



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:43 AM UTC

PDB ID : 6V86 / pdb_00006v86
EMDB ID : EMD-21096
Title : Parainfluenza virus 5 L-P complex with an alternate conformation of the CD-MTase-CTD module
Authors : Abdella, R.; He, Y.
Deposited on : 2019-12-10
Resolution : 4.63 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
MolProbity : 4-5-2 with Phenix2.0
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

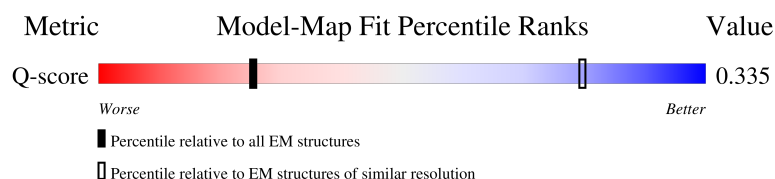
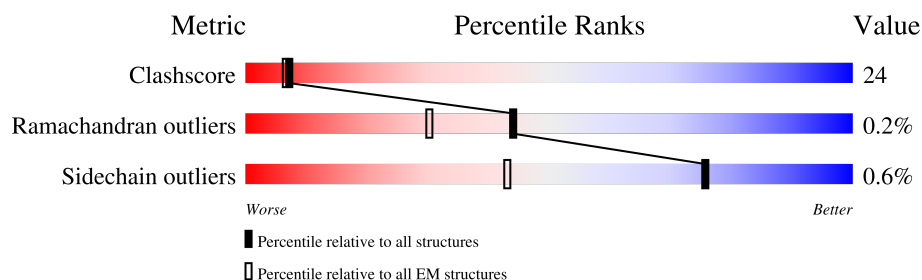
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 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	2068 (4.13 - 5.13)

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	2255	17% 46% 37% 16%
2	B	392	14% 9% 9% 82%
2	C	392	16% 8% 10% 81%
2	D	392	15% 9% 9% 82%

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Mol	Chain	Length	Quality of chain
2	E	392	13%10%9%81%
2	F	392	8%88%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17781 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1890	Total	C	N	O	S	0	0
			15103	9712	2555	2753	83		

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	72	Total	C	N	O	S	4	0
			569	350	101	115	3		
2	C	74	Total	C	N	O	S	4	0
			582	357	103	119	3		
2	D	72	Total	C	N	O	S	4	0
			569	350	101	115	3		
2	E	74	Total	C	N	O	S	4	0
			582	357	103	119	3		
2	F	47	Total	C	N	O	S	0	0
			374	238	64	70	2		

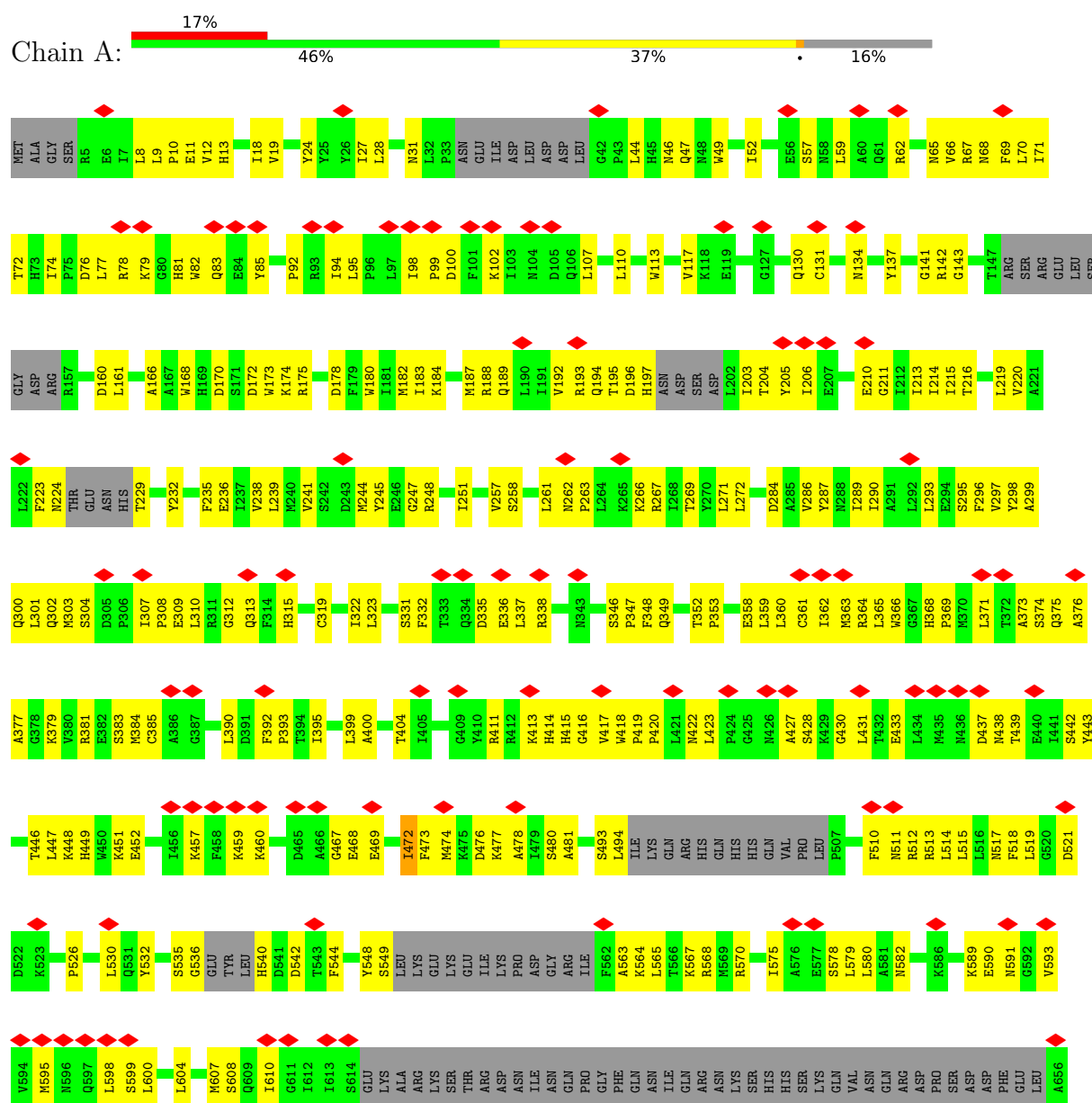
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

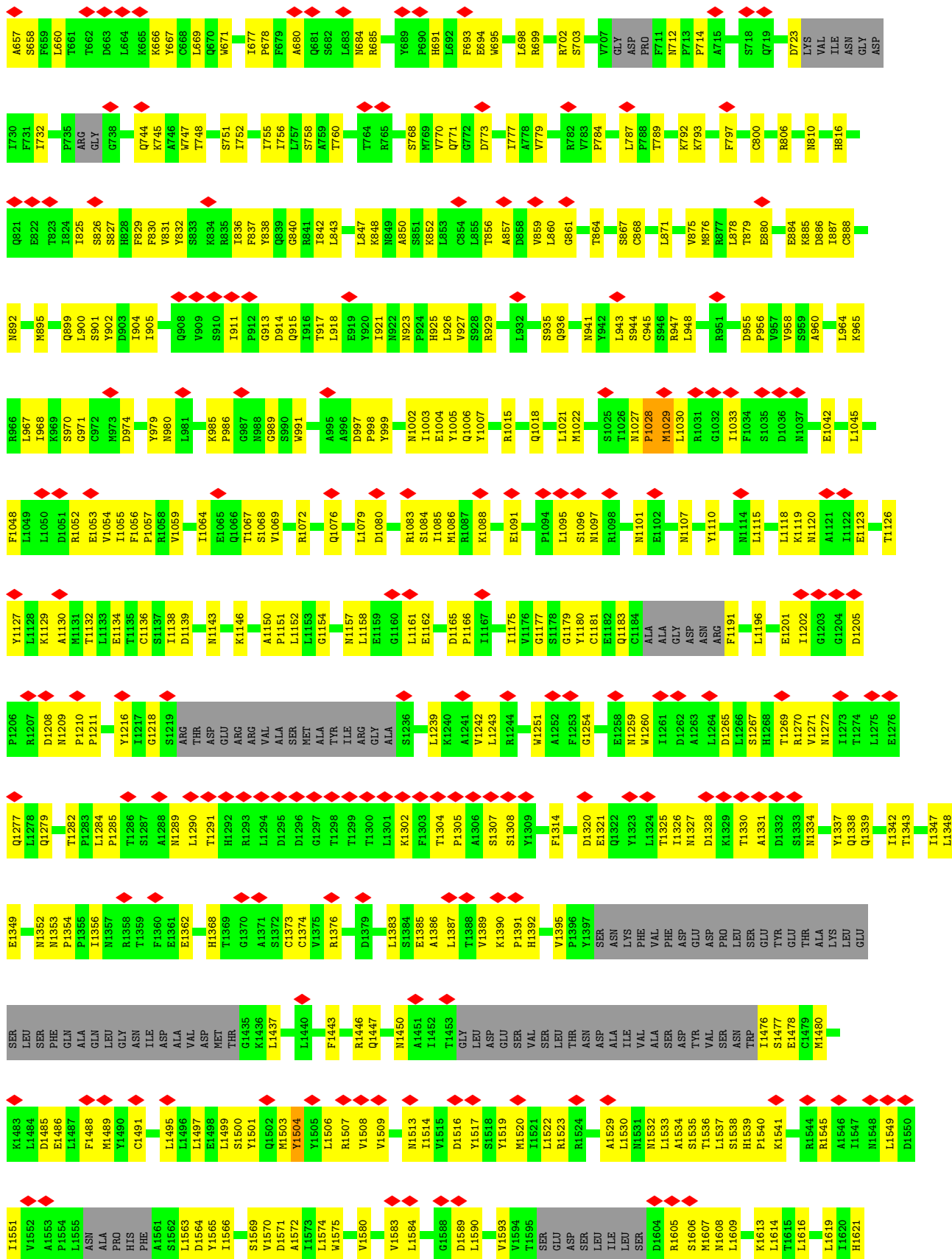
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

3 Residue-property plots

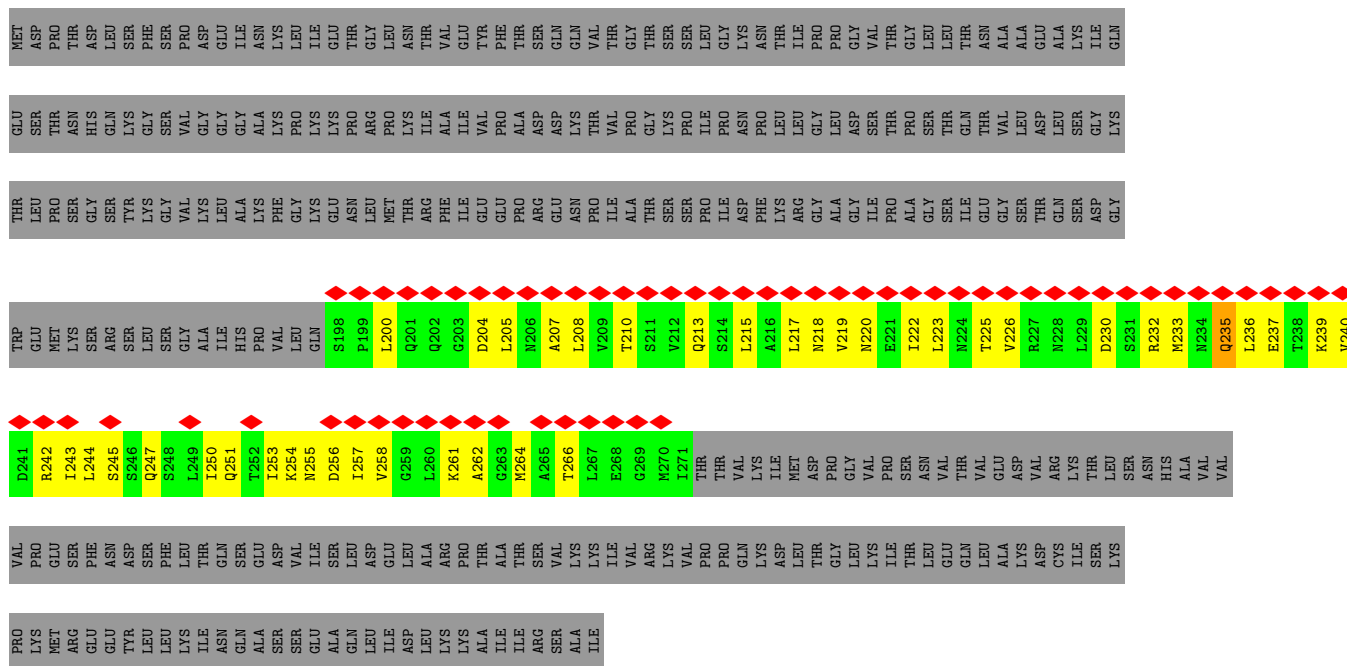
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA-directed RNA polymerase L

