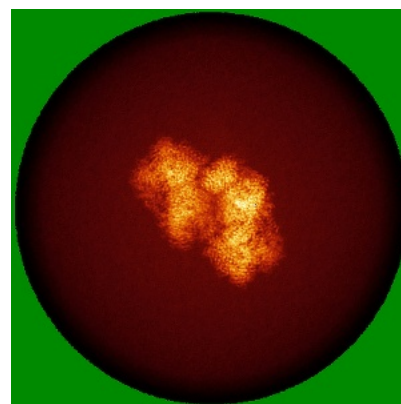
6.4.1 Primary map



X

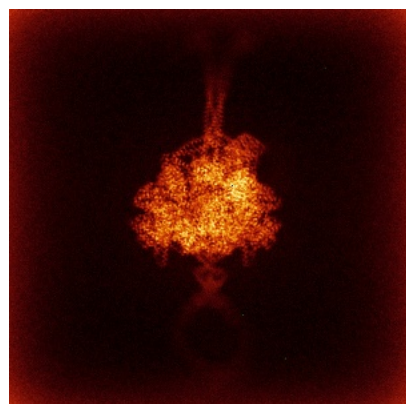


Y

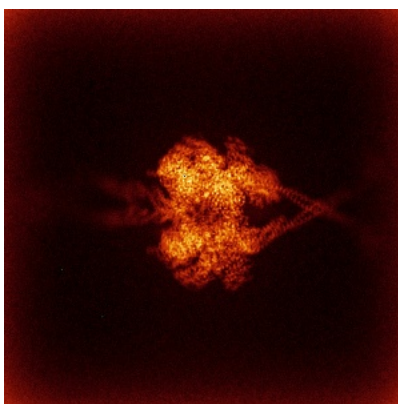


Z

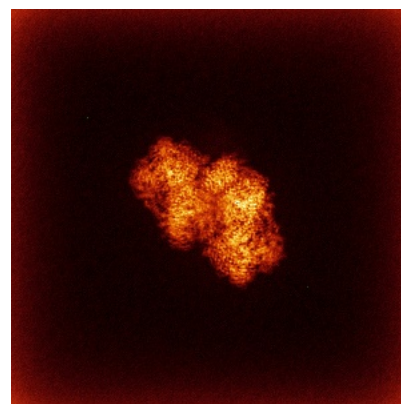
6.4.2 Raw map



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](#)

This section was not generated.

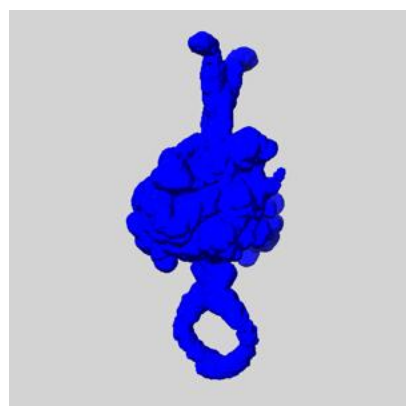
6.6 Mask visualisation [i](#)

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

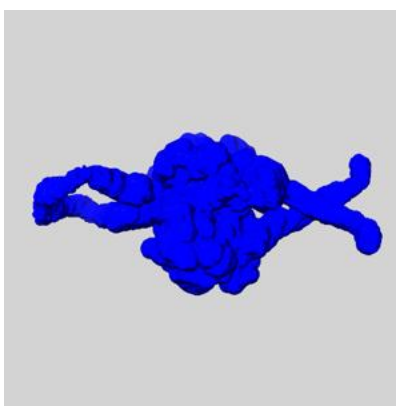
A mask typically either:

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

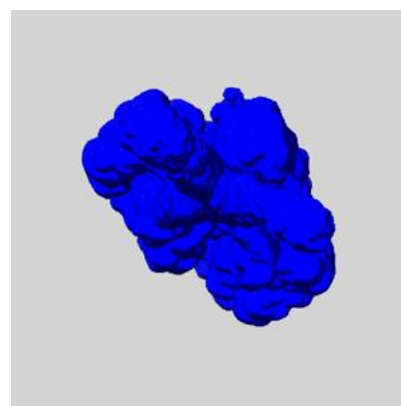
6.6.1 emd_47380_msk_1.map [i](#)



