WORLDWIDE wwPDB
PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

May 15, 2024 – 05:38 PM EDT

PDB ID	:	7UMZ
EMDB ID	:	EMD-26610
Title	:	Cryo-EM structure of rabbit RyR1 in the presence of high Mg2+ and AMP-PCP in nanodisc
Authors	:	Nayak, A.R.; Samso, M.
Deposited on	:	2022-04-08
Resolution	:	3.09 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.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.09 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.7%
Sidechain outliers		4.4%

Worse ——— Better

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
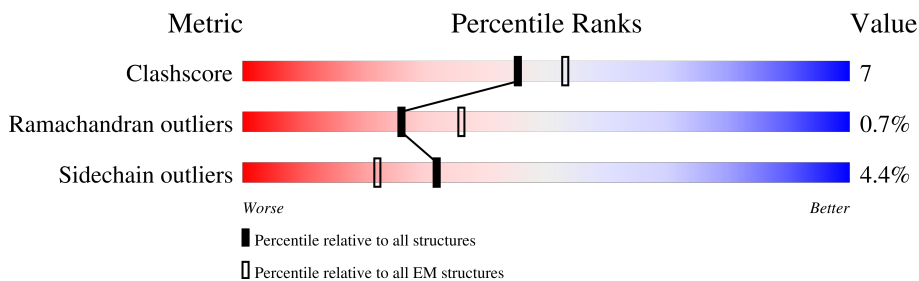
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

| Mol	Chain	Length	Quality of chain
1	A	5037	9% / 67% / 10% · 22%
1	B	5037	9% / 66% / 10% · 22%
1	C	5037	9% / 67% / 10% · 22%
1	D	5037	9% / 67% / 10% · 22%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 111396 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3927	Total	C	N	O	S	0	0
			27759	17494	4909	5192	164		
1	B	3927	Total	C	N	O	S	0	0
			27785	17506	4915	5202	162		
1	C	3927	Total	C	N	O	S	0	0
			27661	17427	4896	5175	163		
1	D	3927	Total	C	N	O	S	0	0
			27670	17436	4891	5180	163		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).
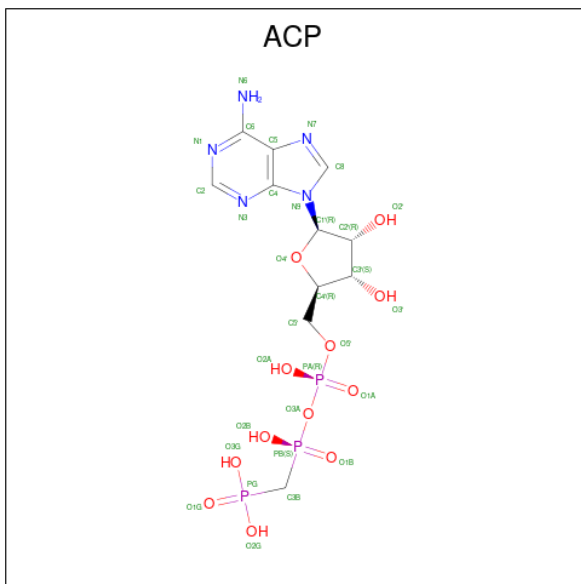
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	B	1	Total	C	N	O	P	0
			31	11	5	12	3	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total 31	C 11	N 5	O 12	P 3	0
2	D	1	Total 31	C 11	N 5	O 12	P 3	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	4	Total 4	Mg 4	0
4	B	3	Total 3	Mg 3	0
4	C	3	Total 3	Mg 3	0
4	D	3	Total 3	Mg 3	0

- Molecule 5 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: $C_{42}H_{82}NO_8P$).

LBN

Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 47	C 37	N 1	O 8	P 1	0
5	A	1	Total 46	C 36	N 1	O 8	P 1	0
5	B	1	Total 46	C 36	N 1	O 8	P 1	0
5	B	1	Total 47	C 37	N 1	O 8	P 1	0
5	C	1	Total 47	C 37	N 1	O 8	P 1	0
5	C	1	Total 46	C 36	N 1	O 8	P 1	0
5	D	1	Total 47	C 37	N 1	O 8	P 1	0
5	D	1	Total 46	C 36	N 1	O 8	P 1	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total 2	O 2	0
6	B	2	Total 2	O 2	0
6	C	2	Total 2	O 2	0
6	D	2	Total 2	O 2	0

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.
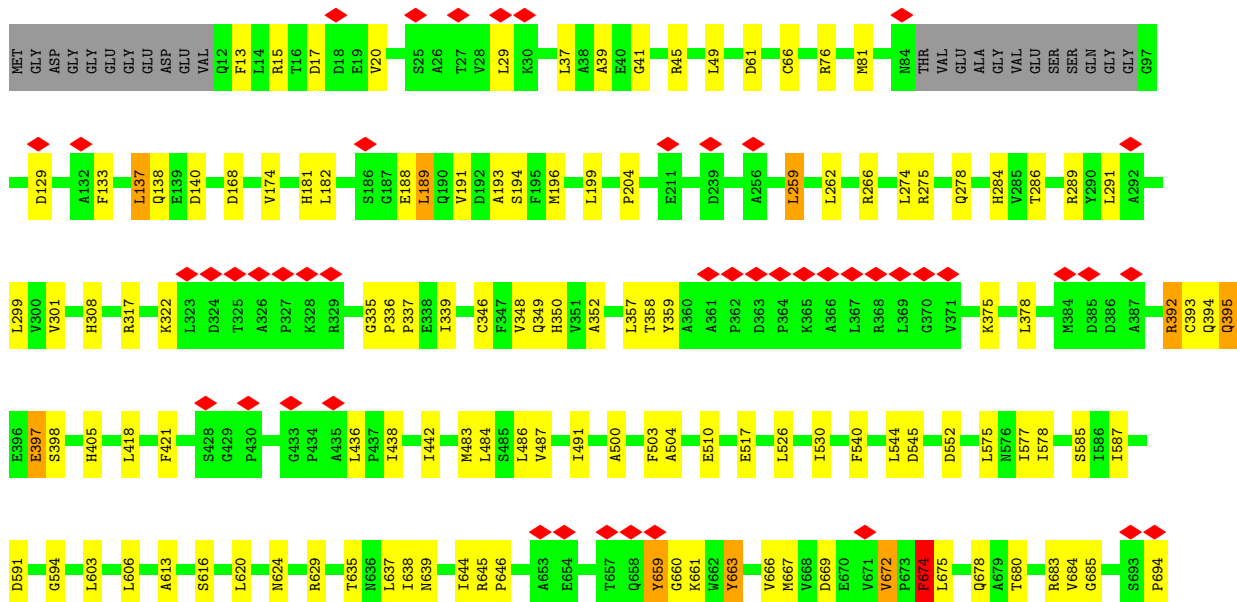
• Molecule 1: Ryanodine receptor 1

• Molecule 1: Ryanodine receptor 1

• Molecule 1: Ryanodine receptor 1

Chain C:

9%

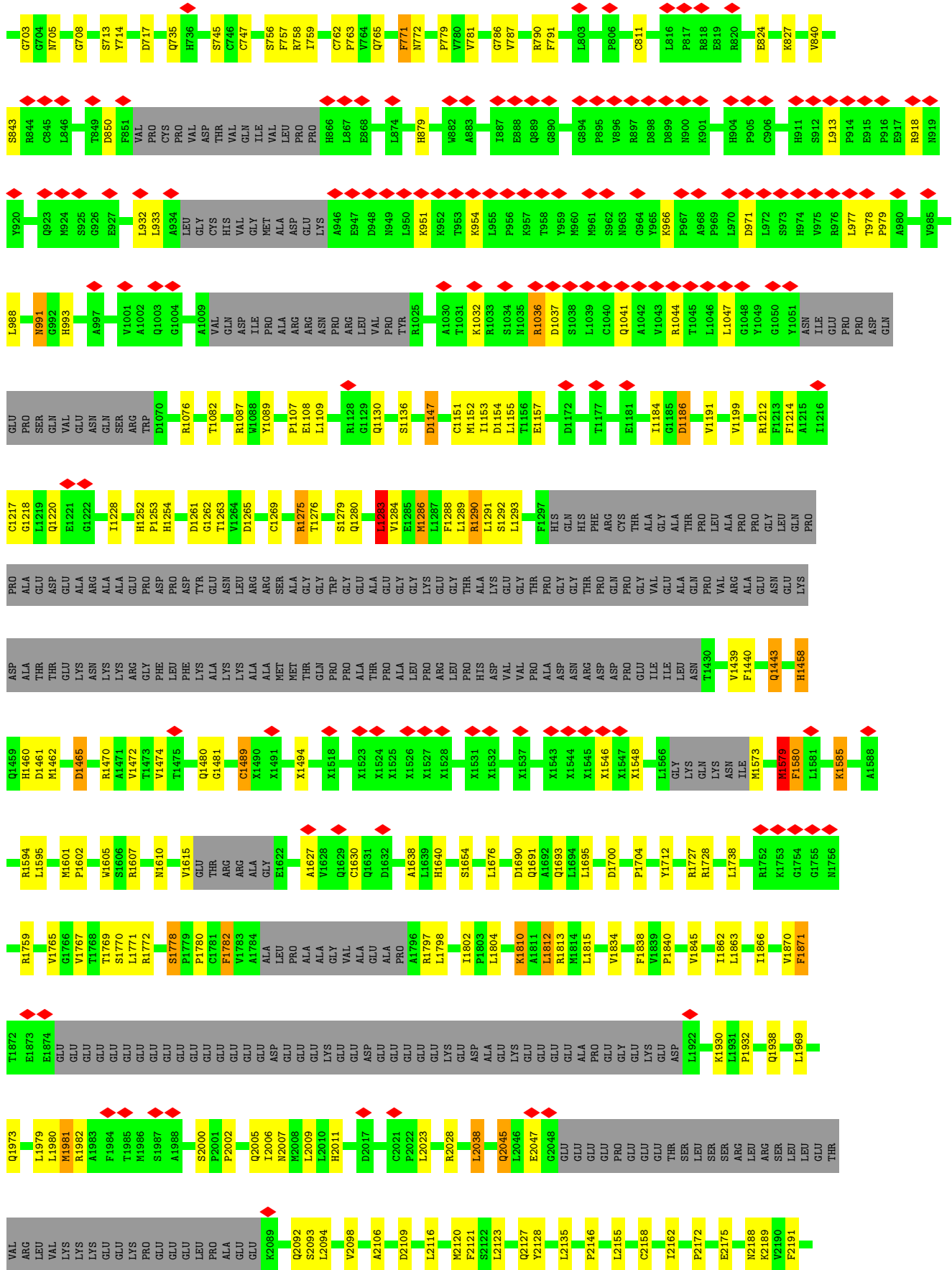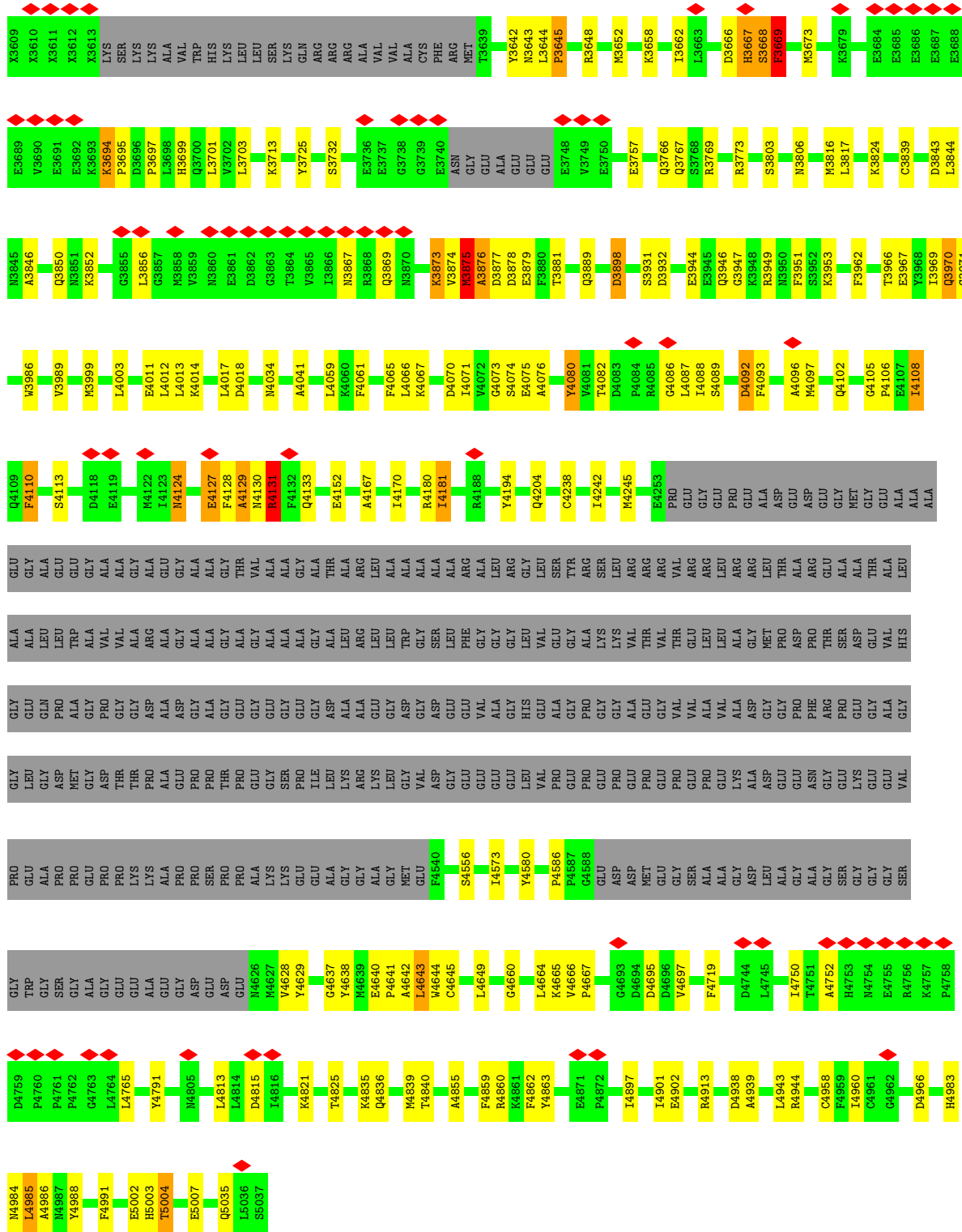