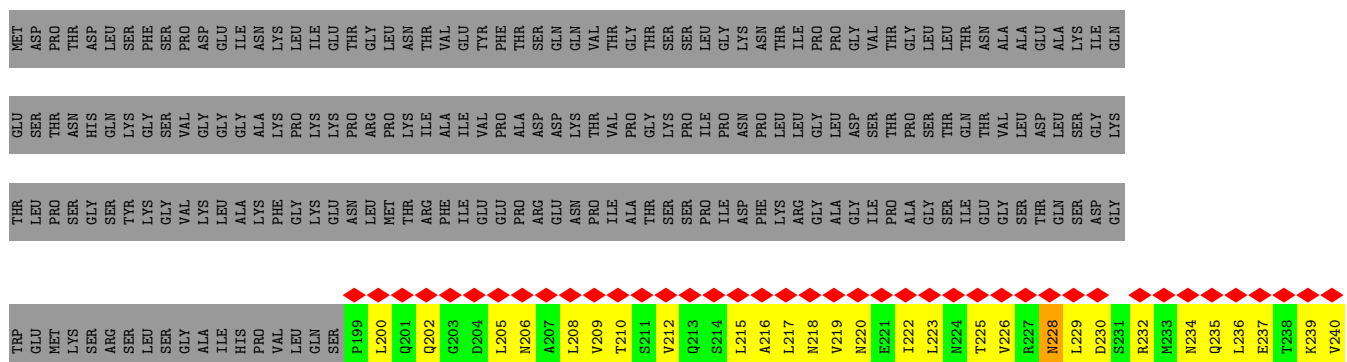




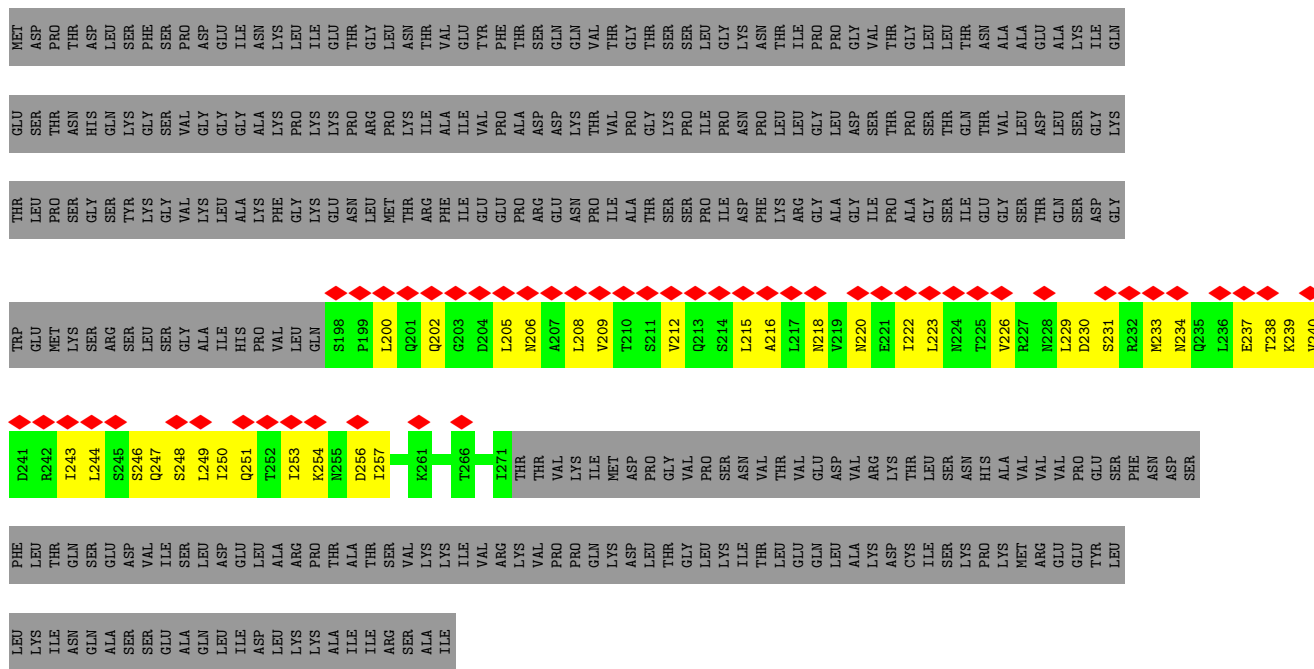
- Molecule 2: Phosphoprotein



- Molecule 2: Phosphoprotein

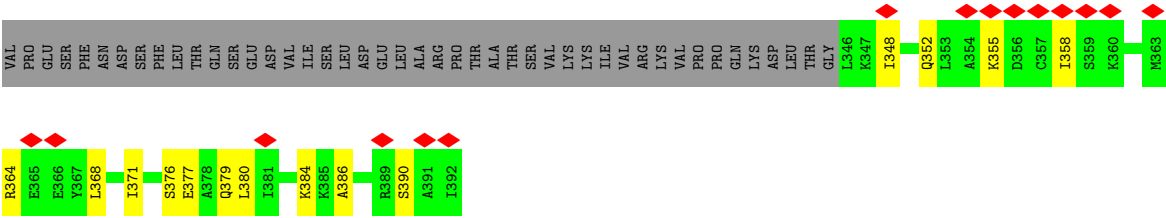


- Molecule 2: Phosphoprotein



- Molecule 2: Phosphoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	403.2, 403.2, 403.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/15416	0.53	5/20905 (0.0%)
2	B	0.18	0/575	0.42	0/776
2	C	0.18	0/588	0.44	0/794
2	D	0.16	0/575	0.43	0/776
2	E	0.17	0/588	0.43	0/794
2	F	0.14	0/375	0.44	0/498
All	All	0.22	0/18117	0.51	5/24543 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1737	ILE	N-CA-C	-5.83	108.17	113.71
1	A	1736	ILE	CA-C-N	5.24	128.87	121.53
1	A	1736	ILE	C-N-CA	5.24	128.87	121.53
1	A	304	SER	CA-C-N	5.04	127.24	120.58
1	A	304	SER	C-N-CA	5.04	127.24	120.58

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	15103	0	15272	717	0
2	B	569	0	600	41	0
2	C	582	0	611	43	0
2	D	569	0	600	39	0
2	E	582	0	611	34	0
2	F	374	0	414	9	0
3	A	2	0	0	0	0
All	All	17781	0	18108	847	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 24.