X



Y

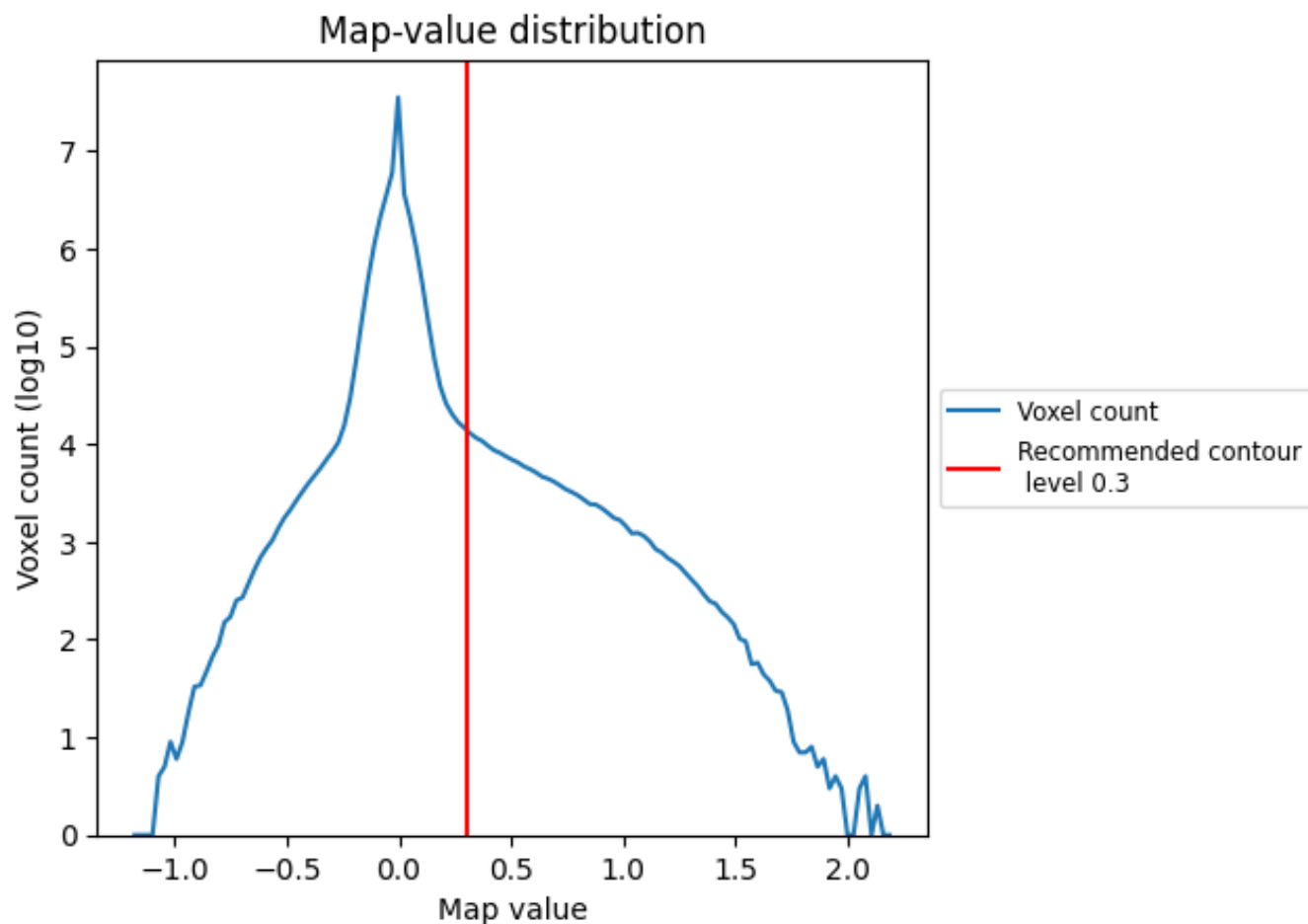


Z

7 Map analysis [i](#)