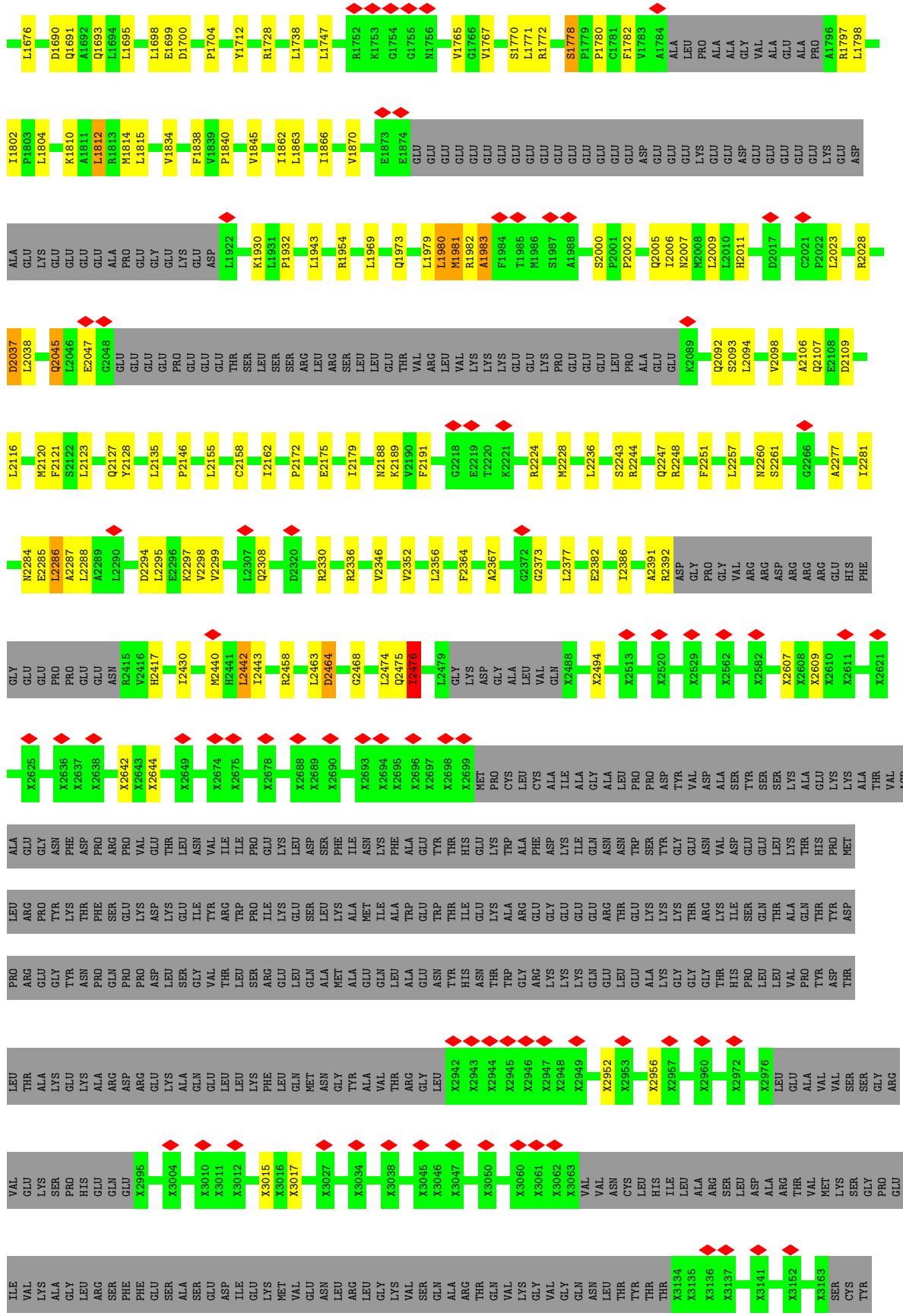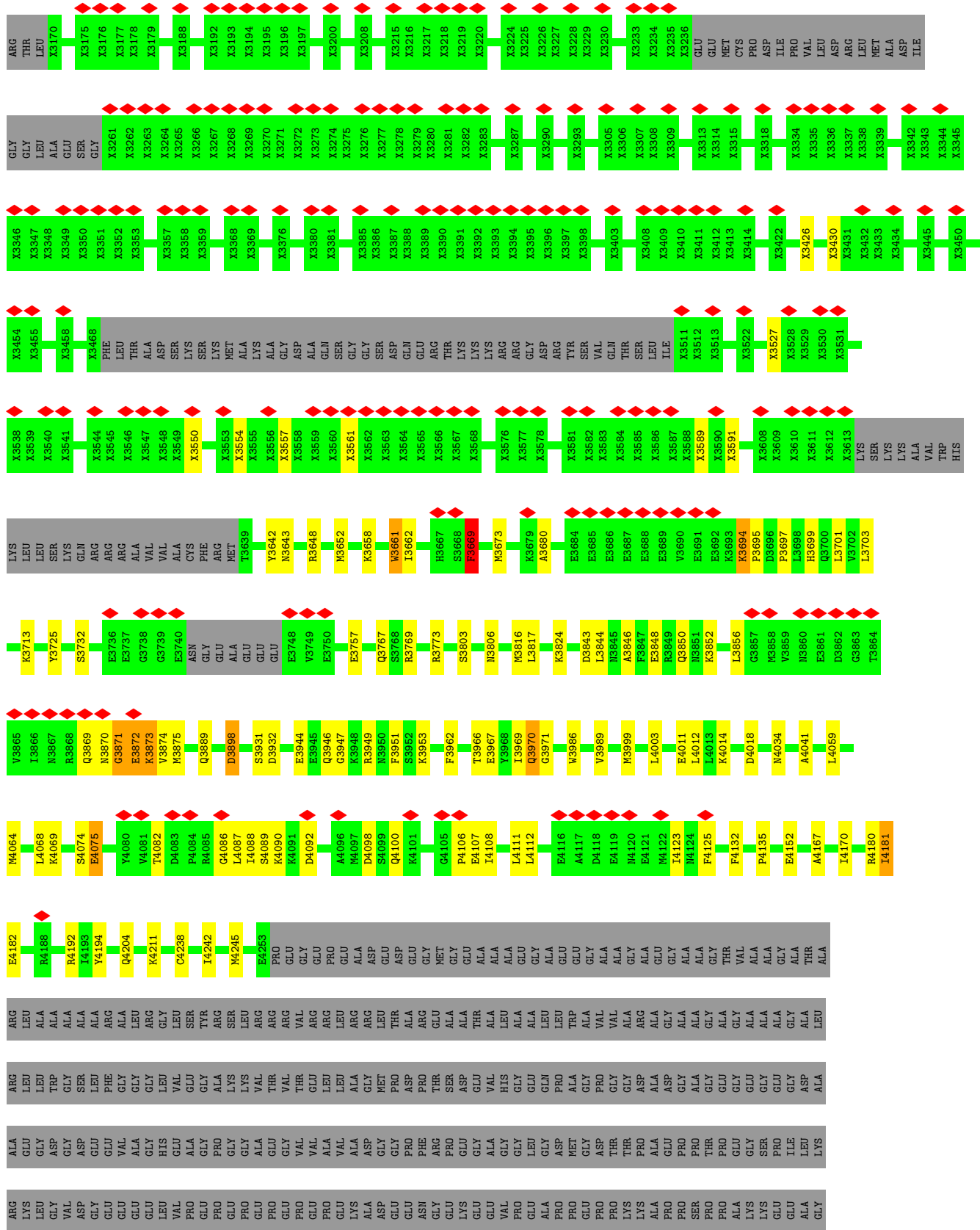67%   10%   •   22%