All (847) 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:1739:ILE:HD11	1:A:1972:VAL:CG1	1.47	1.43
1:A:1744:ALA:O	1:A:1964:TRP:CE2	1.89	1.25
1:A:1739:ILE:CD1	1:A:1972:VAL:HG12	1.69	1.22
1:A:1744:ALA:O	1:A:1964:TRP:CZ2	2.03	1.10
1:A:1971:THR:HG22	1:A:1988:ILE:HD13	1.34	1.09
1:A:1744:ALA:O	1:A:1964:TRP:NE1	1.89	1.06
1:A:1737:ILE:CG2	1:A:1972:VAL:CG1	2.34	1.05
1:A:1191:PHE:O	1:A:1321:GLU:HB2	1.57	1.05
1:A:1737:ILE:CG2	1:A:1972:VAL:HG12	1.88	1.03
1:A:1191:PHE:O	1:A:1321:GLU:CB	2.06	1.02
1:A:1737:ILE:HG23	1:A:1739:ILE:HD13	1.37	1.01
1:A:1954:THR:O	1:A:1958:THR:HG23	1.60	1.01
1:A:1739:ILE:HD11	1:A:1972:VAL:HG12	0.99	0.96
1:A:1956:PHE:O	1:A:1960:ILE:HG12	1.67	0.94
1:A:1619:LEU:O	1:A:1623:ASN:HB2	1.66	0.94
1:A:1971:THR:HG22	1:A:1988:ILE:CD1	1.98	0.94
1:A:211:GLY:HA2	1:A:223:PHE:O	1.67	0.94
1:A:1739:ILE:CD1	1:A:1972:VAL:CG1	2.37	0.92
1:A:1737:ILE:HG21	1:A:1972:VAL:CG1	2.02	0.88
1:A:1191:PHE:O	1:A:1321:GLU:CG	2.22	0.87
1:A:1745:ASN:HB3	1:A:1964:TRP:CZ2	2.09	0.86
1:A:1739:ILE:HD11	1:A:1972:VAL:HG11	1.55	0.86
1:A:1745:ASN:HB3	1:A:1964:TRP:CH2	2.10	0.85
1:A:1737:ILE:HG22	1:A:1972:VAL:CG1	2.06	0.85
1:A:457:LYS:H	1:A:685:ARG:HG2	1.40	0.85
1:A:1660:LEU:O	1:A:1663:PHE:HB2	1.78	0.84
1:A:1743:ASN:O	1:A:1743:ASN:ND2	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1183:GLN:HE21	1:A:1183:GLN:HA	1.44	0.83
1:A:590:GLU:HG3	1:A:756:ILE:HD11	1.63	0.81
1:A:1030:LEU:HA	1:A:1033:ILE:HD13	1.62	0.80
1:A:1737:ILE:CG2	1:A:1972:VAL:HG13	2.13	0.78
1:A:332:PHE:HB3	1:A:336:GLU:HB2	1.66	0.78
1:A:1737:ILE:HG22	1:A:1972:VAL:HG13	1.66	0.78
1:A:1816:THR:HG22	1:A:1851:PHE:HD1	1.49	0.77
1:A:1737:ILE:HD11	1:A:2022:ARG:HB3	1.65	0.77
1:A:1971:THR:CG2	1:A:1988:ILE:HD13	2.14	0.76
1:A:418:TRP:O	1:A:420:PRO:HD3	1.85	0.76
1:A:1181:CYS:SG	1:A:1368:HIS:NE2	2.58	0.76
1:A:1920:GLN:NE2	1:A:1922:CYS:SG	2.59	0.76
1:A:1737:ILE:CG2	1:A:1739:ILE:HD13	2.16	0.75
2:B:212:VAL:HG21	2:C:208:LEU:HD12	1.68	0.75
1:A:2158:GLN:O	1:A:2161:GLU:O	2.04	0.75
1:A:1737:ILE:HG23	1:A:1739:ILE:CD1	2.16	0.74
1:A:1243:LEU:HG	1:A:1285:PRO:HG3	1.68	0.74
1:A:1744:ALA:C	1:A:1964:TRP:CZ2	2.66	0.74
1:A:10:PRO:O	1:A:188:ARG:NH2	2.20	0.73
1:A:1745:ASN:CA	1:A:1964:TRP:CZ2	2.71	0.73
1:A:1539:HIS:CE1	1:A:1766:LEU:H	2.05	0.73
1:A:514:LEU:O	1:A:518:PHE:HB3	1.88	0.73
1:A:1519:TYR:HB3	1:A:1523:ARG:HH21	1.54	0.73
1:A:1745:ASN:HA	1:A:1964:TRP:CZ2	2.24	0.72
2:F:386:ALA:O	2:F:390:SER:HB2	1.89	0.72
1:A:2158:GLN:O	1:A:2161:GLU:C	2.32	0.72
1:A:684:ASN:HD21	1:A:691:HIS:H	1.36	0.72
1:A:11:GLU:O	1:A:188:ARG:NH1	2.23	0.71
1:A:1897:ILE:O	1:A:1899:ARG:NH1	2.23	0.71
1:A:784:PRO:O	1:A:792:LYS:NZ	2.24	0.71
1:A:206:ILE:HB	1:A:213:ILE:HB	1.72	0.71
1:A:287:TYR:O	1:A:290:ILE:HB	1.91	0.71
1:A:1191:PHE:C	1:A:1321:GLU:HB2	2.14	0.71
2:F:355:LYS:HA	2:F:364:ARG:HD3	1.72	0.71
1:A:1500:SER:HA	1:A:1503:MET:HG2	1.73	0.70
1:A:1533:LEU:HD11	1:A:1565:TYR:HB3	1.72	0.70
1:A:1569:SER:O	1:A:1572:ALA:HB3	1.92	0.70
1:A:1254:GLY:O	1:A:1259:ASN:ND2	2.25	0.70
2:C:243:ILE:O	2:C:247:GLN:NE2	2.24	0.70
1:A:374:SER:OG	1:A:375:GLN:OE1	2.07	0.70
1:A:1744:ALA:H	1:A:1964:TRP:HE1	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1768:ALA:HB3	1:A:1979:ASP:HB2	1.75	0.69
1:A:346:SER:O	1:A:349:GLN:NE2	2.25	0.69
1:A:1537:LEU:O	1:A:1763:ASN:ND2	2.25	0.69
1:A:1743:ASN:HD22	1:A:1743:ASN:C	2.01	0.69
1:A:885:LYS:NZ	1:A:948:LEU:O	2.24	0.69
1:A:1183:GLN:HA	1:A:1183:GLN:NE2	2.06	0.69
1:A:2207:LEU:N	1:A:2207:LEU:HD23	2.08	0.69
1:A:92:PRO:HB2	1:A:95:LEU:HB2	1.75	0.68
1:A:82:TRP:HB3	1:A:85:TYR:HB3	1.74	0.68
1:A:847:LEU:O	1:A:850:ALA:HB3	1.93	0.68
1:A:1571:ASP:O	1:A:1574:LEU:HB3	1.91	0.68
1:A:307:ILE:HD12	1:A:308:PRO:HD2	1.76	0.68
1:A:257:VAL:HG11	1:A:887:ILE:HD12	1.75	0.68
1:A:417:VAL:HG23	1:A:419:PRO:HD3	1.75	0.68
1:A:204:THR:HB	1:A:215:ILE:HB	1.76	0.68
1:A:1022:MET:HE3	1:A:1076:GLN:HA	1.74	0.68
1:A:1270:ARG:NH1	1:A:1270:ARG:O	2.27	0.68
1:A:323:LEU:HD13	1:A:337:LEU:HD21	1.75	0.68
1:A:1745:ASN:CB	1:A:1964:TRP:CZ2	2.78	0.68
1:A:1771:HIS:O	1:A:1775:ARG:NH1	2.27	0.68
1:A:1784:TRP:HB3	1:A:1814:SER:HA	1.75	0.68
1:A:1971:THR:H	1:A:1988:ILE:HG12	1.59	0.68
1:A:1446:ARG:NH1	1:A:1593:VAL:O	2.27	0.67
1:A:871:LEU:HD21	1:A:895:MET:HG3	1.76	0.67
1:A:1737:ILE:CG2	1:A:1739:ILE:CD1	2.73	0.67
1:A:1747:GLU:HG3	1:A:2016:THR:HG23	1.76	0.67
2:C:254:LYS:HA	2:C:257:ILE:HD12	1.77	0.67
2:B:219:VAL:HG21	2:C:215:LEU:HD12	1.75	0.67
1:A:11:GLU:HA	1:A:859:VAL:HG23	1.77	0.67
1:A:1731:CYS:N	1:A:1785:TYR:HH	1.93	0.67
1:A:1827:ILE:HD13	1:A:1851:PHE:CE2	2.29	0.67
1:A:1501:TYR:HB2	1:A:1614:LEU:HG	1.75	0.67
2:D:251:GLN:O	2:D:255:ASN:ND2	2.28	0.66
1:A:1680:TYR:HB3	1:A:1684:ARG:HH21	1.60	0.66
1:A:189:GLN:HE22	1:A:193:ARG:HE	1.42	0.66
1:A:1629:LYS:NZ	1:A:1630:ILE:O	2.28	0.66
1:A:864:THR:H	1:A:1107:ASN:HD21	1.41	0.66
1:A:196:ASP:O	1:A:197:HIS:ND1	2.29	0.66
1:A:1534:ALA:HB2	1:A:1760:ASN:HB2	1.78	0.66
1:A:1745:ASN:CB	1:A:1964:TRP:CH2	2.78	0.66
2:B:258:VAL:HA	2:B:261:LYS:HE2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:ASN:ND2	1:A:691:HIS:H	1.94	0.65
1:A:1739:ILE:HD11	1:A:1972:VAL:CB	2.26	0.65
1:A:1750:PRO:HA	1:A:2017:LEU:HB2	1.78	0.65
1:A:880:GLU:HG3	1:A:1308:SER:HB3	1.78	0.65
1:A:980:ASN:HD21	1:A:1120:ASN:HA	1.62	0.65
1:A:658:SER:OG	1:A:779:VAL:O	2.14	0.65
1:A:2225:CYS:SG	1:A:2226:HIS:N	2.70	0.65
1:A:1905:CYS:HB2	1:A:1933:THR:HA	1.79	0.65
2:D:200:LEU:HD21	2:E:200:LEU:H	1.62	0.65
1:A:413:LYS:O	1:A:414:HIS:ND1	2.31	0.64
1:A:1021:LEU:HD23	1:A:1079:LEU:HD13	1.79	0.64
1:A:1476:ILE:O	1:A:1535:SER:OG	2.11	0.64
1:A:1943:VAL:HG11	1:A:1988:ILE:HD12	1.79	0.64
1:A:400:ALA:HB1	1:A:452:GLU:HG2	1.79	0.64
1:A:476:ASP:HB2	1:A:515:LEU:HB2	1.79	0.64
1:A:1731:CYS:SG	1:A:1733:ASN:ND2	2.70	0.64
1:A:856:THR:HG22	1:A:857:ALA:H	1.61	0.64
1:A:1566:ILE:O	1:A:1569:SER:OG	2.13	0.64
1:A:1129:LYS:HA	1:A:1132:THR:HG22	1.79	0.63
1:A:1741:GLU:HG3	1:A:1744:ALA:HB2	1.80	0.63
2:D:257:ILE:HG13	2:E:256:ASP:HB3	1.80	0.63
1:A:137:TYR:HD1	1:A:141:GLY:HA2	1.62	0.63
1:A:1744:ALA:N	1:A:1964:TRP:HE1	1.95	0.63
1:A:258:SER:HA	1:A:261:LEU:HD13	1.79	0.63
1:A:2208:THR:OG1	1:A:2210:PRO:HD2	1.98	0.63
1:A:1284:LEU:O	1:A:1681:TYR:OH	2.16	0.63
1:A:876:MET:O	1:A:879:THR:OG1	2.12	0.63
1:A:31:ASN:O	1:A:67:ARG:NH2	2.30	0.62
1:A:1762:HIS:ND1	1:A:1762:HIS:O	2.31	0.62
1:A:447:LEU:HD22	1:A:760:THR:HG22	1.81	0.62
1:A:299:ALA:O	1:A:302:GLN:HB3	1.99	0.62
1:A:1030:LEU:O	1:A:1033:ILE:HB	2.00	0.62
1:A:1746:LEU:CB	1:A:1748:LYS:NZ	2.63	0.62
1:A:695:TRP:O	1:A:698:LEU:HB3	2.00	0.62
1:A:1331:ALA:HA	1:A:1334:ASN:HB2	1.81	0.62
2:C:257:ILE:HD13	2:D:253:ILE:HG12	1.82	0.62
2:D:200:LEU:HD13	2:D:202:GLN:HB2	1.81	0.62
2:D:205:LEU:HD13	2:D:208:LEU:HD12	1.82	0.62
1:A:838:TYR:HB3	1:A:843:LEU:HD21	1.81	0.62
1:A:1042:GLU:HG2	1:A:1064:ILE:HD11	1.81	0.62
1:A:1054:VAL:H	1:A:1383:LEU:HD13	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1136:CYS:SG	1:A:1374:CYS:HB3	2.39	0.61
1:A:1210:PRO:HG2	1:A:1211:PRO:HD3	1.82	0.61
1:A:1854:SER:O	1:A:1858:LYS:NZ	2.33	0.61
1:A:399:LEU:HD13	1:A:678:PRO:HB2	1.82	0.61
2:E:218:ASN:O	2:E:222:ILE:HG12	2.00	0.61
1:A:519:LEU:O	1:A:1027:ASN:ND2	2.32	0.61
1:A:806:ARG:O	1:A:810:ASN:ND2	2.34	0.61
1:A:411:ARG:NH1	1:A:415:HIS:O	2.34	0.61
2:D:248:SER:HB3	2:D:251:GLN:HE21	1.64	0.61
1:A:1613:LYS:NZ	1:A:1634:SER:O	2.28	0.61
2:E:253:ILE:O	2:E:257:ILE:HG12	2.00	0.60
1:A:768:SER:HB2	1:A:777:ILE:HG13	1.83	0.60
1:A:657:ALA:HB1	1:A:827:SER:HB2	1.82	0.60
1:A:986:PRO:HB2	1:A:1151:PRO:HG3	1.83	0.60
1:A:332:PHE:HE2	1:A:335:ASP:HB2	1.65	0.60
1:A:904:ILE:HD11	1:A:917:THR:HA	1.81	0.60
1:A:1028:PRO:O	1:A:1030:LEU:N	2.34	0.60
2:C:213:GLN:O	2:C:217:LEU:HG	2.01	0.60
1:A:381:ARG:NE	1:A:723:ASP:OD2	2.35	0.60
1:A:476:ASP:OD1	1:A:477:LYS:N	2.34	0.60
1:A:945:CYS:O	1:A:948:LEU:CB	2.50	0.60
1:A:1029:MET:HE2	1:A:1395:VAL:HA	1.84	0.60
1:A:1541:LYS:O	1:A:1545:ARG:N	2.27	0.60
1:A:287:TYR:HD1	1:A:290:ILE:HD12	1.66	0.60
1:A:549:SER:OG	1:A:564:LYS:NZ	2.34	0.60
1:A:1820:TYR:CZ	1:A:2060:ILE:HB	2.37	0.60
1:A:1272:ASN:HB3	1:A:1395:VAL:O	2.01	0.60
1:A:1022:MET:HG3	1:A:1076:GLN:HG2	1.83	0.60
2:E:216:ALA:O	2:E:220[B]:ASN:ND2	2.35	0.60
1:A:130:GLN:O	1:A:134:ASN:ND2	2.35	0.59
1:A:235:PHE:O	1:A:238:VAL:HG22	2.02	0.59
1:A:964:LEU:O	1:A:968:ILE:HG12	2.02	0.59
2:B:261:LYS:NZ	2:C:256:ASP:OD1	2.34	0.59
1:A:914:ASP:OD1	1:A:915:GLN:N	2.35	0.59
1:A:1772:HIS:HA	1:A:1775:ARG:HH22	1.67	0.59
1:A:1739:ILE:HD13	1:A:1972:VAL:HG12	1.78	0.59
1:A:1201:GLU:HG3	1:A:1202:ILE:H	1.67	0.59
1:A:251:ILE:HG21	1:A:362:ILE:HG21	1.83	0.59
1:A:418:TRP:NE1	1:A:437:ASP:OD1	2.35	0.59
1:A:433:GLU:HG3	1:A:438:ASN:HD22	1.68	0.59
1:A:1191:PHE:O	1:A:1321:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:THR:OG1	1:A:219:LEU:N	2.36	0.58
2:E:222:ILE:O	2:E:226:VAL:HG23	2.03	0.58
1:A:184:LYS:O	1:A:188:ARG:HG3	2.03	0.58
1:A:1744:ALA:C	1:A:1964:TRP:HZ2	2.10	0.58
1:A:12:VAL:O	1:A:13:HIS:ND1	2.36	0.58
1:A:875:VAL:O	1:A:878:LEU:HB3	2.03	0.58
1:A:1265:ASP:OD2	1:A:1390:LYS:NZ	2.35	0.58
1:A:78:ARG:NH2	1:A:79:LYS:O	2.37	0.58
1:A:384:MET:HG3	1:A:385:CYS:H	1.68	0.58
1:A:1564:ASP:OD1	1:A:1565:TYR:N	2.36	0.58
1:A:457:LYS:O	1:A:685:ARG:NE	2.37	0.58
1:A:536:GLY:O	1:A:540:HIS:N	2.37	0.58
1:A:2100:ILE:HD11	1:A:2192:ALA:HB2	1.84	0.58
1:A:358:GLU:CD	1:A:847:LEU:H	2.10	0.58
2:E:240:VAL:HA	2:E:243:ILE:HG22	1.84	0.58
1:A:298:TYR:O	1:A:302:GLN:N	2.36	0.58
1:A:319:CYS:O	1:A:323:LEU:HG	2.03	0.58
1:A:901:SER:O	1:A:905:ILE:HG12	2.03	0.58
1:A:1045:LEU:HD22	1:A:1064:ILE:HD12	1.86	0.58
1:A:1745:ASN:HB3	1:A:1964:TRP:HZ2	1.67	0.58
1:A:99:PRO:HB3	1:A:102:LYS:HD3	1.85	0.57
1:A:286:VAL:HA	1:A:289:ILE:HG12	1.85	0.57
1:A:989:GLY:HA3	1:A:1002:ASN:HD21	1.68	0.57
1:A:1136:CYS:SG	1:A:1373:CYS:SG	3.01	0.57
2:C:215:LEU:O	2:C:219:VAL:HG23	2.04	0.57
1:A:219:LEU:HD11	1:A:232:TYR:HB3	1.86	0.57
1:A:166:ALA:O	1:A:170:ASP:N	2.37	0.57
1:A:1539:HIS:CE1	1:A:1763:ASN:HA	2.40	0.57
1:A:1793:TYR:OH	1:A:1971:THR:HG21	2.04	0.57
1:A:2148:LEU:HB2	1:A:2153:ARG:HH11	1.68	0.57
1:A:1816:THR:HG22	1:A:1851:PHE:CD1	2.37	0.57
1:A:1959:LEU:HD23	1:A:1959:LEU:O	2.04	0.57
2:B:200:LEU:HD11	2:C:200:LEU:HD22	1.87	0.57
1:A:1737:ILE:HG23	1:A:1972:VAL:HG12	1.84	0.57
1:A:1832:LEU:HB2	1:A:1887:ILE:HG13	1.87	0.57
1:A:595:MET:HG2	1:A:599:SER:HB2	1.87	0.57
1:A:1177:GLY:HA2	1:A:1919:ASN:HD21	1.69	0.57
1:A:1746:LEU:HB2	1:A:1748:LYS:NZ	2.20	0.57
1:A:892:ASN:ND2	1:A:944:SER:OG	2.38	0.57
1:A:991:TRP:NE1	1:A:1152:LEU:HD11	2.20	0.57
1:A:925:HIS:HE1	1:A:929:ARG:HE	1.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:VAL:HG21	1:A:771:GLN:HE21	1.70	0.56
1:A:468:GLU:OE1	1:A:468:GLU:N	2.38	0.56
1:A:1813:ALA:HB3	1:A:1815:MET:HE1	1.86	0.56
1:A:1911:ASP:OD1	1:A:1911:ASP:N	2.38	0.56
1:A:1951:LEU:HB3	1:A:1952:PRO:HD3	1.86	0.56
1:A:71:ILE:HD13	1:A:74:ILE:HD11	1.87	0.56
1:A:1538:SER:HA	1:A:1763:ASN:ND2	2.20	0.56
1:A:1138:ILE:HD12	1:A:1138:ILE:H	1.71	0.56
1:A:1507:ARG:NH2	1:A:1621:HIS:O	2.35	0.56
1:A:2001:SER:HB3	1:A:2004:THR:HG23	1.88	0.56
1:A:1807:ILE:HB	1:A:1910:VAL:HG12	1.87	0.56
2:B:249:LEU:O	2:B:253:ILE:HG12	2.06	0.56
1:A:137:TYR:HA	1:A:141:GLY:HA2	1.86	0.56
1:A:1499:LEU:HD11	1:A:1517:TYR:HE2	1.71	0.56
1:A:364:ARG:HH21	1:A:368:HIS:CE1	2.24	0.56
2:E:230:ASP:O	2:E:233:MET:HG3	2.05	0.56
1:A:9:LEU:HD12	1:A:188:ARG:HE	1.72	0.55
1:A:1068:SER:OG	1:A:1072:ARG:NH2	2.39	0.55
1:A:411:ARG:HD3	1:A:418:TRP:CD1	2.42	0.55
1:A:1115:LEU:O	1:A:1118:LEU:HB2	2.06	0.55
1:A:1497:LEU:HB3	1:A:1614:LEU:HD23	1.86	0.55
1:A:1734:ASP:HB2	1:A:1974:ARG:HG3	1.89	0.55
1:A:1158:LEU:H	1:A:1158:LEU:HD23	1.71	0.55
2:B:229:LEU:O	2:B:233:MET:HG3	2.07	0.55
1:A:1745:ASN:HB3	1:A:1964:TRP:HH2	1.65	0.55
1:A:160:ASP:OD1	1:A:161:LEU:N	2.37	0.55
1:A:1920:GLN:OE1	1:A:1923:LEU:N	2.40	0.55
1:A:1052:ARG:NH1	1:A:1386:ALA:O	2.39	0.55
1:A:400:ALA:O	1:A:404:THR:HG23	2.07	0.55
1:A:542:ASP:OD1	1:A:542:ASP:N	2.40	0.55
1:A:544:PHE:CZ	1:A:699:ARG:HB3	2.42	0.55
1:A:789:THR:O	1:A:793:LYS:HG2	2.07	0.55
1:A:979:TYR:HH	1:A:1132:THR:HG1	1.51	0.55
1:A:1769:PRO:HB2	1:A:2216:TRP:CD1	2.42	0.55
1:A:113:TRP:CH2	1:A:902:TYR:HB2	2.42	0.55
1:A:1539:HIS:NE2	1:A:1763:ASN:HA	2.21	0.55
1:A:1632:GLY:H	1:A:1638:LYS:HZ2	1.53	0.54
1:A:1658:GLU:O	1:A:1661:SER:OG	2.15	0.54
1:A:1849:THR:O	1:A:1853:GLU:HG2	2.08	0.54
1:A:955:ASP:OD2	1:A:958:VAL:N	2.30	0.54
1:A:864:THR:H	1:A:1107:ASN:ND2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1499:LEU:HD21	1:A:1517:TYR:HD2	1.72	0.54
2:D:253:ILE:HG21	2:E:253:ILE:HG23	1.88	0.54
1:A:31:ASN:HB2	1:A:67:ARG:HD2	1.89	0.54
1:A:469:GLU:OE1	1:A:582:ASN:ND2	2.40	0.54
1:A:1827:ILE:HD13	1:A:1851:PHE:HE2	1.71	0.54
1:A:1963:LEU:HD23	1:A:1970:ILE:HD12	1.90	0.54
2:D:250:ILE:HD12	2:E:249:LEU:HD22	1.88	0.54
1:A:49:TRP:CE3	1:A:52:ILE:HD11	2.43	0.54
1:A:476:ASP:OD1	1:A:514:LEU:HB3	2.07	0.54