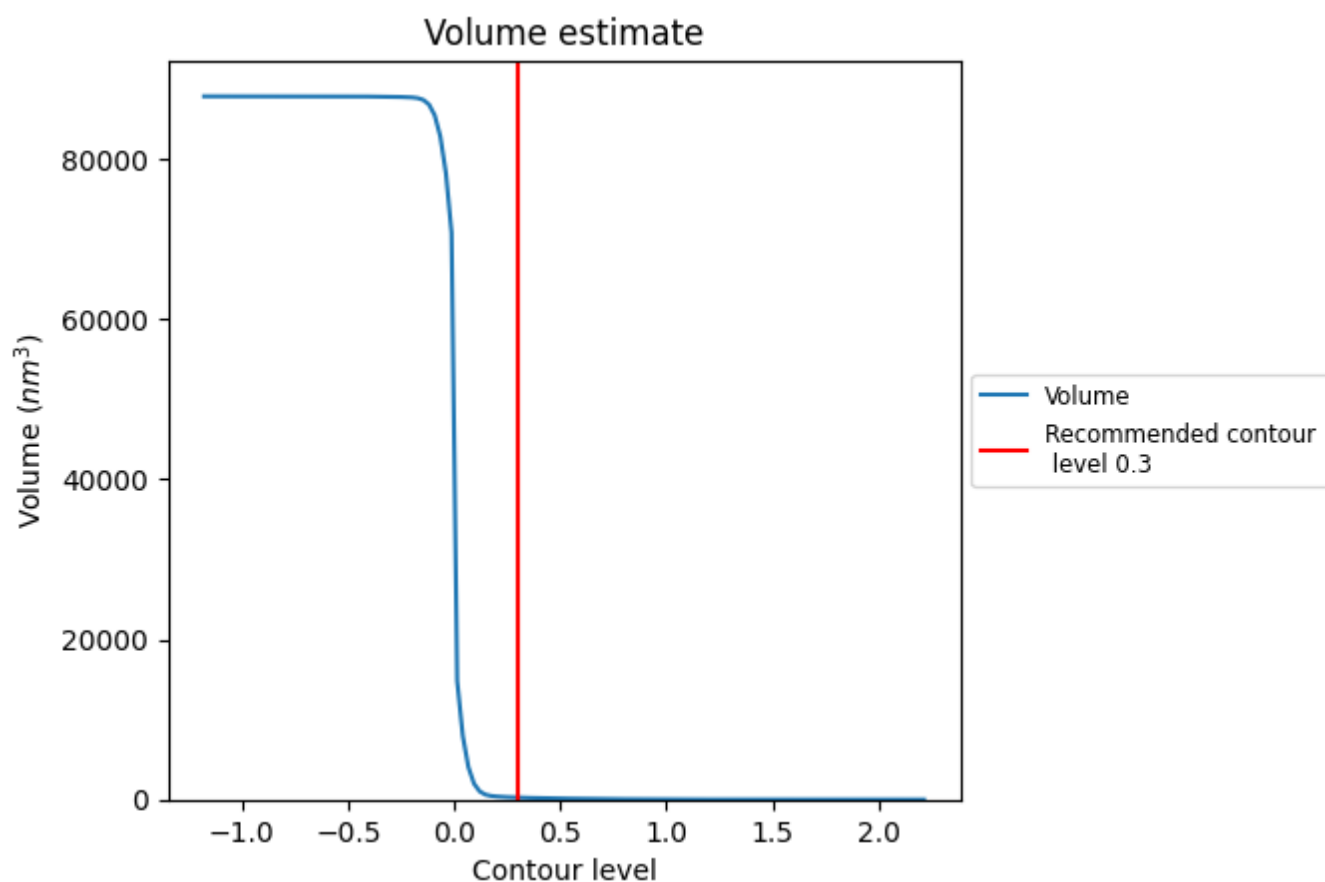
This section contains the results of statistical analysis of the map.