• Molecule 1: Ryanodine receptor 1

Chain D:
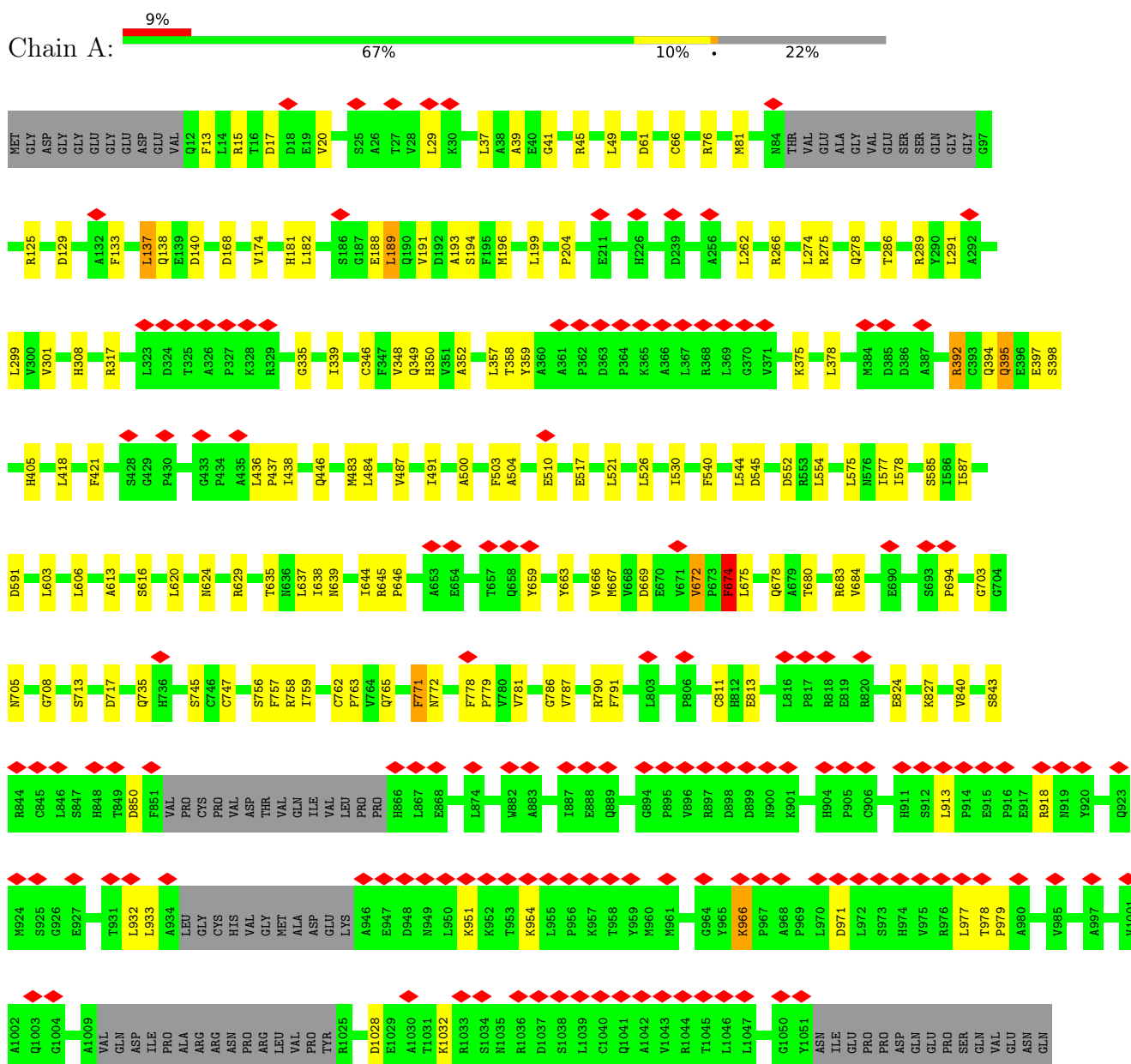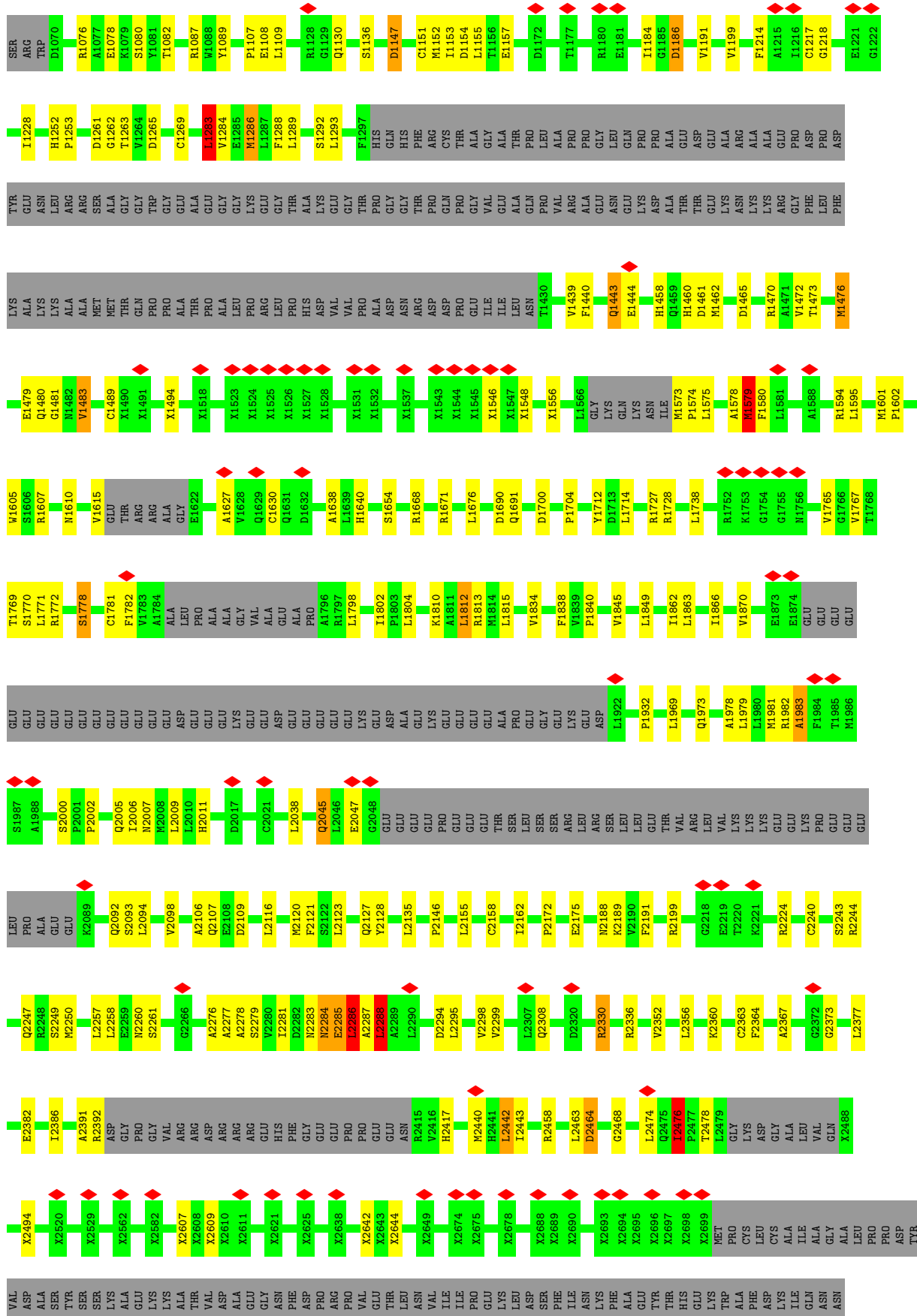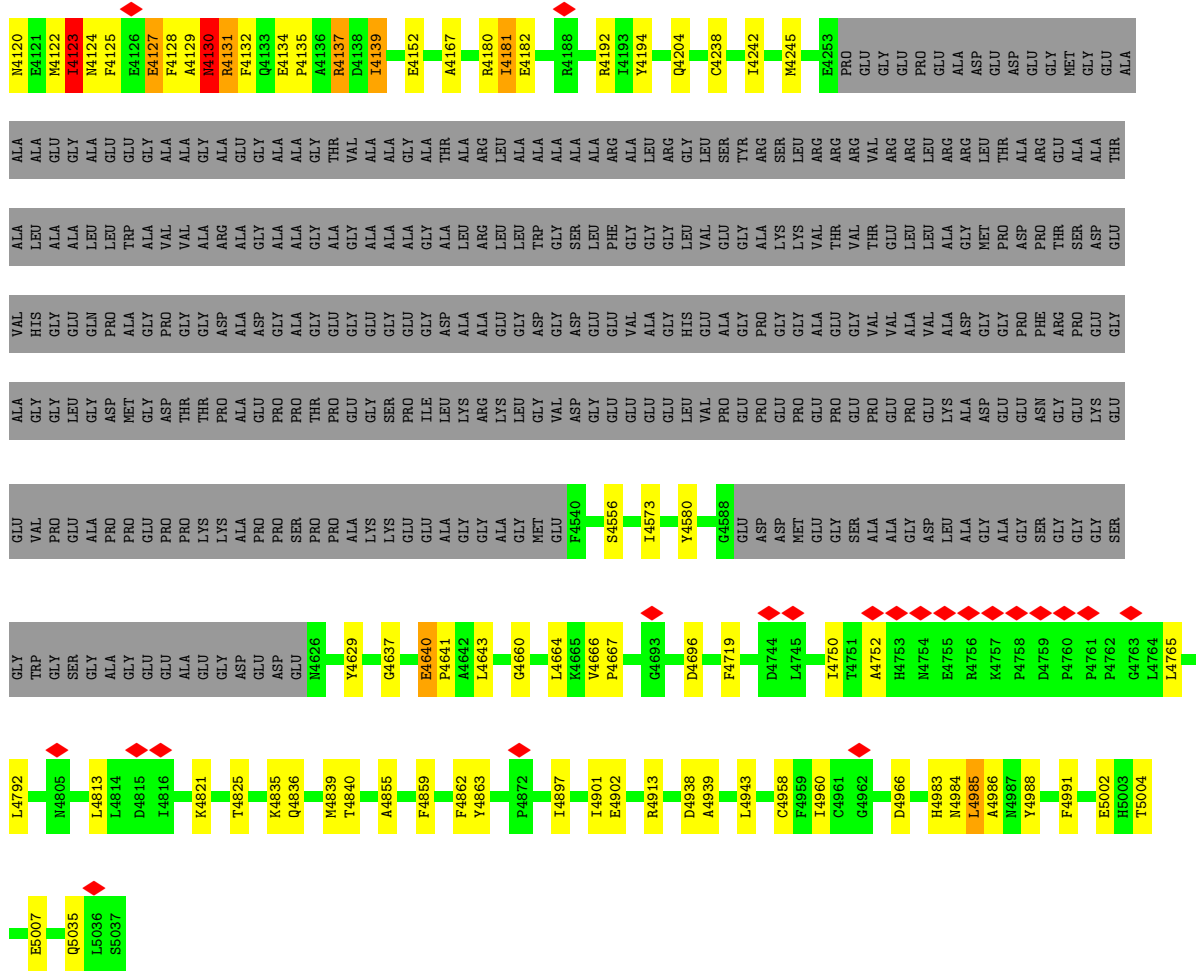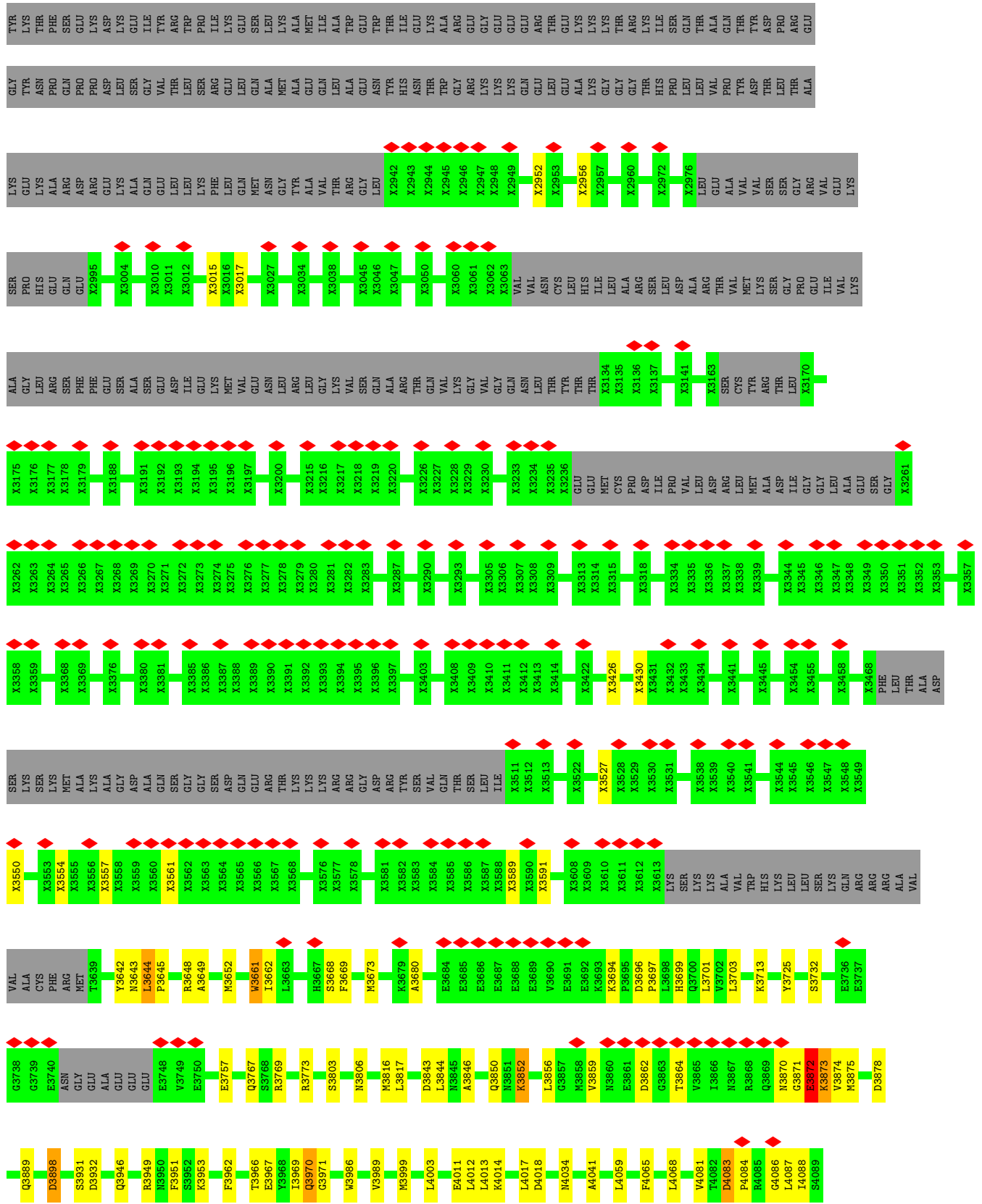
4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	167778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.171	Depositor
Minimum map value	-0.700	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	474.72, 474.72, 474.72	wwPDB
Map dimensions	552, 552, 552	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LBN, ACP, MG, 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	0.31	0/24263	0.59	16/32920 (0.0%)
1	B	0.30	0/24291	0.57	11/32959 (0.0%)
1	C	0.30	0/24161	0.56	9/32790 (0.0%)
1	D	0.30	0/24170	0.57	9/32806 (0.0%)
All	All	0.30	0/96885	0.57	45/131475 (0.0%)