1:A:472:ILE:HG21	1:A:578:SER:HB3	1.89	0.54
1:A:2029:GLY:HA2	1:A:2032:LYS:HD2	1.90	0.54
2:C:251:GLN:O	2:C:254:LYS:HG2	2.07	0.54
1:A:192:VAL:O	1:A:195:THR:OG1	2.17	0.54
1:A:2096:LEU:HD11	1:A:2188:ALA:HB1	1.89	0.54
2:C:232:ARG:HH21	2:C:236:LEU:HD23	1.71	0.54
2:E:237:GLU:HA	2:E:240:VAL:HG12	1.89	0.54
1:A:1055:ILE:HG13	1:A:1158:LEU:HA	1.89	0.54
2:E:202:GLN:HB2	2:E:206:ASN:OD1	2.07	0.54
1:A:1509:VAL:H	1:A:1513:ASN:HB2	1.72	0.53
1:A:1619:LEU:O	1:A:1623:ASN:CB	2.48	0.53
2:B:248:SER:O	2:B:252:THR:HG23	2.08	0.53
1:A:353:PRO:HB2	1:A:843:LEU:HD11	1.90	0.53
1:A:580:LEU:HD22	1:A:745:LYS:HB2	1.88	0.53
1:A:1530:LEU:HG	1:A:1760:ASN:HB3	1.90	0.53
1:A:1478:GLU:C	1:A:1480:MET:H	2.16	0.53
1:A:1532:ASN:O	1:A:1536:THR:HG22	2.08	0.53
1:A:2041:ILE:O	1:A:2045:VAL:HG23	2.08	0.53
1:A:886:ASP:OD1	1:A:887:ILE:N	2.40	0.53
1:A:956:PRO:O	1:A:960:ALA:N	2.35	0.53
1:A:1605:ARG:HA	1:A:1608:ASN:ND2	2.23	0.53
1:A:272:LEU:HA	1:A:366:TRP:HZ2	1.73	0.53
1:A:1852:ILE:HG13	1:A:1856:PRO:HG3	1.90	0.53
1:A:2054:SER:HA	1:A:2057:ASN:ND2	2.23	0.53
2:D:225:THR:O	2:D:228[A]:ASN:ND2	2.41	0.53
1:A:247:GLY:O	1:A:251:ILE:HG12	2.08	0.53
1:A:224:ASN:OD1	1:A:229:THR:OG1	2.26	0.53
1:A:332:PHE:CE2	1:A:335:ASP:HB2	2.43	0.53
1:A:1115:LEU:HD12	1:A:1118:LEU:HD13	1.90	0.53
1:A:1362:GLU:H	1:A:1362:GLU:CD	2.16	0.53
1:A:580:LEU:HB3	1:A:745:LYS:HD2	1.90	0.53
1:A:2024:ASN:OD1	1:A:2025:GLN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLN:OE1	1:A:375:GLN:N	2.40	0.53
1:A:476:ASP:OD2	1:A:515:LEU:N	2.38	0.53
1:A:518:PHE:CD2	1:A:519:LEU:HD12	2.44	0.53
2:B:215:LEU:O	2:B:219:VAL:HG22	2.09	0.53
2:D:248:SER:O	2:D:252:THR:HG23	2.09	0.53
1:A:411:ARG:HD3	1:A:418:TRP:HD1	1.73	0.52
2:B:251:GLN:O	2:B:255:ASN:ND2	2.41	0.52
1:A:95:LEU:O	1:A:98:ILE:HB	2.10	0.52
1:A:381:ARG:HB2	1:A:732:ILE:HG12	1.89	0.52
1:A:1056:PHE:HB2	1:A:1059:VAL:HG12	1.91	0.52
1:A:1745:ASN:CA	1:A:1964:TRP:HZ2	2.20	0.52
2:B:254:LYS:O	2:B:258:VAL:HG23	2.09	0.52
2:D:249:LEU:O	2:D:253:ILE:HG13	2.09	0.52
1:A:517:ASN:OD1	1:A:518:PHE:N	2.42	0.52
2:F:358:ILE:O	2:F:364:ARG:NH1	2.30	0.52
1:A:671:TRP:CH2	1:A:747:TRP:HA	2.45	0.52
1:A:1516:ASP:O	1:A:1520:MET:HG2	2.09	0.52
1:A:1737:ILE:HG22	1:A:1972:VAL:HG12	1.73	0.52
1:A:1745:ASN:HA	1:A:1964:TRP:CH2	2.45	0.52
2:C:230:ASP:OD1	2:D:225:THR:HG23	2.10	0.52
2:C:250:ILE:O	2:C:253:ILE:HG22	2.09	0.52
1:A:411:ARG:HD2	1:A:416:GLY:HA3	1.90	0.52
1:A:1731:CYS:N	1:A:1785:TYR:OH	2.41	0.52
1:A:1740:ILE:HD13	1:A:1741:GLU:H	1.75	0.52
2:B:234:ASN:OD1	2:B:235:GLN:N	2.42	0.52
1:A:945:CYS:O	1:A:948:LEU:HB2	2.09	0.52
1:A:967:LEU:O	1:A:971:GLY:N	2.39	0.52
2:B:219:VAL:HA	2:B:222:ILE:HG22	1.90	0.52
2:C:205:LEU:HD21	2:D:205:LEU:HD11	1.92	0.52
1:A:76:ASP:HA	1:A:79:LYS:HE3	1.91	0.52
1:A:472:ILE:HG13	1:A:473:PHE:H	1.74	0.52
1:A:567:LYS:HG3	1:A:568:ARG:N	2.24	0.52
1:A:831:VAL:HG13	1:A:836:ILE:HG22	1.92	0.52
2:C:258:VAL:HA	2:C:261:LYS:HE3	1.91	0.52
1:A:427:ALA:HB1	1:A:430:GLY:H	1.75	0.52
1:A:481:ALA:HB2	1:A:510:PHE:CE1	2.45	0.52
1:A:671:TRP:NE1	1:A:816:HIS:HE1	2.08	0.52
1:A:1971:THR:HG23	1:A:1988:ILE:HG21	1.92	0.52
2:C:242:ARG:O	2:C:245:SER:OG	2.26	0.52
1:A:11:GLU:OE1	1:A:1083:ARG:NH2	2.35	0.51
1:A:1637:GLU:HG3	1:A:1638:LYS:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:SER:HB3	1:A:1269:THR:HG22	1.90	0.51
1:A:2148:LEU:HD13	1:A:2153:ARG:NH1	2.25	0.51
1:A:1972:VAL:HG22	1:A:1985:VAL:HG22	1.92	0.51
1:A:480:SER:HB3	1:A:564:LYS:HG3	1.92	0.51
1:A:830:PHE:HB3	1:A:837:PHE:HB2	1.93	0.51
1:A:1953:PHE:HZ	1:A:2019:SER:HB2	1.76	0.51
2:B:218:ASN:ND2	2:E:220[B]:ASN:HD21	2.08	0.51
2:C:204:ASP:O	2:C:208:LEU:HB2	2.09	0.51
2:F:368:LEU:HA	2:F:371:ILE:HG22	1.93	0.51
1:A:62:ARG:NH2	1:A:194:GLN:OE1	2.26	0.51
1:A:172:ASP:HB3	1:A:173:TRP:CE3	2.45	0.51
1:A:837:PHE:CE1	1:A:842:ILE:HG12	2.45	0.51
1:A:1971:THR:HG23	1:A:1988:ILE:CG2	2.41	0.51
1:A:1485:ASP:HB2	1:A:1575:TRP:CH2	2.45	0.51
1:A:1606:SER:OG	1:A:1607:MET:SD	2.68	0.51
1:A:1915:SER:O	1:A:1955:ARG:NH1	2.39	0.51
1:A:65:ASN:HD21	1:A:203:ILE:HD11	1.75	0.51
1:A:107:LEU:HB2	1:A:110:LEU:HD13	1.93	0.51
2:C:258:VAL:O	2:C:261:LYS:HG2	2.10	0.51
1:A:442:SER:O	1:A:446:THR:HG23	2.11	0.51
1:A:1343:THR:O	1:A:1347:ILE:HG12	2.11	0.51
1:A:2208:THR:HG23	1:A:2211:ILE:HG12	1.93	0.51
1:A:459:LYS:HG3	1:A:460:LYS:HG2	1.92	0.51
1:A:789:THR:O	1:A:792:LYS:HB2	2.11	0.51
1:A:979:TYR:OH	1:A:1132:THR:OG1	2.22	0.51
1:A:1339:GLN:HA	1:A:1342:ILE:HD12	1.93	0.51
1:A:287:TYR:CD2	1:A:369:PRO:HB3	2.46	0.51
1:A:1745:ASN:CB	1:A:1964:TRP:HH2	2.21	0.51
1:A:245:TYR:HD1	1:A:248:ARG:HD2	1.75	0.50
1:A:1127:TYR:HA	1:A:1130:ALA:HB3	1.91	0.50
2:B:249:LEU:HD22	2:E:254:LYS:HD3	1.93	0.50
2:D:215:LEU:O	2:D:219:VAL:HG23	2.11	0.50
1:A:57:SER:C	1:A:59:LEU:H	2.19	0.50
1:A:364:ARG:HH21	1:A:368:HIS:HE1	1.60	0.50
1:A:1136:CYS:SG	1:A:1373:CYS:HB2	2.51	0.50
1:A:1920:GLN:OE1	1:A:1922:CYS:N	2.45	0.50
2:C:237:GLU:HA	2:D:236:LEU:HD21	1.92	0.50
1:A:580:LEU:HD22	1:A:745:LYS:HD2	1.93	0.50
1:A:867:SER:OG	1:A:868:CYS:N	2.44	0.50
1:A:214:ILE:O	1:A:220:VAL:HA	2.11	0.50
1:A:359:LEU:HD23	1:A:363:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1690:ILE:HG23	1:A:1691:ARG:HE	1.76	0.50
1:A:332:PHE:HD2	1:A:336:GLU:H	1.60	0.50
1:A:589:LYS:O	1:A:591:ASN:ND2	2.45	0.50
1:A:751:SER:O	1:A:755:ILE:HG12	2.12	0.50
2:D:219:VAL:HB	2:E:215:LEU:HD12	1.94	0.50
1:A:826:SER:OG	1:A:827:SER:N	2.44	0.50
1:A:1118:LEU:HG	1:A:1119:LYS:H	1.75	0.50
1:A:1772:HIS:HA	1:A:1775:ARG:NH2	2.26	0.50
1:A:2219:LEU:O	1:A:2223:VAL:HG23	2.12	0.50
2:C:261:LYS:HA	2:C:264:MET:HG2	1.94	0.50
1:A:771:GLN:HB2	1:A:832:TYR:OH	2.12	0.50
1:A:945:CYS:O	1:A:948:LEU:HB3	2.11	0.50
1:A:968:ILE:HD12	1:A:974:ASP:O	2.11	0.50
1:A:998:PRO:HB3	1:A:1057:PRO:HB2	1.94	0.50
1:A:1980:PRO:HB3	1:A:2034:GLU:HG3	1.94	0.50
1:A:2207:LEU:N	1:A:2207:LEU:CD2	2.73	0.50
1:A:474:MET:HA	1:A:518:PHE:CE2	2.47	0.49
1:A:467:GLY:HA2	1:A:526:PRO:HG2	1.94	0.49
1:A:1540:PRO:HG3	1:A:2162:PHE:CD2	2.47	0.49
2:B:254:LYS:NZ	2:C:256:ASP:OD2	2.32	0.49
1:A:28:LEU:HB3	1:A:49:TRP:CH2	2.47	0.49
2:E:234:ASN:O	2:E:237:GLU:HG2	2.13	0.49
1:A:296:PHE:O	1:A:299:ALA:HB3	2.13	0.49
1:A:567:LYS:HG3	1:A:568:ARG:H	1.76	0.49
1:A:1616:LEU:HD22	1:A:1642:LEU:HB2	1.94	0.49
1:A:1735:TYR:HB2	1:A:1974:ARG:HH12	1.77	0.49
1:A:1849:THR:O	1:A:1852:ILE:HG22	2.12	0.49
1:A:1779:LEU:HD11	1:A:1850:GLN:HG3	1.95	0.49
1:A:1947:LYS:HB2	1:A:1986:TYR:CE1	2.47	0.49
1:A:2054:SER:HA	1:A:2057:ASN:HD21	1.78	0.49
1:A:1139:ASP:O	1:A:1143:ASN:ND2	2.38	0.49
1:A:1856:PRO:HB2	1:A:1860:TRP:CZ2	2.48	0.49
1:A:1894:GLU:O	1:A:1897:ILE:HG22	2.13	0.49
2:B:234:ASN:HA	2:B:237:GLU:HG3	1.93	0.49
1:A:299:ALA:HB1	1:A:315:HIS:HA	1.95	0.49
1:A:513:ARG:CZ	1:A:1084:SER:HB3	2.43	0.49
1:A:1180:TYR:OH	1:A:1921:GLN:O	2.21	0.49
1:A:81:HIS:CE1	1:A:83:GLN:HG3	2.48	0.49
1:A:1334:ASN:HA	1:A:1337:TYR:HB3	1.94	0.49
1:A:8:LEU:HD11	1:A:860:LEU:HA	1.94	0.49
1:A:348:PHE:CE1	1:A:359:LEU:HD22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1507:ARG:HH21	1:A:1508:VAL:C	2.21	0.49
2:B:252:THR:HA	2:B:255:ASN:HD21	1.78	0.49
2:C:223:LEU:HA	2:C:226:VAL:HG12	1.93	0.49
1:A:315:HIS:CE1	2:F:352:GLN:HE22	2.30	0.49
1:A:744:GLN:HA	1:A:747:TRP:HB2	1.94	0.49
1:A:2152:LEU:HD11	1:A:2168:THR:HG22	1.94	0.49
1:A:297:VAL:HG11	1:A:360:LEU:HB2	1.93	0.48
1:A:352:THR:HB	1:A:353:PRO:HD2	1.94	0.48
1:A:361:CYS:HB2	1:A:848:LYS:HB2	1.95	0.48
1:A:1015:ARG:O	1:A:1018:GLN:NE2	2.46	0.48
1:A:251:ILE:HD12	1:A:847:LEU:HG	1.95	0.48
1:A:515:LEU:HD23	1:A:1085:ILE:HG12	1.95	0.48
1:A:1929:ASN:HA	1:A:1932:ILE:HG22	1.94	0.48
2:C:222:ILE:HA	2:C:225:THR:HG22	1.95	0.48
1:A:364:ARG:O	1:A:364:ARG:HD3	2.13	0.48
1:A:918:LEU:HA	1:A:921:ILE:HG22	1.95	0.48
2:B:250:ILE:HG13	2:B:251:GLN:N	2.28	0.48
2:D:234:ASN:O	2:D:237:GLU:HG2	2.12	0.48
1:A:513:ARG:HH12	1:A:1088:LYS:HB2	1.79	0.48
1:A:677:ILE:N	1:A:678:PRO:HD2	2.27	0.48
1:A:110:LEU:O	1:A:113:TRP:HB3	2.14	0.48
1:A:113:TRP:O	1:A:117:VAL:HG22	2.13	0.48
1:A:1808:ALA:N	1:A:1830:ASN:OD1	2.46	0.48
1:A:2090:THR:O	1:A:2094:THR:HG23	2.13	0.48
2:C:240:VAL:HG21	2:D:236:LEU:HD13	1.94	0.48
2:B:247:GLN:O	2:B:250:ILE:HG12	2.14	0.48
1:A:478:ALA:O	1:A:570:ARG:NH1	2.47	0.48
1:A:1806:TYR:CZ	1:A:1815:MET:HB2	2.49	0.48
1:A:44:LEU:HD23	1:A:44:LEU:H	1.78	0.48
1:A:261:LEU:HG	1:A:262:ASN:H	1.78	0.48
1:A:289:ILE:O	1:A:293:LEU:N	2.46	0.48
1:A:667:TYR:HB3	1:A:773:ASP:OD2	2.12	0.48
1:A:1353:ASN:N	1:A:1354:PRO:HD3	2.29	0.48
1:A:1920:GLN:CD	1:A:1922:CYS:H	2.22	0.48
2:C:262:ALA:O	2:C:266:THR:HG23	2.14	0.48
1:A:911:ILE:HG12	1:A:913:GLY:H	1.79	0.48
1:A:1216:TYR:OH	1:A:1338:GLN:NE2	2.47	0.48
2:B:246:SER:O	2:B:249:LEU:HG	2.14	0.48
1:A:130:GLN:HG3	1:A:134:ASN:HD21	1.78	0.48
1:A:271:LEU:HD21	1:A:363:MET:HG2	1.96	0.48
1:A:1146:LYS:HG3	1:A:1157:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1793:TYR:OH	1:A:1971:THR:CG2	2.61	0.48
1:A:2167:ILE:HD12	1:A:2199:ILE:HA	1.96	0.48
2:B:257:ILE:HG12	2:B:261:LYS:NZ	2.29	0.48
2:E:240:VAL:O	2:E:244:LEU:HD23	2.14	0.48
1:A:1088:LYS:O	1:A:1091:GLU:HB3	2.14	0.47
1:A:1165:ASP:OD1	1:A:1166:PRO:HD2	2.14	0.47
1:A:1304:THR:OG1	1:A:1305:PRO:HD3	2.14	0.47
1:A:2159:ASP:HB3	1:A:2165:PHE:H	1.79	0.47
2:D:216:ALA:HA	2:E:215:LEU:HG	1.95	0.47
1:A:10:PRO:C	1:A:188:ARG:HH22	2.23	0.47
1:A:71:ILE:HD12	1:A:77:LEU:HB2	1.95	0.47
1:A:263:PRO:O	1:A:267:ARG:HG2	2.14	0.47
1:A:535:SER:OG	1:A:536:GLY:N	2.48	0.47
1:A:1563:LEU:HB3	1:A:2027:TRP:CZ2	2.49	0.47
1:A:1739:ILE:HD13	1:A:1739:ILE:H	1.79	0.47
1:A:1818:ILE:O	1:A:1822:PHE:N	2.47	0.47
1:A:2084:PHE:HA	1:A:2087:LEU:HB3	1.97	0.47
1:A:548:TYR:HD1	1:A:563:ALA:HB2	1.79	0.47
1:A:1290:LEU:HD21	1:A:1328:ASP:HB2	1.94	0.47
1:A:1589:ASP:O	1:A:1590:LEU:HG	2.15	0.47
1:A:244:MET:HG3	1:A:365:LEU:O	2.14	0.47
1:A:1658:GLU:HG2	1:A:1659:ASN:N	2.30	0.47
2:C:261:LYS:HB2	2:C:264:MET:HE2	1.96	0.47
2:C:233:MET:HG2	2:D:229:LEU:HD22	1.97	0.47
1:A:575:ILE:O	1:A:579:LEU:HG	2.15	0.47
1:A:1181:CYS:HG	1:A:1368:HIS:CD2	2.33	0.47
1:A:1563:LEU:HG	1:A:1755:PRO:HG2	1.95	0.47
1:A:1739:ILE:HB	1:A:1970:ILE:HG12	1.96	0.47
1:A:301:LEU:HD11	1:A:353:PRO:HB3	1.96	0.47
1:A:667:TYR:HB3	1:A:773:ASP:CG	2.40	0.47
1:A:1893:VAL:HB	1:A:1928:ILE:HD11	1.96	0.47
1:A:1924:SER:O	1:A:1928:ILE:HG12	2.15	0.47
1:A:1949:SER:HB2	1:A:1984:GLU:HA	1.96	0.47
1:A:238:VAL:HA	1:A:241:VAL:HG12	1.97	0.47
1:A:376:ALA:HA	1:A:379:LYS:HD2	1.96	0.47
1:A:1211:PRO:HG2	1:A:1314:PHE:CG	2.50	0.47
1:A:1608:ASN:OD1	1:A:1609:LEU:N	2.48	0.47
1:A:1735:TYR:HB2	1:A:1974:ARG:NH1	2.30	0.47
2:C:207:ALA:O	2:C:210:THR:HG22	2.14	0.47
1:A:210:GLU:HG3	1:A:224:ASN:HB2	1.97	0.47
1:A:1126:THR:OG1	1:A:1127:TYR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1506:LEU:O	1:A:1508:VAL:HG23	2.15	0.47
1:A:2170:ILE:HG22	1:A:2199:ILE:HG21	1.96	0.47
2:B:210:THR:O	2:B:213:GLN:HG3	2.14	0.47
1:A:867:SER:OG	1:A:899:GLN:NE2	2.48	0.46
1:A:1580:VAL:O	1:A:1583:VAL:HB	2.15	0.46
1:A:1750:PRO:O	1:A:2017:LEU:HD12	2.14	0.46
1:A:1779:LEU:HG	1:A:1784:TRP:CH2	2.50	0.46
2:B:222:ILE:HD12	2:E:223:LEU:HB3	1.97	0.46
1:A:359:LEU:O	1:A:363:MET:HG3	2.15	0.46
1:A:1067:THR:HG23	1:A:1069:VAL:HG22	1.96	0.46
1:A:1320:ASP:OD1	1:A:1320:ASP:N	2.47	0.46
1:A:1437:LEU:HG	1:A:1690:ILE:HD12	1.98	0.46
1:A:1783:ALA:O	1:A:1786:LYS:HG2	2.15	0.46
2:D:209:VAL:O	2:D:212:VAL:HG22	2.16	0.46
2:E:246:SER:O	2:E:250:ILE:HG12	2.15	0.46
1:A:1267:SER:O	1:A:1271:VAL:HB	2.16	0.46
1:A:1950:TRP:HD1	1:A:1950:TRP:O	1.98	0.46
1:A:2170:ILE:HG13	1:A:2171:LEU:H	1.81	0.46
1:A:68:ASN:O	1:A:72:THR:HG23	2.14	0.46
1:A:1022:MET:HE2	1:A:1079:LEU:HD11	1.97	0.46
1:A:1028:PRO:C	1:A:1030:LEU:H	2.23	0.46
1:A:98:ILE:O	1:A:100:ASP:N	2.49	0.46
1:A:183:ILE:O	1:A:187:MET:HG3	2.15	0.46
1:A:448:LYS:O	1:A:449:HIS:ND1	2.48	0.46
1:A:694:GLU:OE1	1:A:694:GLU:N	2.49	0.46
1:A:1739:ILE:C	1:A:2022:ARG:HH12	1.93	0.46
1:A:1752:PRO:HB3	1:A:2017:LEU:HD11	1.97	0.46
1:A:658:SER:HB2	1:A:800:CYS:HB3	1.97	0.46
1:A:1048:PHE:CD2	1:A:1389:VAL:HG12	2.50	0.46
1:A:1150:ALA:O	1:A:1154:GLY:N	2.46	0.46
1:A:1643:THR:O	1:A:1647:ARG:HG2	2.14	0.46
1:A:1950:TRP:HB2	1:A:1953:PHE:HA	1.97	0.46
1:A:2051:LEU:HG	1:A:2052:PHE:H	1.79	0.46
2:B:250:ILE:HG22	2:C:250:ILE:HD11	1.97	0.46
1:A:312:GLY:HA3	2:F:384:LYS:NZ	2.31	0.46
1:A:353:PRO:HG3	1:A:838:TYR:CE1	2.50	0.46
1:A:985:LYS:HD3	1:A:986:PRO:HD2	1.97	0.46
1:A:1386:ALA:O	1:A:1387:LEU:HD22	2.16	0.46
1:A:1981:ALA:H	1:A:2030:HIS:HE1	1.63	0.46
2:B:257:ILE:HG23	2:B:261:LYS:HZ1	1.79	0.46
1:A:142:ARG:NH1	1:A:143:GLY:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:ASN:HB3	1:A:1356:ILE:HD13	1.98	0.46
2:C:210:THR:O	2:C:213:GLN:HG2	2.16	0.46
2:E:248:SER:O	2:E:251:GLN:HG3	2.15	0.46
2:E:215:LEU:HD13	2:E:218:ASN:HD22	1.81	0.46
1:A:443:TYR:O	1:A:446:THR:OG1	2.24	0.45
1:A:600:LEU:HD21	1:A:1302:LYS:HZ3	1.81	0.45
2:D:235:GLN:O	2:D:239:LYS:HG2	2.16	0.45
2:D:257:ILE:HD11	2:E:257:ILE:HD13	1.97	0.45