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.

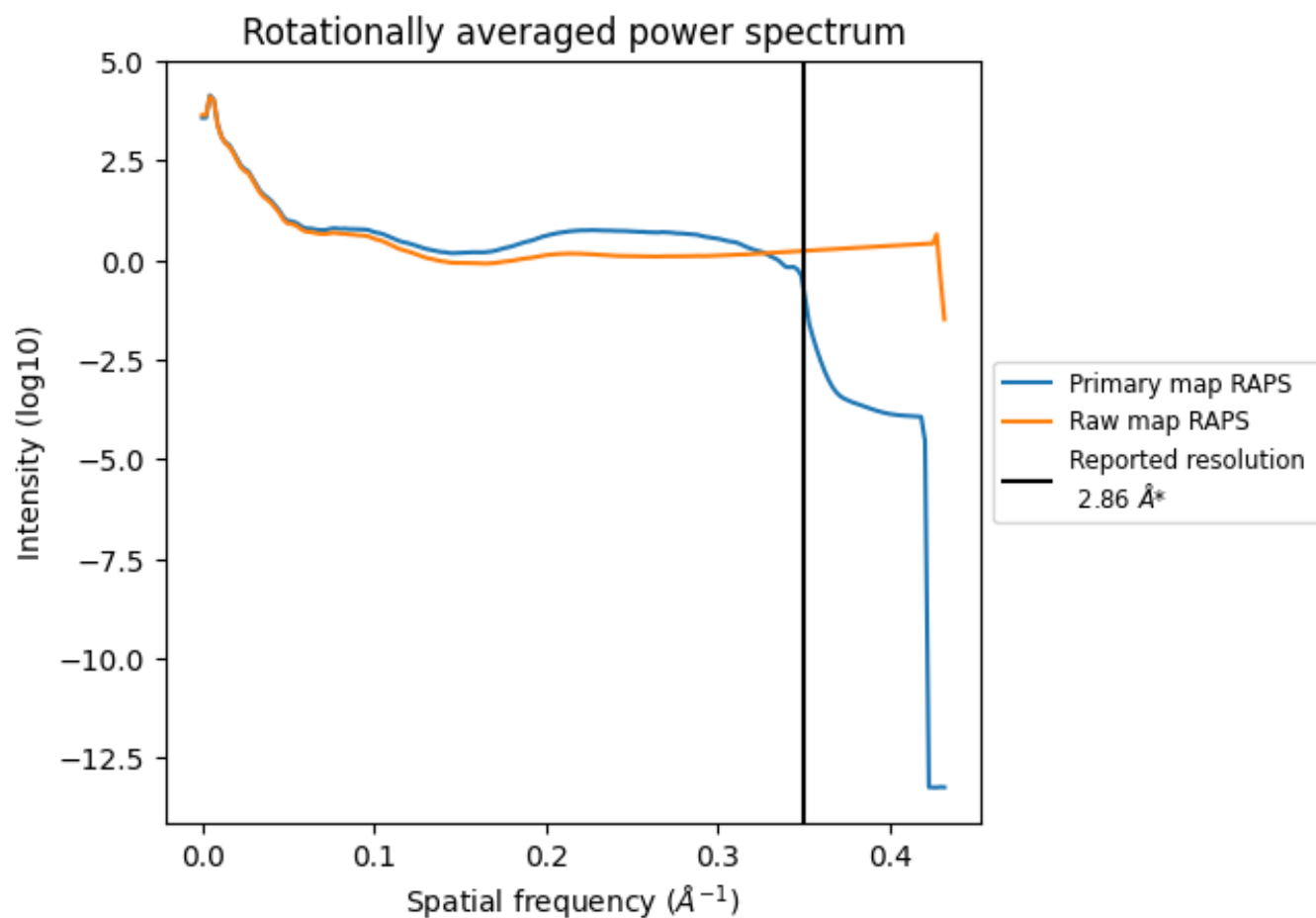
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm³; this corresponds to an approximate mass of 228 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 ⓘ