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

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

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4139	ILE	C-N-CA	8.47	140.10	122.30
1	A	4137	ARG	CB-CA-C	-8.20	94.00	110.40
1	A	4088	ILE	N-CA-C	-7.85	89.81	111.00
1	D	2308	GLN	CA-CB-CG	5.90	126.37	113.40
1	C	2308	GLN	CA-CB-CG	5.89	126.36	113.40
1	B	2308	GLN	CA-CB-CG	5.89	126.36	113.40
1	A	2308	GLN	CA-CB-CG	5.89	126.35	113.40
1	A	1579	MET	CB-CG-SD	5.75	129.65	112.40
1	D	1579	MET	CB-CG-SD	5.75	129.64	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1579	MET	CB-CG-SD	5.74	129.63	112.40
1	B	1579	MET	CB-CG-SD	5.74	129.62	112.40
1	A	2464	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	2464	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	4123	ILE	N-CA-C	-5.64	95.77	111.00
1	C	2464	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	2464	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	4130	ASN	CB-CA-C	5.55	121.50	110.40
1	C	4765	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	4139	ILE	CA-C-N	5.50	127.20	116.20
1	D	4765	LEU	CA-CB-CG	5.50	127.94	115.30
1	B	4765	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	4765	LEU	CA-CB-CG	5.49	127.92	115.30
1	D	1579	MET	CA-CB-CG	5.47	122.59	113.30
1	B	1579	MET	CA-CB-CG	5.46	122.59	113.30
1	A	1579	MET	CA-CB-CG	5.46	122.59	113.30
1	C	1579	MET	CA-CB-CG	5.46	122.59	113.30
1	B	4129	ALA	N-CA-C	-5.43	96.33	111.00
1	A	1465	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	932	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	2442	LEU	CA-CB-CG	5.35	127.60	115.30
1	B	932	LEU	CA-CB-CG	5.35	127.60	115.30
1	D	932	LEU	CA-CB-CG	5.34	127.58	115.30
1	D	2442	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	2442	LEU	CA-CB-CG	5.32	127.53	115.30
1	C	2442	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	932	LEU	CA-CB-CG	5.31	127.50	115.30
1	B	933	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	933	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	933	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	933	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	1871	PHE	CB-CG-CD1	-5.25	117.12	120.80
1	A	1283	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	1283	LEU	CA-CB-CG	5.12	127.09	115.30
1	C	1283	LEU	CA-CB-CG	5.12	127.07	115.30
1	D	1283	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4131	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	4137	ARG	Sidechain
1	B	4131	ARG	Sidechain
1	D	4131	ARG	Sidechain