1:A:390:LEU:HD23	1:A:390:LEU:H	1.81	0.45
1:A:404:THR:HG21	1:A:446:THR:HG21	1.98	0.45
1:A:595:MET:SD	1:A:598:LEU:HB3	2.56	0.45
1:A:607:MET:HA	1:A:610:ILE:HG12	1.98	0.45
1:A:997:ASP:OD2	1:A:1007:TYR:OH	2.34	0.45
1:A:1052:ARG:HG3	1:A:1385:GLU:HA	1.98	0.45
1:A:1097:ASN:OD1	1:A:1101:ASN:ND2	2.44	0.45
1:A:1136:CYS:HB2	1:A:1139:ASP:OD2	2.17	0.45
1:A:1210:PRO:CG	1:A:1211:PRO:HD3	2.44	0.45
1:A:1826:LYS:HA	1:A:1826:LYS:HD2	1.78	0.45
2:B:223:LEU:HD23	2:C:218:ASN:HD21	1.81	0.45
2:D:232:ARG:O	2:D:236:LEU:HG	2.16	0.45
1:A:284:ASP:O	1:A:287:TYR:HB2	2.16	0.45
1:A:935:SER:OG	1:A:941:ASN:N	2.50	0.45
1:A:1633:PHE:O	1:A:1637:GLU:HB3	2.16	0.45
1:A:1889:MET:SD	1:A:1889:MET:N	2.89	0.45
1:A:860:LEU:HD22	1:A:1086:MET:SD	2.56	0.45
1:A:2041:ILE:HA	1:A:2044:VAL:HG22	1.98	0.45
1:A:46:ASN:N	1:A:47:GLN:OE1	2.49	0.45
1:A:1123:GLU:N	1:A:1123:GLU:OE1	2.49	0.45
1:A:1150:ALA:N	1:A:1151:PRO:HD2	2.32	0.45
1:A:2130:VAL:O	1:A:2134:THR:HG23	2.16	0.45
1:A:1095:LEU:HG	1:A:1096:SER:H	1.82	0.45
1:A:1443:PHE:HB3	1:A:1683:THR:HG22	1.99	0.45
2:C:261:LYS:O	2:C:264:MET:HG2	2.17	0.45
1:A:189:GLN:NE2	1:A:193:ARG:HE	2.13	0.45
1:A:295:SER:HA	1:A:298:TYR:CD1	2.52	0.45
1:A:298:TYR:HD2	1:A:829:PHE:CZ	2.34	0.45
1:A:1067:THR:OG1	1:A:1068:SER:N	2.49	0.45
1:A:1956:PHE:CE1	1:A:1960:ILE:HD11	2.52	0.45
2:E:244:LEU:HA	2:E:247:GLN:HG2	1.99	0.45
1:A:110:LEU:HD23	1:A:178:ASP:HB3	1.99	0.45
1:A:187:MET:SD	1:A:238:VAL:HG21	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:SER:OG	1:A:669:LEU:O	2.35	0.45
1:A:1749:TYR:CE2	1:A:1751:ILE:HB	2.52	0.45
2:B:208:LEU:HG	2:C:208:LEU:HG	1.99	0.45
1:A:1736:ILE:HD12	1:A:1738:TRP:HB3	1.99	0.45
1:A:1803:ASP:CG	1:A:1906:SER:HB2	2.42	0.45
1:A:702:ARG:O	1:A:703:SER:OG	2.26	0.45
1:A:1509:VAL:O	1:A:1514:ILE:HG12	2.17	0.45
1:A:1851:PHE:O	1:A:1855:VAL:HG12	2.16	0.45
1:A:2164:ILE:HD12	1:A:2164:ILE:H	1.81	0.45
1:A:695:TRP:HE1	1:A:699:ARG:NE	2.15	0.44
1:A:1175:ILE:HD12	1:A:1179:GLY:C	2.42	0.44
1:A:510:PHE:CG	1:A:511:ASN:N	2.85	0.44
1:A:1390:LYS:O	1:A:1392:HIS:NE2	2.49	0.44
1:A:1529:ALA:HB1	1:A:1566:ILE:HD11	1.98	0.44
1:A:1584:LEU:HD21	1:A:1619:LEU:HA	1.99	0.44
1:A:1745:ASN:CB	1:A:1964:TRP:HZ2	2.24	0.44
2:C:239:LYS:O	2:C:243:ILE:HG23	2.17	0.44
1:A:1538:SER:HA	1:A:1763:ASN:CG	2.43	0.44
1:A:1950:TRP:O	1:A:1950:TRP:CD1	2.70	0.44
1:A:2167:ILE:HB	1:A:2199:ILE:HG23	1.97	0.44
2:D:225:THR:O	2:D:229:LEU:HG	2.18	0.44
1:A:19:VAL:HA	1:A:371:LEU:H	1.82	0.44
1:A:514:LEU:O	1:A:518:PHE:CB	2.60	0.44
1:A:677:ILE:HD12	1:A:680:ALA:HB3	1.98	0.44
1:A:712:ASN:O	1:A:714:PRO:HD3	2.18	0.44
1:A:1003:ILE:HG22	1:A:1004:GLU:H	1.82	0.44
1:A:1805:LEU:HA	1:A:1828:TYR:O	2.17	0.44
1:A:2035:ARG:HD3	1:A:2035:ARG:HA	1.72	0.44
1:A:2051:LEU:HD12	1:A:2054:SER:HB2	2.00	0.44
1:A:24:TYR:HA	1:A:27:ILE:HG12	1.99	0.44
1:A:1374:CYS:HB2	1:A:1376:ARG:HG2	2.00	0.44
1:A:362:ILE:HD11	1:A:847:LEU:C	2.43	0.44
1:A:836:ILE:O	1:A:843:LEU:HD23	2.18	0.44
1:A:1279:GLN:HE22	1:A:1282:THR:N	2.16	0.44
1:A:70:LEU:O	1:A:74:ILE:N	2.51	0.44
1:A:660:LEU:HB2	1:A:825:ILE:HG22	1.99	0.44
1:A:1052:ARG:HE	1:A:1386:ALA:H	1.66	0.44
1:A:1801:GLN:CD	1:A:1801:GLN:H	2.25	0.44
1:A:1983:HIS:HE1	1:A:2033:GLN:HE22	1.65	0.44
2:D:200:LEU:HD11	2:E:200:LEU:HB2	1.99	0.44
1:A:62:ARG:HA	1:A:65:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:OD1	1:A:457:LYS:NZ	2.51	0.44
1:A:666:LYS:HG3	1:A:669:LEU:HD11	1.98	0.44
1:A:1005:TYR:HD2	1:A:1110:TYR:HA	1.83	0.44
1:A:1889:MET:HG2	1:A:1890:THR:N	2.32	0.44
1:A:2089:CYS:O	1:A:2092:LEU:HG	2.17	0.44
2:B:208:LEU:O	2:B:212:VAL:HG23	2.18	0.44
1:A:18:ILE:HD13	1:A:236:GLU:HB2	1.98	0.43
1:A:28:LEU:HB3	1:A:49:TRP:CZ2	2.53	0.43
1:A:131:CYS:HA	1:A:970:SER:HB2	2.00	0.43
1:A:287:TYR:CD1	1:A:290:ILE:HD12	2.50	0.43
1:A:510:PHE:O	1:A:512:ARG:HD3	2.18	0.43
1:A:1033:ILE:O	1:A:1072:ARG:HG2	2.18	0.43
1:A:1488:PHE:HA	1:A:1491:CYS:SG	2.58	0.43
1:A:1639:CYS:O	1:A:1643:THR:HG23	2.18	0.43
2:C:250:ILE:HA	2:C:253:ILE:HG22	2.00	0.43
1:A:530:LEU:HD13	1:A:530:LEU:HA	1.81	0.43
1:A:915:GLN:HG3	1:A:918:LEU:HD21	2.00	0.43
1:A:1326:ILE:HD12	1:A:1477:SER:OG	2.18	0.43
1:A:1659:ASN:HA	1:A:1662:ASN:HD22	1.82	0.43
1:A:2008:MET:HE2	1:A:2008:MET:HB2	1.92	0.43
2:E:208:LEU:O	2:E:212:VAL:HG22	2.18	0.43
1:A:936:GLN:O	1:A:1006:GLN:NE2	2.51	0.43
1:A:1307:SER:OG	1:A:1308:SER:N	2.51	0.43
1:A:1734:ASP:HB2	1:A:1974:ARG:O	2.18	0.43
1:A:1747:GLU:HG2	1:A:2017:LEU:O	2.19	0.43
1:A:2091:MET:HE1	1:A:2140:HIS:HE1	1.83	0.43
2:E:206:ASN:HA	2:E:209:VAL:HB	2.00	0.43
1:A:955:ASP:OD1	1:A:999:TYR:HD2	2.01	0.43
1:A:1119:LYS:HD2	1:A:1120:ASN:H	1.82	0.43
2:F:376:SER:HB3	2:F:379:GLN:HB2	2.00	0.43
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.84	0.43
1:A:338:ARG:HD2	2:F:348:ILE:HD11	2.01	0.43
1:A:411:ARG:HG2	1:A:439:THR:HA	2.01	0.43
2:B:222:ILE:O	2:B:226:VAL:HG13	2.18	0.43
1:A:360:LEU:HD23	1:A:361:CYS:N	2.34	0.43
1:A:428:SER:O	1:A:431:LEU:HB3	2.19	0.43
1:A:879:THR:HG22	1:A:888:CYS:SG	2.59	0.43
1:A:965:LYS:HE2	1:A:1134:GLU:HB2	2.01	0.43
1:A:1889:MET:HG2	1:A:1890:THR:H	1.83	0.43
1:A:310:LEU:HD21	1:A:797:PHE:CE1	2.54	0.43
1:A:847:LEU:HD12	1:A:847:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:ASP:HA	1:A:1639:CYS:SG	2.59	0.43
1:A:2208:THR:CG2	1:A:2211:ILE:HG12	2.47	0.43
1:A:943:LEU:HB3	1:A:947:ARG:HD2	2.00	0.43
1:A:1291:THR:HG21	1:A:1330:THR:O	2.19	0.43
1:A:1965:CYS:SG	1:A:1966:TYR:N	2.88	0.43
1:A:1974:ARG:HD3	1:A:2033:GLN:OE1	2.19	0.43
1:A:451:LYS:HD2	1:A:451:LYS:HA	1.77	0.43
1:A:797:PHE:HA	1:A:800:CYS:SG	2.58	0.43
1:A:1849:THR:OG1	1:A:1850:GLN:N	2.52	0.43
2:D:226:VAL:HB	2:E:226:VAL:HG22	2.00	0.43
1:A:236:GLU:HA	1:A:239:LEU:HD13	2.01	0.43
1:A:476:ASP:N	1:A:1080:ASP:OD2	2.36	0.43
1:A:532:TYR:CD2	1:A:568:ARG:HG2	2.54	0.43
1:A:884:GLU:HG3	1:A:887:ILE:HG22	2.01	0.43
1:A:1239:LEU:O	1:A:1242:VAL:HG12	2.19	0.43
1:A:1805:LEU:HB3	1:A:1908:VAL:HG13	2.01	0.43
1:A:1954:THR:O	1:A:1958:THR:CG2	2.49	0.43
1:A:2018:ILE:O	1:A:2020:PRO:HD3	2.19	0.43
1:A:2163:GLY:H	1:A:2164:ILE:HD12	1.84	0.43
2:B:250:ILE:HG13	2:B:251:GLN:H	1.84	0.43
1:A:422:ASN:HB3	1:A:423:LEU:H	1.69	0.42
1:A:517:ASN:O	1:A:521:ASP:N	2.52	0.42
1:A:604:LEU:HB3	1:A:837:PHE:HE2	1.84	0.42
1:A:608:SER:OG	1:A:840:GLY:HA2	2.19	0.42
1:A:1770:SER:OG	1:A:1771:HIS:N	2.51	0.42
1:A:99:PRO:CB	1:A:102:LYS:HB2	2.49	0.42
1:A:267:ARG:HD2	1:A:347:PRO:HA	2.01	0.42
1:A:748:THR:O	1:A:752:ILE:HG13	2.19	0.42
1:A:923:ASN:ND2	1:A:926:LEU:HB2	2.34	0.42
2:B:265:ALA:HA	2:B:268:GLU:CD	2.44	0.42
1:A:180:TRP:CD1	1:A:245:TYR:HD2	2.37	0.42
1:A:1196:LEU:HB2	1:A:1348:LEU:HD21	2.01	0.42
1:A:411:ARG:NH1	1:A:416:GLY:HA3	2.34	0.42
1:A:580:LEU:HD12	1:A:693:PHE:CE2	2.55	0.42
1:A:1271:VAL:HG11	1:A:1277:GLN:HG2	2.01	0.42
1:A:1504:TYR:HD1	1:A:1504:TYR:HA	1.74	0.42
1:A:1549:LEU:HD23	1:A:1551:ILE:HD11	2.01	0.42
1:A:81:HIS:HE1	1:A:83:GLN:HG3	1.85	0.42
1:A:130:GLN:HG3	1:A:134:ASN:ND2	2.34	0.42
1:A:301:LEU:HD23	1:A:829:PHE:HE1	1.85	0.42
1:A:806:ARG:HG3	1:A:810:ASN:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1349:GLU:O	1:A:1353:ASN:N	2.52	0.42
1:A:1737:ILE:HG21	1:A:1972:VAL:HG13	1.87	0.42
1:A:1959:LEU:HD23	1:A:1959:LEU:C	2.45	0.42
1:A:2038:ALA:HA	1:A:2041:ILE:HD12	2.01	0.42
1:A:2159:ASP:HB3	1:A:2165:PHE:N	2.34	0.42
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.88	0.42
1:A:1390:LYS:HB2	1:A:1392:HIS:CE1	2.55	0.42
1:A:1522:LEU:HD12	1:A:1570:VAL:HG23	2.01	0.42
1:A:1740:ILE:HD12	1:A:1744:ALA:HB3	2.02	0.42
1:A:1974:ARG:HA	1:A:1985:VAL:HG23	2.02	0.42
2:D:222:ILE:HD12	2:E:222:ILE:HG21	2.02	0.42
1:A:875:VAL:O	1:A:879:THR:HG23	2.19	0.42
1:A:1251:TRP:HD1	1:A:1289:ASN:HD21	1.67	0.42
1:A:1767:ASN:OD1	1:A:1767:ASN:N	2.50	0.42
1:A:174:LYS:HE2	1:A:174:LYS:HB3	1.89	0.42
1:A:309:GLU:O	1:A:313:GLN:HB2	2.20	0.42
1:A:755:ILE:O	1:A:758:SER:OG	2.32	0.42
1:A:787:LEU:O	1:A:792:LYS:HE2	2.20	0.42
1:A:1815:MET:SD	1:A:1815:MET:N	2.93	0.42
1:A:1911:ASP:HB2	1:A:1947:LYS:HD2	2.02	0.42
1:A:1973:LEU:HD23	1:A:1974:ARG:O	2.19	0.42
1:A:1983:HIS:NE2	1:A:2033:GLN:OE1	2.51	0.42
1:A:2095:HIS:CG	1:A:2133:LEU:HD13	2.55	0.42
1:A:1486:GLU:HA	1:A:1489:MET:HE2	2.02	0.42
1:A:1747:GLU:CD	1:A:2016:THR:HA	2.44	0.42
1:A:1983:HIS:CE1	1:A:2033:GLN:HE22	2.38	0.42
1:A:2012:ASP:HB3	1:A:2016:THR:HB	2.02	0.42
1:A:2095:HIS:O	1:A:2099:ILE:HG12	2.20	0.42
2:E:202:GLN:HA	2:E:205:LEU:HB3	2.02	0.42
1:A:8:LEU:HD13	1:A:861:GLY:H	1.85	0.41
1:A:107:LEU:HD13	1:A:182:MET:HG2	2.02	0.41
1:A:245:TYR:HD1	1:A:245:TYR:HA	1.76	0.41
1:A:1205:ASP:HB2	1:A:1208:ASP:HB3	2.01	0.41
1:A:1739:ILE:CD1	1:A:1972:VAL:HG11	2.33	0.41
1:A:245:TYR:CD1	1:A:248:ARG:HD2	2.54	0.41
1:A:900:LEU:HD23	1:A:927:VAL:HG23	2.01	0.41
2:D:237:GLU:HA	2:D:240:VAL:HG12	2.02	0.41
1:A:392:PHE:HA	1:A:395:ILE:HG22	2.02	0.41
2:D:206:ASN:O	2:D:210:THR:HG22	2.20	0.41
1:A:392:PHE:N	1:A:393:PRO:HD2	2.35	0.41
1:A:925:HIS:CE1	1:A:929:ARG:HE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211[A]:SER:OG	2:E:212:VAL:HG23	2.21	0.41
2:B:223:LEU:HA	2:B:226:VAL:HG22	2.03	0.41
2:C:223:LEU:HD22	2:D:218:ASN:CG	2.46	0.41
1:A:69:PHE:HB3	1:A:205:TYR:CE1	2.56	0.41
1:A:373:ALA:O	1:A:377:ALA:HB3	2.20	0.41
1:A:695:TRP:HE1	1:A:699:ARG:CZ	2.34	0.41
1:A:793:LYS:HG2	1:A:793:LYS:H	1.63	0.41
1:A:1446:ARG:O	1:A:1450:ASN:HB2	2.21	0.41
1:A:1509:VAL:N	1:A:1513:ASN:HB2	2.35	0.41
2:B:233:MET:O	2:B:237:GLU:HG3	2.21	0.41
2:B:235:GLN:O	2:B:238:THR:OG1	2.31	0.41
2:C:226:VAL:HG22	2:D:225:THR:HG21	2.03	0.41
2:C:232:ARG:NH2	2:C:235[A]:GLN:HB3	2.35	0.41
2:D:230:ASP:OD1	2:E:229:LEU:HD13	2.21	0.41
1:A:1161:LEU:HG	1:A:1162:GLU:CD	2.45	0.41
1:A:1495:LEU:HD11	1:A:1522:LEU:HD21	2.03	0.41
1:A:1745:ASN:OD1	1:A:1745:ASN:N	2.53	0.41
1:A:1851:PHE:CE2	1:A:1855:VAL:HG11	2.56	0.41
2:C:220[B]:ASN:OD1	2:D:218:ASN:ND2	2.54	0.41
1:A:1021:LEU:HD12	1:A:1021:LEU:HA	1.78	0.41
1:A:1265:ASP:O	1:A:1269:THR:OG1	2.28	0.41
1:A:1325:THR:OG1	1:A:1327:ASN:ND2	2.54	0.41
1:A:1391:PRO:C	1:A:1392:HIS:CG	2.98	0.41
1:A:1632:GLY:H	1:A:1638:LYS:NZ	2.19	0.41
2:C:208:LEU:HD13	2:C:208:LEU:HA	1.98	0.41
1:A:9:LEU:CG	1:A:188:ARG:HH21	2.34	0.41
1:A:102:LYS:HE3	1:A:175:ARG:HD2	2.01	0.41
1:A:300:GLN:O	1:A:303:MET:HG2	2.20	0.41
1:A:1053:GLU:H	1:A:1053:GLU:CD	2.28	0.41
1:A:1928:ILE:HD13	1:A:1928:ILE:HA	1.97	0.41
1:A:2033:GLN:O	1:A:2037:VAL:HG13	2.20	0.41
1:A:2081:PHE:CE2	1:A:2083:GLU:HB2	2.55	0.41
2:B:234:ASN:O	2:B:238:THR:HG23	2.20	0.41
2:C:240:VAL:O	2:C:244:LEU:HD23	2.21	0.41
2:C:255:ASN:HA	2:C:258:VAL:HG22	2.03	0.41
2:F:377:GLU:HA	2:F:380:LEU:HG	2.03	0.41
1:A:62:ARG:O	1:A:66:VAL:HG23	2.21	0.41
1:A:1745:ASN:CA	1:A:1964:TRP:CH2	3.04	0.41
1:A:1947:LYS:HB2	1:A:1986:TYR:HE1	1.85	0.41
1:A:2128:THR:O	1:A:2131:ARG:HG2	2.20	0.41
2:B:226:VAL:HG21	2:C:222:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HG13	1:A:95:LEU:HD22	2.03	0.40
1:A:1191:PHE:C	1:A:1321:GLU:CB	2.82	0.40
1:A:1816:THR:HG21	1:A:1850:GLN:NE2	2.36	0.40
1:A:1893:VAL:HG11	1:A:1924:SER:HB2	2.03	0.40
1:A:2025:GLN:HA	1:A:2028:ASP:OD2	2.21	0.40
1:A:2214:GLN:O	1:A:2217:LYS:HG2	2.22	0.40
2:D:208:LEU:H	2:D:208:LEU:HG	1.74	0.40
2:D:257:ILE:HG22	2:D:261:LYS:HE2	2.03	0.40
1:A:168:TRP:CH2	1:A:895:MET:HE1	2.56	0.40
1:A:331:SER:OG	1:A:332:PHE:N	2.53	0.40
1:A:770:VAL:O	1:A:771:GLN:HG2	2.21	0.40
1:A:997:ASP:OD1	1:A:997:ASP:N	2.52	0.40
1:A:1259:ASN:OD1	1:A:1260:TRP:N	2.54	0.40
1:A:1632:GLY:CA	1:A:1637:GLU:HG2	2.51	0.40
1:A:2085:GLU:HG2	1:A:2086:GLN:H	1.86	0.40
1:A:2148:LEU:HD12	1:A:2148:LEU:O	2.21	0.40
1:A:302:GLN:HG3	1:A:302:GLN:O	2.22	0.40
1:A:1447:GLN:NE2	1:A:1679:ASN:HB3	2.37	0.40
1:A:1499:LEU:HD21	1:A:1517:TYR:CD2	2.54	0.40
1:A:1545:ARG:HH21	1:A:1700:VAL:HB	1.86	0.40
2:B:236:LEU:HA	2:B:239:LYS:HD2	2.03	0.40
1:A:9:LEU:HA	1:A:10:PRO:HD3	1.93	0.40
1:A:493:SER:OG	1:A:494:LEU:N	2.54	0.40
1:A:564:LYS:C	1:A:565:LEU:HD12	2.46	0.40
1:A:691:HIS:ND1	1:A:694:GLU:OE2	2.55	0.40
1:A:1209:ASN:HB3	1:A:1314:PHE:CZ	2.56	0.40
2:B:223:LEU:O	2:B:227:ARG:HG2	2.21	0.40
1:A:266:LYS:HA	1:A:269:THR:HG22	2.04	0.40
1:A:319:CYS:O	1:A:322:ILE:HG22	2.21	0.40
1:A:852:LYS:HD3	1:A:852:LYS:HA	1.86	0.40
1:A:1629:LYS:HD2	1:A:1629:LYS:HA	1.87	0.40
1:A:1644:GLU:O	1:A:1648:LYS:HG3	2.22	0.40
1:A:1771:HIS:NE2	1:A:1977:TYR:O	2.54	0.40
1:A:1851:PHE:CZ	1:A:1855:VAL:HG11	2.57	0.40
1:A:1917:SER:OG	1:A:1919:ASN:OD1	2.39	0.40
1:A:1929:ASN:ND2	1:A:1944:LEU:HB3	2.36	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	1832/2255 (81%)	1555 (85%)	272 (15%)	5 (0%)	36	71
2	B	74/392 (19%)	71 (96%)	3 (4%)	0	100	100
2	C	76/392 (19%)	74 (97%)	2 (3%)	0	100	100
2	D	74/392 (19%)	72 (97%)	2 (3%)	0	100	100
2	E	76/392 (19%)	72 (95%)	4 (5%)	0	100	100
2	F	45/392 (12%)	44 (98%)	1 (2%)	0	100	100
All	All	2177/4215 (52%)	1888 (87%)	284 (13%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1739	ILE
1	A	1029	MET
1	A	1028	PRO
1	A	1218	GLY
1	A	1827	ILE