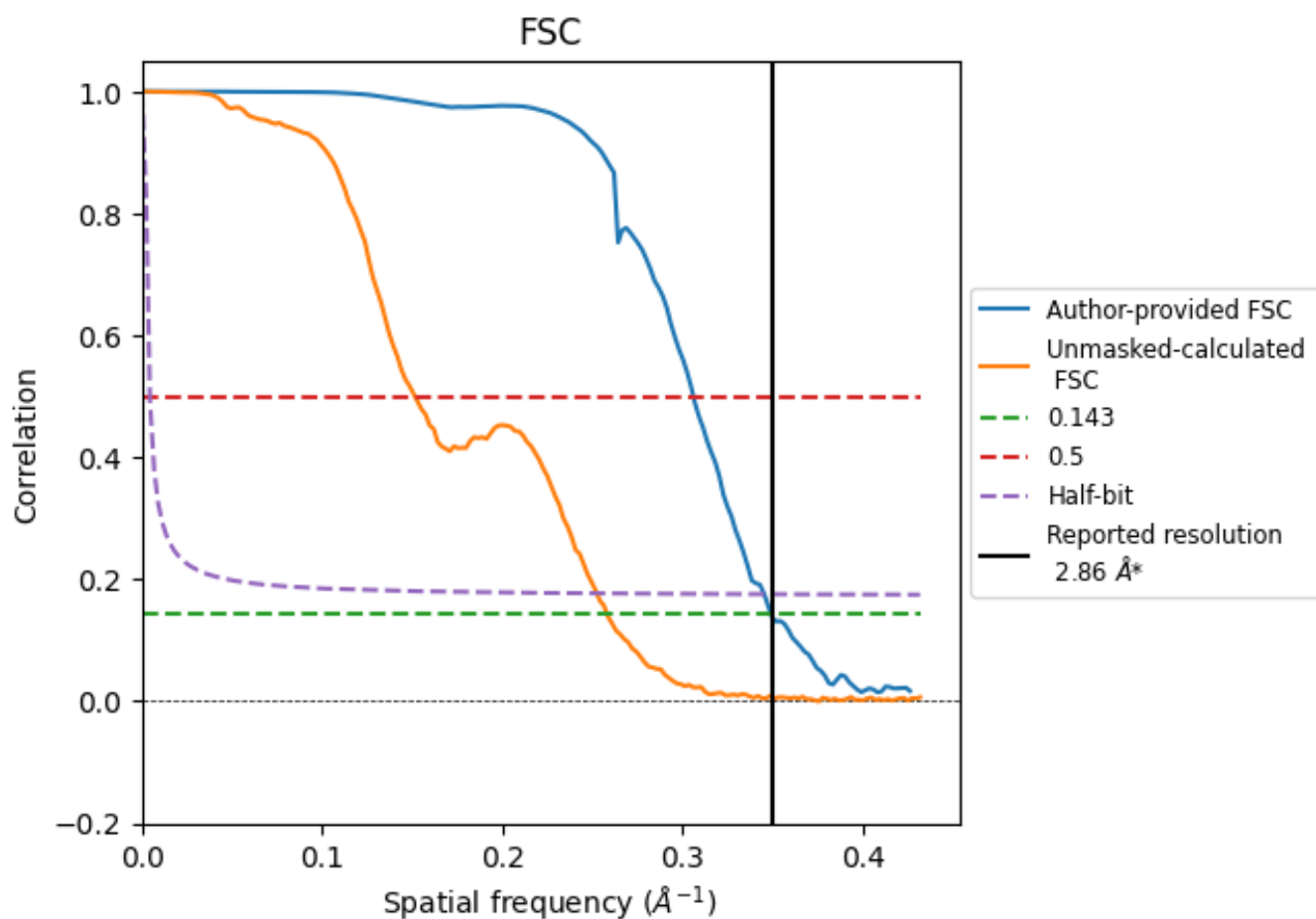


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.27	2.89
Unmasked-calculated*	3.87	6.60	3.96