5.2　Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	27759	0	23608	369	0
1	B	27785	0	23648	356	0
1	C	27661	0	23455	315	0
1	D	27670	0	23479	351	0
2	A	31	0	14	1	0
2	B	31	0	14	1	0
2	C	31	0	14	1	0
2	D	31	0	14	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	93	0	0	0	0
5	B	93	0	0	0	0
5	C	93	0	0	3	0
5	D	93	0	0	1	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	111396	0	94246	1382	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 (1382) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2128:TYR:HB3	1:D:3669:PHE:CZ	1.61	1.35
1:A:2128:TYR:HB3	1:A:3669:PHE:CZ	1.63	1.33
1:D:2128:TYR:CD2	1:D:3673:MET:HE3	1.67	1.28
1:A:2128:TYR:CD2	1:A:3673:MET:HE3	1.73	1.22
1:C:2128:TYR:CG	1:C:3673:MET:CE	2.27	1.18
1:B:2128:TYR:CG	1:B:3673:MET:CE	2.26	1.18
1:D:1483:VAL:CG2	1:D:1575:LEU:HD23	1.74	1.16
1:D:2128:TYR:CG	1:D:3673:MET:CE	2.28	1.16
1:B:2128:TYR:CD2	1:B:3673:MET:HE3	1.80	1.15
1:A:2128:TYR:CG	1:A:3673:MET:CE	2.29	1.15
1:D:2106:ALA:HB1	1:D:3697:PRO:HG3	1.27	1.14
1:A:2106:ALA:HB1	1:A:3697:PRO:HG3	1.31	1.10
1:C:2128:TYR:CD2	1:C:3673:MET:CE	2.34	1.10
1:B:2106:ALA:HB1	1:B:3697:PRO:HG3	1.30	1.09
1:B:2128:TYR:CD2	1:B:3673:MET:CE	2.34	1.08
1:B:2128:TYR:CG	1:B:3673:MET:HE2	1.90	1.07
1:C:2128:TYR:CD2	1:C:3673:MET:HE3	1.90	1.06
1:C:2106:ALA:HB1	1:C:3697:PRO:HG3	1.32	1.06
1:D:2128:TYR:CD2	1:D:3673:MET:CE	2.37	1.06
1:C:2128:TYR:CG	1:C:3673:MET:HE2	1.87	1.05
1:A:1480:GLN:HA	1:A:1573:MET:HA	1.38	1.04
1:A:2128:TYR:CD2	1:A:3673:MET:CE	2.37	1.04
1:B:2121:PHE:CZ	1:B:3701:LEU:HB2	1.94	1.02
1:D:1483:VAL:CG2	1:D:1575:LEU:CD2	2.38	1.02
1:D:2121:PHE:CZ	1:D:3701:LEU:HB2	1.95	1.02
1:C:2121:PHE:CZ	1:C:3701:LEU:HB2	1.95	1.01
1:A:2121:PHE:CZ	1:A:3701:LEU:HB2	1.96	1.01
1:D:1483:VAL:HG12	1:D:1484:HIS:H	1.27	0.99
1:D:2106:ALA:HB1	1:D:3697:PRO:CG	1.92	0.98
1:B:2121:PHE:HD1	1:B:3725:TYR:HH	0.98	0.97
1:D:1483:VAL:HG12	1:D:1484:HIS:N	1.80	0.97
1:C:4090:LYS:HA	1:C:4123:ILE:HG12	1.43	0.96
1:D:2128:TYR:HB3	1:D:3669:PHE:CE1	2.01	0.95
1:A:2128:TYR:CG	1:A:3673:MET:HE2	1.98	0.95
1:D:2128:TYR:CG	1:D:3673:MET:HE2	2.01	0.95
1:B:2106:ALA:HB1	1:B:3697:PRO:CG	1.97	0.95
1:A:2106:ALA:HB1	1:A:3697:PRO:CG	1.96	0.94
1:A:2128:TYR:HB3	1:A:3669:PHE:CE1	2.03	0.94
1:C:2106:ALA:HB1	1:C:3697:PRO:CG	1.97	0.93
1:A:2121:PHE:HD1	1:A:3725:TYR:HH	0.93	0.93
1:C:2128:TYR:CD2	1:C:3673:MET:HE2	1.99	0.92
1:D:2106:ALA:CB	1:D:3697:PRO:HG3	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2121:PHE:HD1	1:D:3725:TYR:HH	0.93	0.92
1:C:2121:PHE:HD1	1:C:3725:TYR:HH	0.94	0.91
1:A:2128:TYR:CD2	1:A:3669:PHE:CE1	2.59	0.91
1:D:2128:TYR:CG	1:D:3673:MET:HE3	1.96	0.90
1:B:2106:ALA:CB	1:B:3697:PRO:HG3	2.00	0.90
1:C:2106:ALA:CB	1:C:3697:PRO:HG3	2.01	0.90
1:D:1483:VAL:HG22	1:D:1575:LEU:HD23	1.52	0.90
1:D:2128:TYR:CD2	1:D:3669:PHE:CE1	2.59	0.90
1:A:2106:ALA:CB	1:A:3697:PRO:HG3	2.01	0.89
1:A:2128:TYR:HB3	1:A:3669:PHE:HZ	1.05	0.88
1:B:2128:TYR:CB	1:B:3673:MET:CE	2.51	0.88
1:D:2128:TYR:CB	1:D:3669:PHE:CZ	2.53	0.88
1:A:2128:TYR:CG	1:A:3673:MET:HE3	2.02	0.88
1:D:1483:VAL:HG23	1:D:1575:LEU:CD2	2.05	0.87
1:B:4124:ASN:HB3	1:B:4127:GLU:HB2	1.56	0.87
1:D:1483:VAL:CG1	1:D:1484:HIS:H	1.88	0.86
1:D:2128:TYR:CB	1:D:3673:MET:CE	2.53	0.86
1:B:1254:HIS:HA	1:B:1275:ARG:HH12	1.39	0.86
1:C:2128:TYR:CB	1:C:3673:MET:CE	2.54	0.85
1:D:1483:VAL:HG23	1:D:1575:LEU:HD22	1.58	0.85
1:A:4181:ILE:HD11	1:A:4988:TYR:HA	1.59	0.85
1:A:2128:TYR:CB	1:A:3669:PHE:CZ	2.55	0.84
1:D:2128:TYR:HB3	1:D:3669:PHE:HZ	1.04	0.84
1:B:4181:ILE:HD11	1:B:4988:TYR:HA	1.58	0.83
1:D:2128:TYR:CB	1:D:3669:PHE:CE1	2.62	0.83
1:A:2128:TYR:CB	1:A:3673:MET:CE	2.55	0.83
1:D:4081:VAL:HG22	1:D:4083:ASP:H	1.42	0.82
1:C:4112:LEU:HD22	1:C:4123:ILE:HD11	1.60	0.82
1:B:2128:TYR:HB3	1:B:3669:PHE:HE1	1.45	0.81
1:D:2106:ALA:CB	1:D:3697:PRO:CG	2.55	0.81
1:B:2128:TYR:CG	1:B:3673:MET:HE3	2.05	0.81
1:B:4130:ASN:O	1:B:4133:GLN:HG2	1.81	0.81
1:B:2128:TYR:CD2	1:B:3673:MET:HE2	2.11	0.81
1:C:4088:ILE:HG13	1:C:4123:ILE:HB	1.63	0.80
1:A:2128:TYR:CB	1:A:3669:PHE:CE1	2.64	0.80
1:C:4181:ILE:HD11	1:C:4988:TYR:HA	1.64	0.80
1:D:4181:ILE:HD11	1:D:4988:TYR:HA	1.61	0.80
1:A:2106:ALA:CB	1:A:3697:PRO:CG	2.58	0.79
1:A:2128:TYR:HD2	1:A:3669:PHE:CE1	2.00	0.79
1:B:2106:ALA:CB	1:B:3697:PRO:CG	2.58	0.78
1:C:2106:ALA:CB	1:C:3697:PRO:CG	2.59	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4115:SER:HA	1:A:4128:PHE:CZ	2.20	0.77
1:D:2128:TYR:HD2	1:D:3669:PHE:CE1	2.01	0.76
1:B:1292:SER:O	1:B:1579:MET:HG3	1.86	0.76
1:C:2285:GLU:O	1:C:2286:LEU:HB2	1.87	0.75
1:C:2128:TYR:CG	1:C:3673:MET:HE3	2.11	0.75
1:D:1292:SER:O	1:D:1579:MET:HG3	1.86	0.75
1:C:1292:SER:O	1:C:1579:MET:HG3	1.86	0.74
1:A:2128:TYR:CD2	1:A:3669:PHE:HE1	2.06	0.74
1:D:3644:LEU:HD21	1:D:3649:ALA:HB2	1.69	0.73
1:A:4069:LYS:HG2	1:A:4130:ASN:HD22	1.51	0.73
1:D:2128:TYR:CB	1:D:3669:PHE:HZ	1.95	0.73
1:A:2287:ALA:O	1:A:2288:LEU:HB3	1.89	0.73
1:A:3870:ASN:C	1:A:3872:GLU:H	1.93	0.72
1:C:2128:TYR:HB3	1:C:3669:PHE:HE1	1.54	0.72
1:D:4096:ALA:O	1:D:4098:ASP:N	2.23	0.72
1:D:2128:TYR:O	1:D:3669:PHE:CE1	2.42	0.71
1:A:1480:GLN:HA	1:A:1573:MET:CA	2.18	0.71
1:B:4637:GLY:O	1:B:4641:PRO:HG2	1.91	0.71
1:A:1480:GLN:CA	1:A:1573:MET:HA	2.17	0.70
1:D:2128:TYR:CD2	1:D:3669:PHE:HE1	2.07	0.70
1:B:1254:HIS:HA	1:B:1275:ARG:NH1	2.05	0.70
1:D:2128:TYR:HD2	1:D:3673:MET:HE3	1.54	0.70
1:A:2128:TYR:O	1:A:3669:PHE:CE1	2.45	0.70
1:A:2285:GLU:O	1:A:2286:LEU:HB2	1.91	0.70
1:D:2128:TYR:CB	1:D:3673:MET:HE1	2.22	0.69
1:A:4089:SER:O	1:A:4093:PHE:N	2.18	0.69
1:B:2286:LEU:O	1:B:2288:LEU:N	2.25	0.68
1:B:2128:TYR:CB	1:B:3673:MET:HE1	2.24	0.68
1:B:2128:TYR:HB2	1:B:3673:MET:HE1	1.76	0.68
1:C:1087:ARG:NH1	1:C:1154:ASP:OD1	2.27	0.68
1:A:1476:MET:HA	1:A:1574:PRO:HA	1.76	0.68
1:B:1087:ARG:NH1	1:B:1154:ASP:OD1	2.27	0.68
1:A:1087:ARG:NH1	1:A:1154:ASP:OD1	2.27	0.68
1:D:2003:GLN:HE22	1:D:3862:ASP:HA	1.58	0.67
1:D:2128:TYR:HB2	1:D:3673:MET:HE1	1.77	0.67
1:A:2128:TYR:CD2	1:A:3673:MET:HE2	2.23	0.67
1:D:4984:ASN:O	1:D:4986:ALA:N	2.28	0.67