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	1692/2019 (84%)	1685 (100%)	7 (0%)	84	82
2	B	68/342 (20%)	68 (100%)	0	100	100
2	C	70/342 (20%)	68 (97%)	2 (3%)	37	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	68/342 (20%)	64 (94%)	4 (6%)	18	40
2	E	70/342 (20%)	68 (97%)	2 (3%)	37	57
2	F	42/342 (12%)	42 (100%)	0	100	100
All	All	2010/3729 (54%)	1995 (99%)	15 (1%)	76	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	ILE
1	A	1504	TYR
1	A	1740	ILE
1	A	1743	ASN
1	A	1967	PHE
1	A	1970	ILE
1	A	2148	LEU
2	C	235[A]	GLN
2	C	235[B]	GLN
2	D	217[A]	LEU
2	D	217[B]	LEU
2	D	228[A]	ASN
2	D	228[B]	ASN
2	E	231[A]	SER
2	E	231[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	73	HIS
1	A	125	ASN
1	A	133	GLN
1	A	134	ASN
1	A	281	GLN
1	A	315	HIS
1	A	368	HIS
1	A	527	ASN
1	A	609	GLN
1	A	670	GLN
1	A	771	GLN
1	A	810	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	A	811	ASN
1	A	816	HIS
1	A	817	HIS
1	A	849	ASN
1	A	892	ASN
1	A	925	HIS
1	A	980	ASN
1	A	1002	ASN
1	A	1044	ASN
1	A	1061	HIS
1	A	1183	GLN
1	A	1289	ASN
1	A	1327	ASN
1	A	1338	GLN
1	A	1352	ASN
1	A	1447	GLN
1	A	1539	HIS
1	A	1582	ASN
1	A	1733	ASN
1	A	1804	HIS
1	A	2030	HIS
2	B	201	GLN
2	B	202	GLN
2	B	235	GLN
2	B	255	ASN
2	C	202	GLN
2	C	218	ASN
2	C	234	ASN
2	C	247	GLN
2	C	251	GLN
2	C	255	ASN
2	D	202	GLN
2	D	251	GLN
2	E	218	ASN
2	E	247	GLN
2	E	255	ASN
2	F	372	ASN