*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 3.87 differs from the reported value 2.86 by more than 10 %

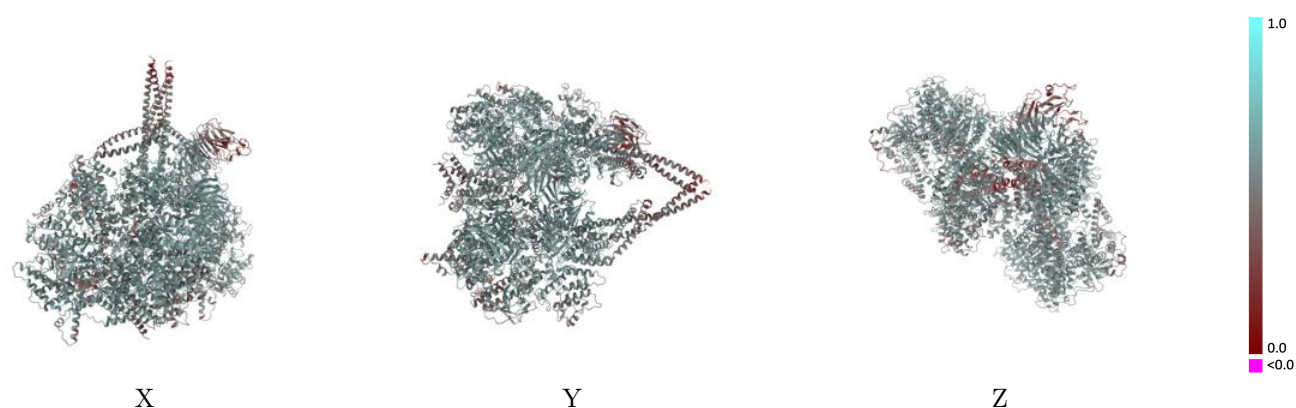
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47380 and PDB model 9E11. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

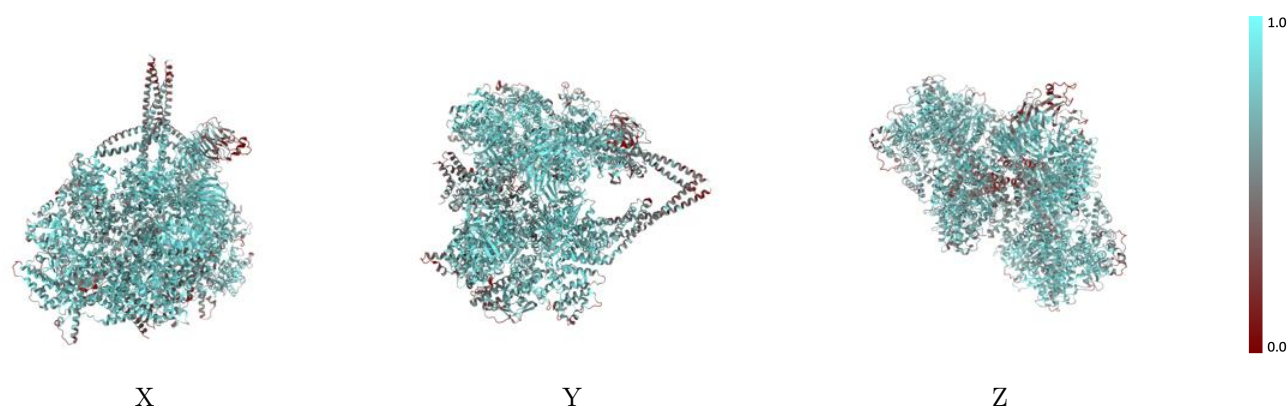
This section was not generated.