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

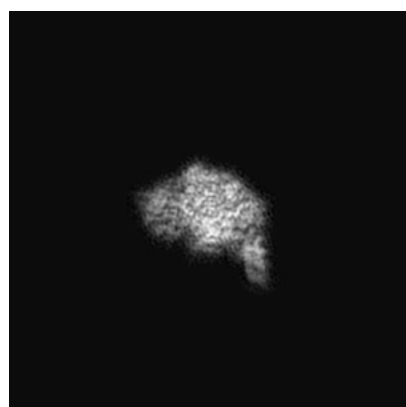
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21096. These allow visual inspection of the internal detail of the map and identification of artifacts.

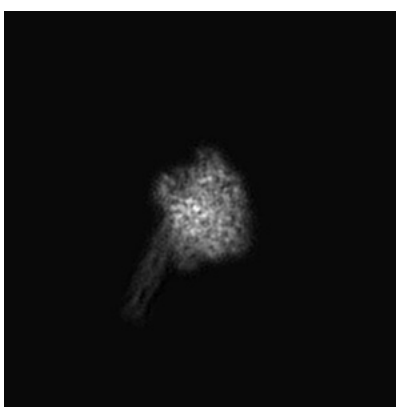
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

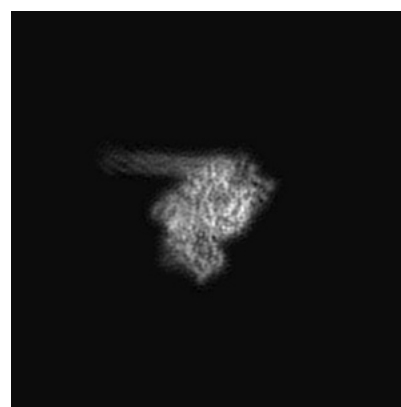
6.1.1 Primary map



X



Y



Z

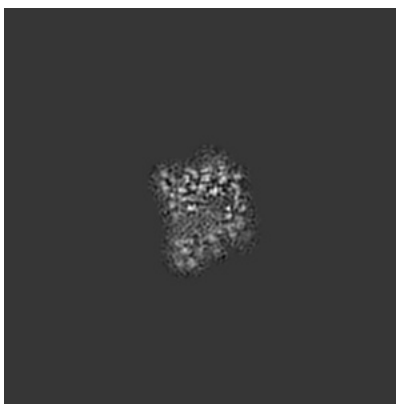
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

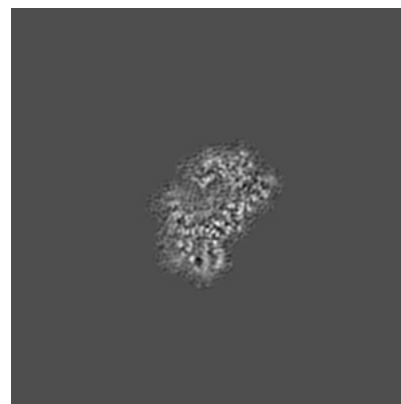
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

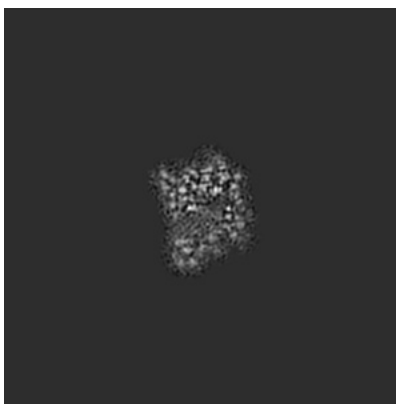
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

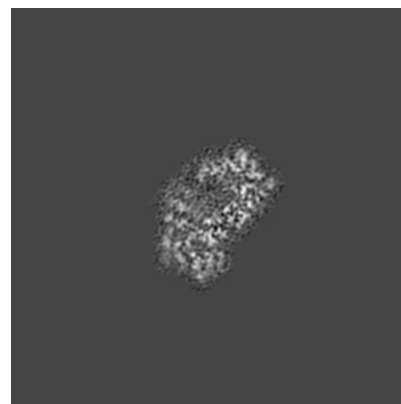
6.3.1 Primary map



X Index: 181



Y Index: 181

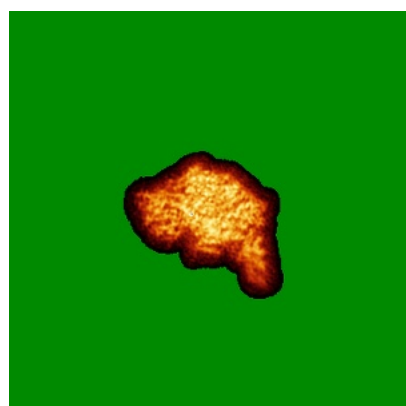


Z Index: 185

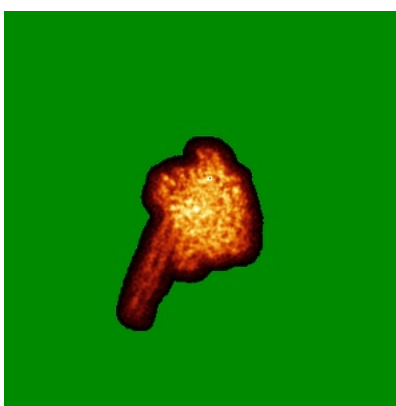
The images above show the largest variance slices of the map in three orthogonal directions.

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

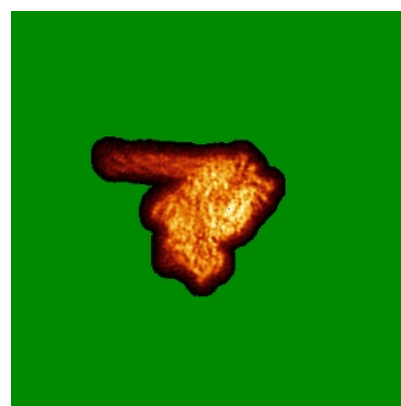
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

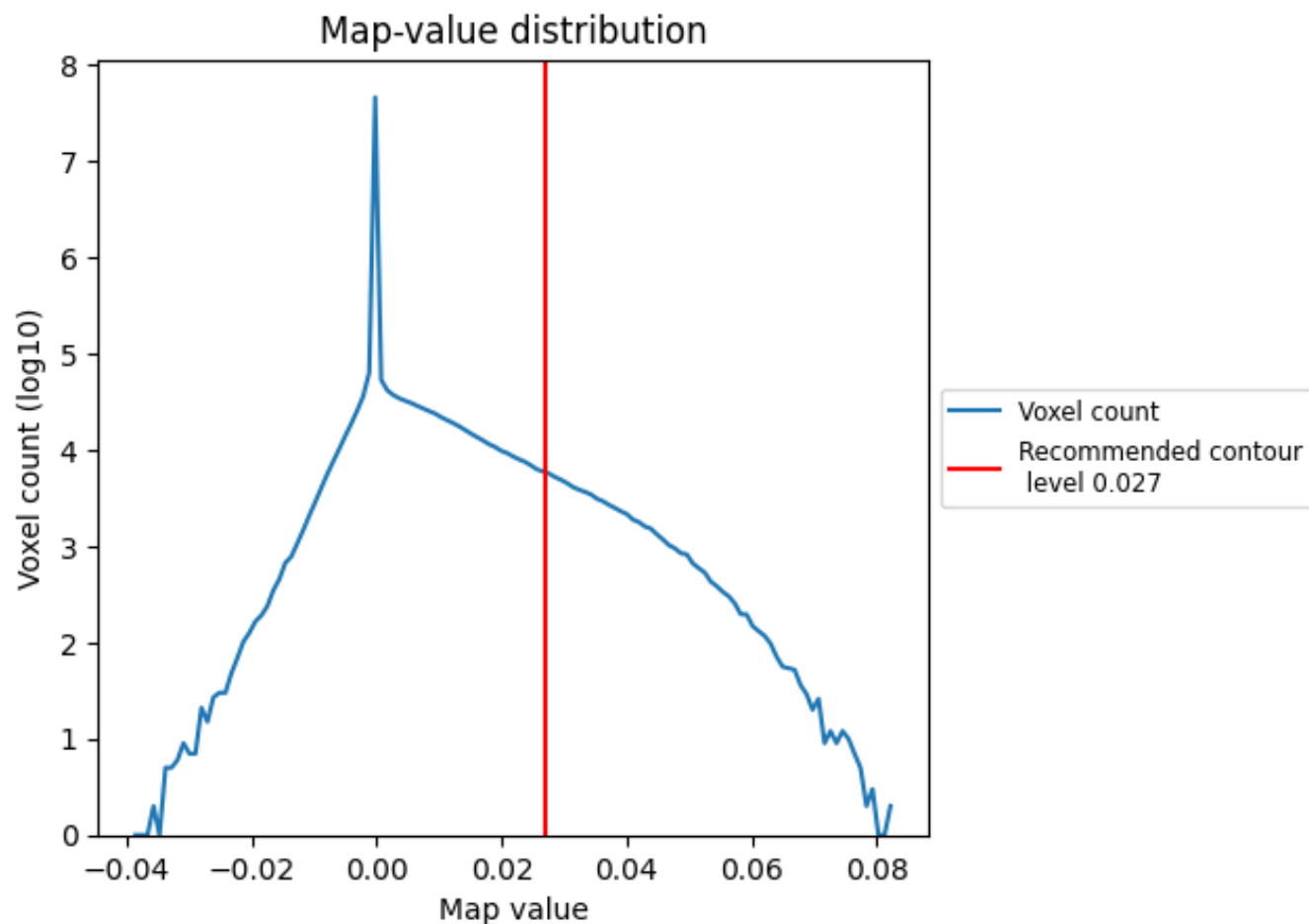
6.6 Mask visualisation

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

7 Map analysis [i](#)

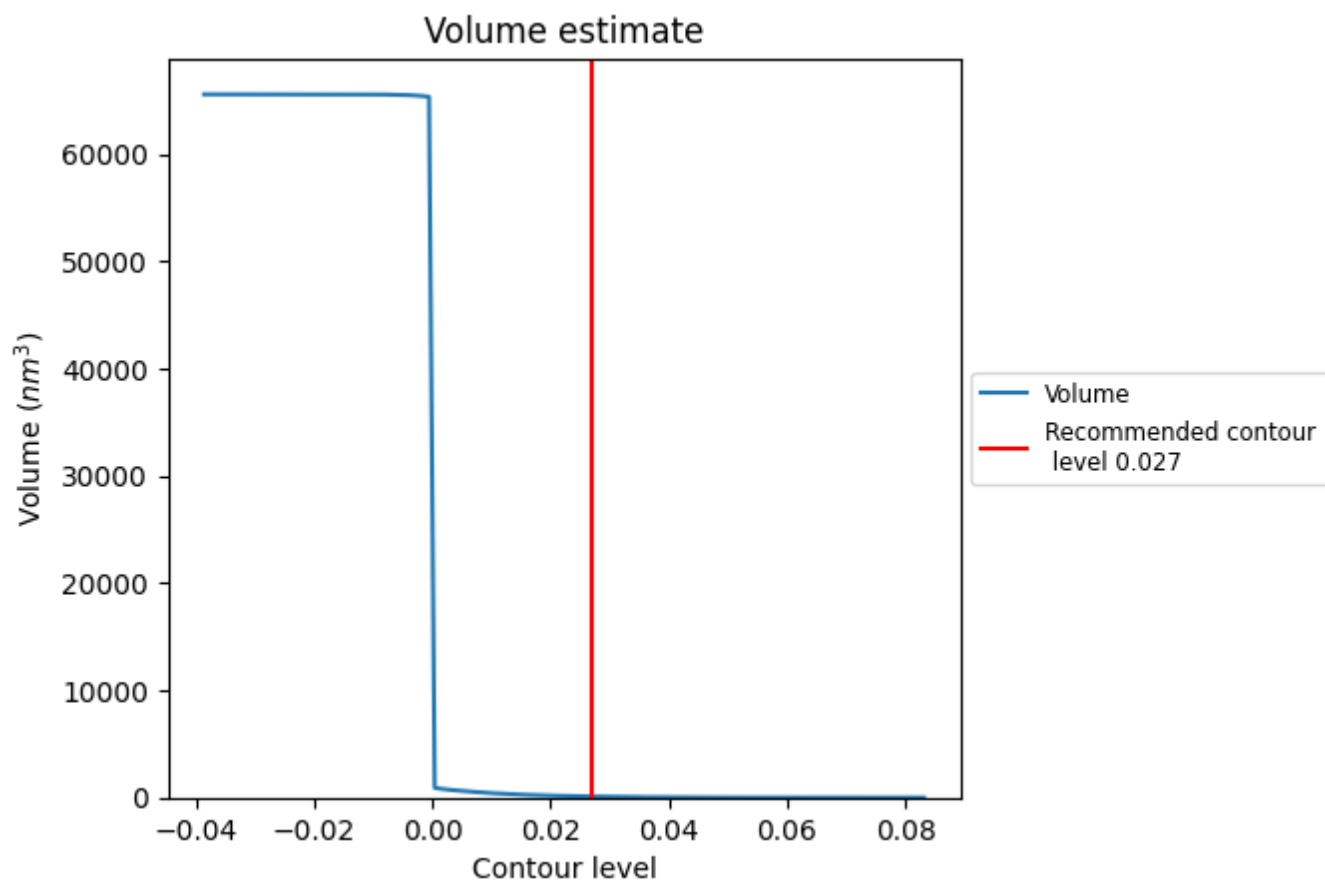
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

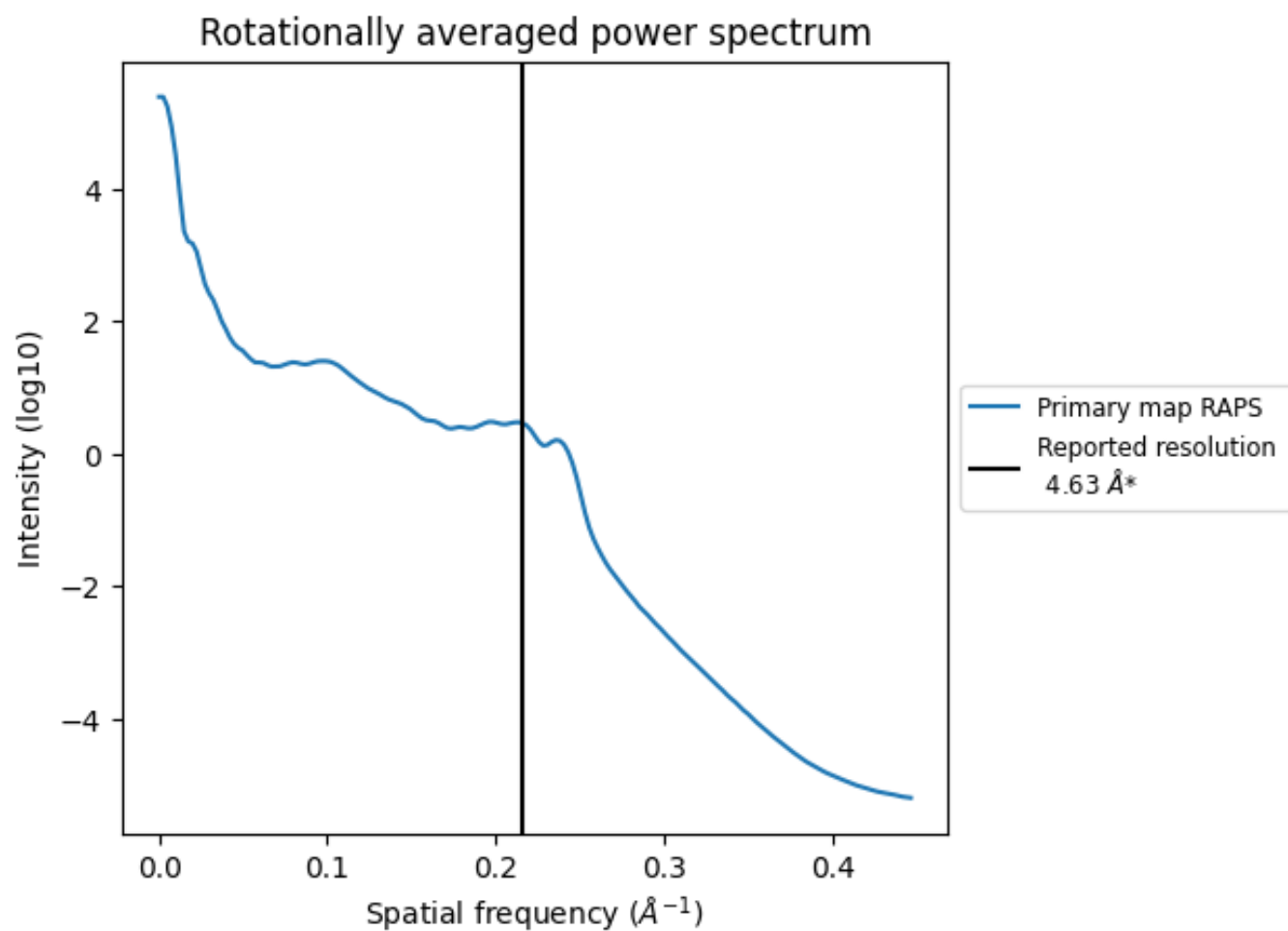
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm³; this corresponds to an approximate mass of 92 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 ⓘ

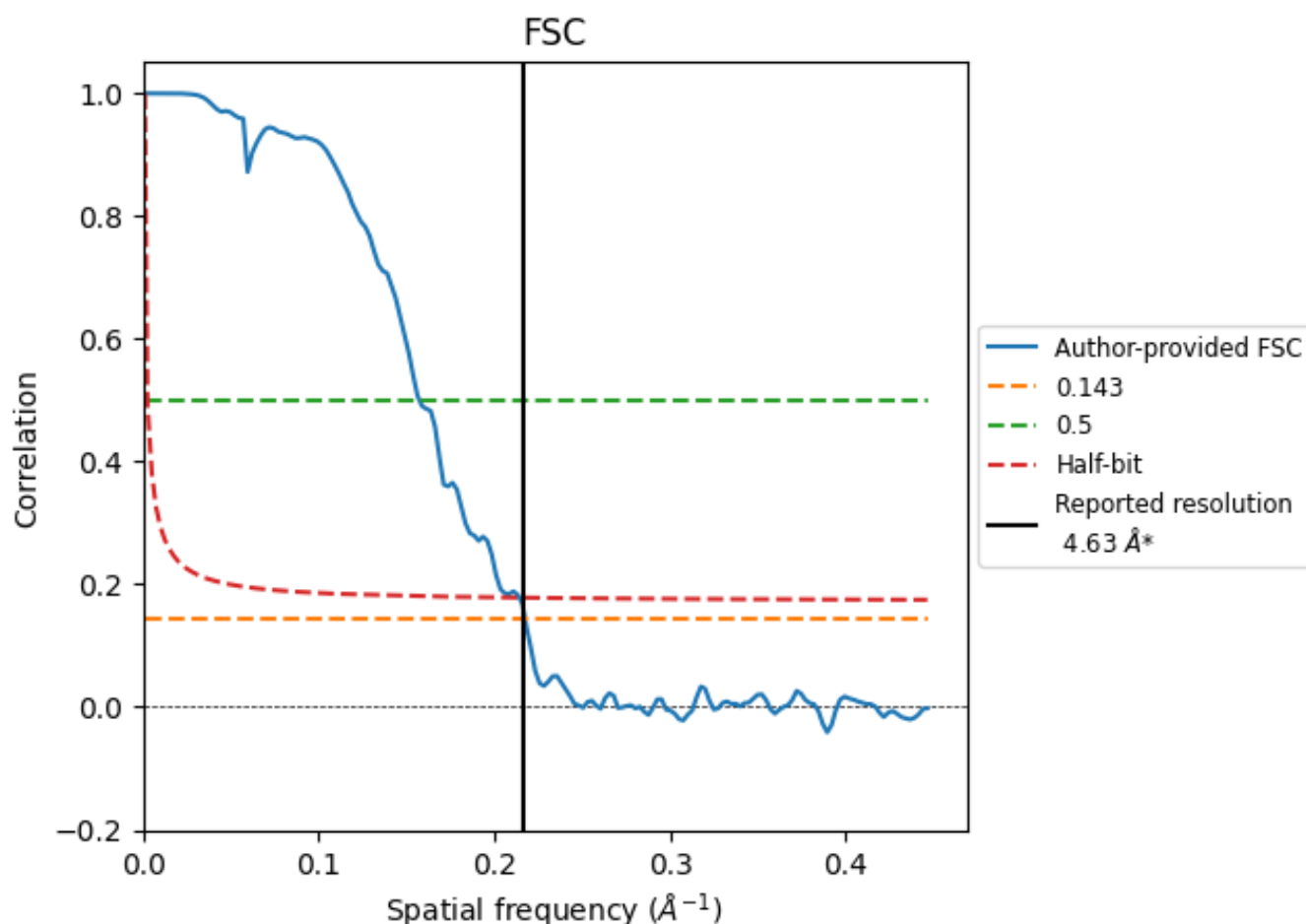


*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

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 0.216 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.60	6.36	4.67
Unmasked-calculated*	-	-	-

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

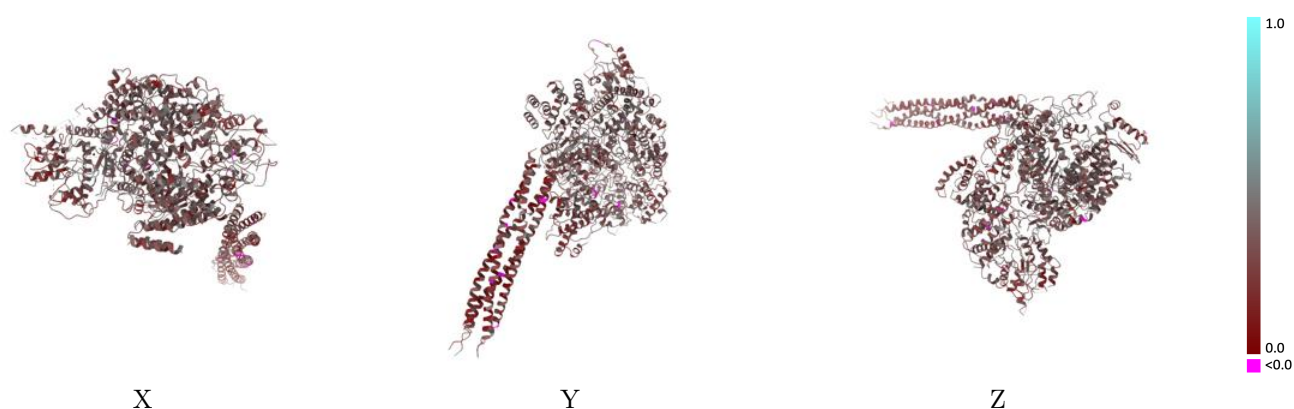
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21096 and PDB model 6V86. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

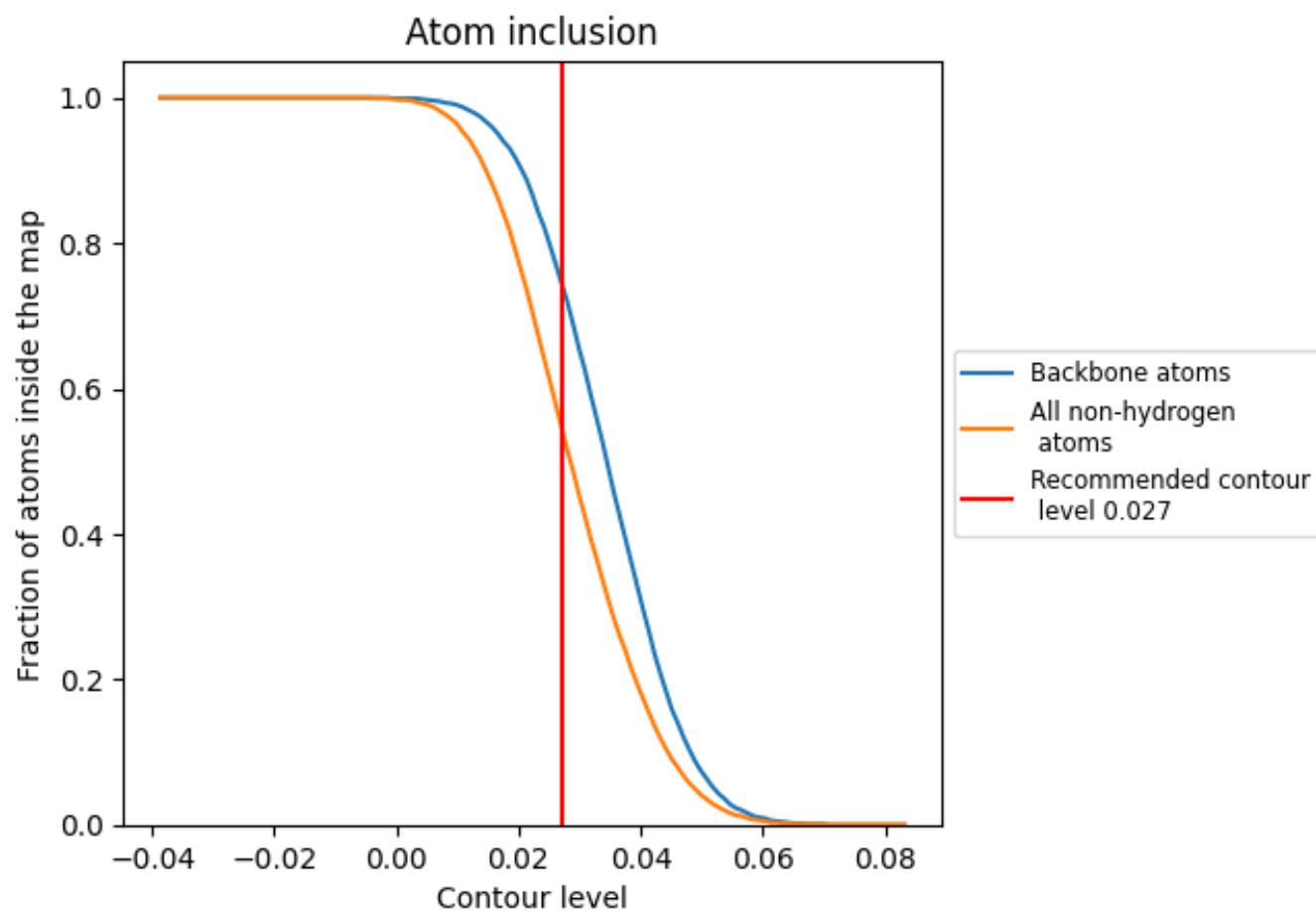


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 55% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.3350
A	0.6000	0.3490
B	0.1910	0.2510
C	0.1660	0.2210
D	0.1760	0.2470
E	0.2460	0.2260
F	0.5390	0.3330

1.0

0.0

<0.0