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



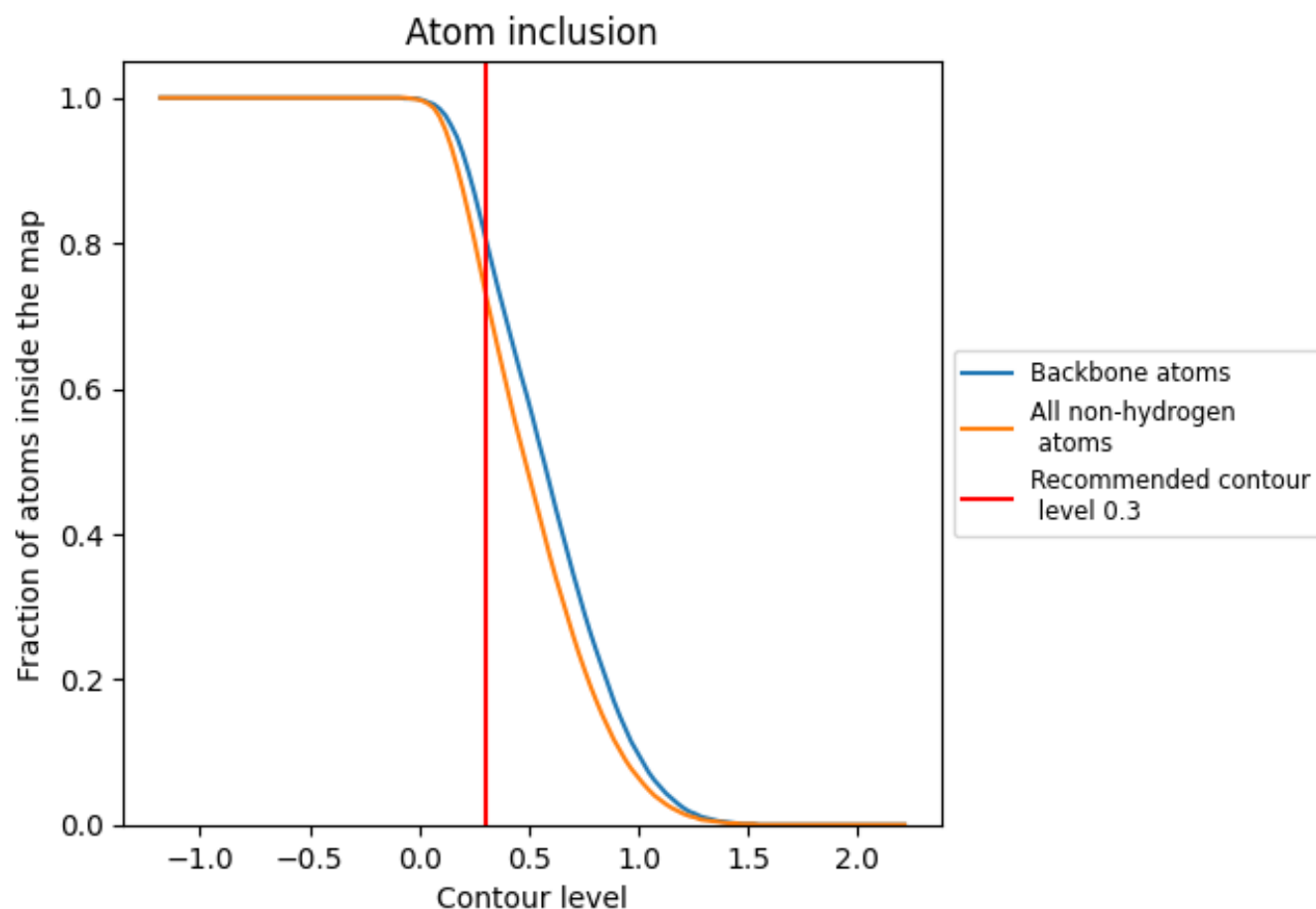
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7360	<div></div> 0.5430
A	<div></div> 0.7130	<div></div> 0.5370
B	<div></div> 0.7660	<div></div> 0.5550
C	<div></div> 0.8490	<div></div> 0.5900
D	<div></div> 0.5620	<div></div> 0.4470