1:A:4984:ASN:O	1:A:4986:ALA:N	2.28	0.67
1:D:1087:ARG:NH1	1:D:1154:ASP:OD1	2.27	0.67
1:D:2128:TYR:C	1:D:3669:PHE:CZ	2.68	0.67
1:A:4660:GLY:O	1:A:4664:LEU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4083:ASP:HA	1:D:4088:ILE:HD11	1.77	0.66
1:B:4105:GLY:N	1:B:4106:PRO:HD2	2.10	0.66
1:D:4660:GLY:O	1:D:4664:LEU:HB2	1.96	0.66
1:A:1483:VAL:HG22	1:A:1575:LEU:HD22	1.78	0.66
1:A:2107:GLN:HB3	1:A:3683:GLN:OE1	1.95	0.66
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.78	0.66
1:A:2128:TYR:CB	1:A:3673:MET:HE1	2.26	0.66
1:B:4660:GLY:O	1:B:4664:LEU:HB2	1.96	0.66
1:C:4660:GLY:O	1:C:4664:LEU:HB2	1.96	0.66
1:A:4087:LEU:O	1:A:4089:SER:N	2.28	0.66
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.78	0.66
1:C:2128:TYR:CB	1:C:3673:MET:HE3	2.24	0.66
1:D:286:THR:HA	1:D:405:HIS:HB2	1.78	0.66
1:A:3642:TYR:O	1:A:3643:ASN:HB2	1.95	0.66
1:A:286:THR:HA	1:A:405:HIS:HB2	1.78	0.66
1:A:3873:LYS:HD3	1:A:3876:ALA:HA	1.78	0.66
1:C:286:THR:HA	1:C:405:HIS:HB2	1.78	0.66
1:B:4984:ASN:O	1:B:4986:ALA:N	2.29	0.65
1:B:286:THR:HA	1:B:405:HIS:HB2	1.78	0.65
1:C:3642:TYR:O	1:C:3643:ASN:HB2	1.95	0.65
1:D:3642:TYR:O	1:D:3643:ASN:HB2	1.97	0.65
1:B:1863:LEU:HG	1:B:1871:PHE:CZ	2.32	0.65
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.78	0.65
1:C:4100:GLN:HB2	1:C:4106:PRO:HG3	1.79	0.65
1:B:4080:TYR:CD2	1:B:4096:ALA:HB1	2.32	0.65
1:C:2458:ARG:HH12	1:C:2463:LEU:HD23	1.62	0.65
1:D:3859:VAL:CB	1:D:3864:THR:HA	2.28	0.64
1:A:2128:TYR:HB2	1:A:3673:MET:HE1	1.79	0.64
1:C:638:ILE:HG12	1:C:703:GLY:HA3	1.78	0.64
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.78	0.64
1:A:638:ILE:HG12	1:A:703:GLY:HA3	1.78	0.64
1:A:2458:ARG:HH12	1:A:2463:LEU:HD23	1.62	0.64
1:C:4960:ILE:HB	1:C:4983:HIS:HD2	1.63	0.64
1:D:638:ILE:HG12	1:D:703:GLY:HA3	1.79	0.64
1:A:667:MET:SD	1:A:790:ARG:NH2	2.71	0.64
1:B:667:MET:SD	1:B:790:ARG:NH2	2.71	0.64
1:B:2128:TYR:CB	1:B:3673:MET:HE3	2.25	0.64
1:B:3867:ASN:HA	1:B:3869:GLN:HE22	1.61	0.64
1:D:2128:TYR:CG	1:D:3669:PHE:HE1	2.16	0.64
1:D:1283:LEU:HG	1:D:1284:VAL:HG12	1.80	0.64
1:C:1082:THR:HG21	1:C:1107:PRO:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1082:THR:HG21	1:D:1107:PRO:HB3	1.80	0.64
1:B:638:ILE:HG12	1:B:703:GLY:HA3	1.79	0.63
1:B:1283:LEU:HG	1:B:1284:VAL:HG12	1.80	0.63
1:C:1283:LEU:HG	1:C:1284:VAL:HG12	1.80	0.63
1:C:4984:ASN:O	1:C:4986:ALA:N	2.30	0.63
1:D:667:MET:SD	1:D:790:ARG:NH2	2.71	0.63
1:A:2128:TYR:C	1:A:3669:PHE:CZ	2.72	0.63
1:C:667:MET:SD	1:C:790:ARG:NH2	2.71	0.63
1:C:4982:GLU:C	1:C:4983:HIS:HD1	2.00	0.63
1:D:2121:PHE:CE1	1:D:3701:LEU:HD22	2.33	0.63
1:D:2458:ARG:HH12	1:D:2463:LEU:HD23	1.62	0.63
1:A:1082:THR:HG21	1:A:1107:PRO:HB3	1.80	0.63
1:C:1954:ARG:HD3	1:C:2038:LEU:HD11	1.79	0.63
1:A:1283:LEU:HG	1:A:1284:VAL:HG12	1.80	0.63
1:B:1082:THR:HG21	1:B:1107:PRO:HB3	1.80	0.63
1:C:2128:TYR:HB2	1:C:3673:MET:HE1	1.81	0.63
1:A:4088:ILE:O	1:A:4089:SER:C	2.37	0.63
1:B:4076:ALA:HB1	1:B:4080:TYR:CG	2.34	0.63
1:C:2121:PHE:CE1	1:C:3701:LEU:HD22	2.34	0.63
1:D:4112:LEU:HD23	1:D:4123:ILE:HD11	1.79	0.63
1:B:639:ASN:HB2	1:B:678:GLN:HG2	1.81	0.63
1:B:2458:ARG:HH12	1:B:2463:LEU:HD23	1.62	0.63
1:C:639:ASN:HB2	1:C:678:GLN:HG2	1.81	0.63
1:B:977:LEU:HD12	1:B:978:THR:HB	1.80	0.62
1:B:4065:PHE:HE2	1:B:4131:ARG:HG2	1.63	0.62
1:D:278:GLN:HG2	1:D:279:PRO:HD2	1.80	0.62
1:D:2003:GLN:NE2	1:D:3862:ASP:HA	2.13	0.62
1:A:639:ASN:HB2	1:A:678:GLN:HG2	1.81	0.62
1:B:3875:MET:O	1:B:3876:ALA:C	2.36	0.62
1:A:2128:TYR:HD2	1:A:3673:MET:HE3	1.57	0.62
1:D:1291:LEU:HD23	1:D:1579:MET:SD	2.40	0.62
1:A:2121:PHE:CE1	1:A:3701:LEU:HD22	2.34	0.62
1:A:2476:ILE:HD11	1:A:2478:THR:HB	1.81	0.62
1:D:639:ASN:HB2	1:D:678:GLN:HG2	1.81	0.62
1:A:1460:HIS:CE1	1:A:1472:VAL:HG21	2.34	0.62
1:A:2107:GLN:CB	1:A:3683:GLN:OE1	2.47	0.62
1:B:1460:HIS:CE1	1:B:1472:VAL:HG21	2.34	0.62
1:D:1460:HIS:CE1	1:D:1472:VAL:HG21	2.34	0.62
1:C:977:LEU:HD12	1:C:978:THR:HB	1.80	0.61
1:C:1460:HIS:CE1	1:C:1472:VAL:HG21	2.34	0.61
1:D:977:LEU:HD12	1:D:978:THR:HB	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD13	1:A:421:PHE:HE1	1.65	0.61
1:A:977:LEU:HD12	1:A:978:THR:HB	1.80	0.61
1:B:394:GLN:CB	1:B:398:SER:HB3	2.29	0.61
1:D:2128:TYR:CB	1:D:3669:PHE:HE1	2.13	0.61
1:D:4204:GLN:HG2	1:D:4245:MET:HG2	1.83	0.61
1:A:2128:TYR:CG	1:A:3669:PHE:HE1	2.17	0.61
1:A:790:ARG:HG3	1:A:1627:ALA:HB2	1.83	0.61
1:D:790:ARG:HG3	1:D:1627:ALA:HB2	1.83	0.61
1:C:275:ARG:HH22	1:C:335:GLY:HA3	1.66	0.61
1:D:418:LEU:HD13	1:D:421:PHE:HE1	1.65	0.61
1:D:275:ARG:HH22	1:D:335:GLY:HA3	1.66	0.61
1:A:3667:HIS:C	1:A:3669:PHE:H	2.04	0.61
1:C:1439:VAL:HA	1:C:1443:GLN:HG2	1.83	0.61
1:C:4204:GLN:HG2	1:C:4245:MET:HG2	1.83	0.61
1:B:275:ARG:HH22	1:B:335:GLY:HA3	1.66	0.61
1:B:790:ARG:HG3	1:B:1627:ALA:HB2	1.83	0.61
1:D:517:GLU:N	1:D:517:GLU:OE1	2.34	0.61
1:A:299:LEU:HG	1:A:357:LEU:HD22	1.83	0.61
1:C:4064:MET:HB3	1:C:4107:GLU:HG2	1.83	0.61
1:D:4090:LYS:HA	1:D:4123:ILE:HB	1.82	0.61
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.83	0.60
1:A:4204:GLN:HG2	1:A:4245:MET:HG2	1.83	0.60
1:B:2121:PHE:CE1	1:B:3701:LEU:HD22	2.36	0.60
1:C:418:LEU:HD13	1:C:421:PHE:HE1	1.66	0.60
1:C:517:GLU:OE1	1:C:517:GLU:N	2.34	0.60
1:A:4088:ILE:HB	1:A:4093:PHE:CB	2.30	0.60
1:A:4129:ALA:O	1:A:4130:ASN:C	2.39	0.60
1:A:4939:ALA:O	1:A:4943:LEU:HG	2.01	0.60
1:B:1291:LEU:HD23	1:B:1579:MET:SD	2.41	0.60
1:C:4637:GLY:O	1:C:4641:PRO:HG2	2.01	0.60
1:C:790:ARG:HG3	1:C:1627:ALA:HB2	1.83	0.60
1:A:275:ARG:HH22	1:A:335:GLY:HA3	1.66	0.60
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.83	0.60
1:D:4065:PHE:HE2	1:D:4131:ARG:HD2	1.65	0.60
1:B:418:LEU:HD13	1:B:421:PHE:HE1	1.65	0.60
1:D:2106:ALA:HB1	1:D:3697:PRO:CB	2.32	0.60
1:D:4637:GLY:O	1:D:4641:PRO:HG2	2.01	0.60
1:A:517:GLU:N	1:A:517:GLU:OE1	2.34	0.60
1:B:663:TYR:HE1	1:B:745:SER:HB3	1.67	0.60
1:B:2128:TYR:HD2	1:B:3673:MET:HE3	1.59	0.60
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ARG:O	1:B:393:CYS:SG	2.56	0.59
1:B:4204:GLN:HG2	1:B:4245:MET:HG2	1.83	0.59
1:A:4556:SER:HB3	1:A:4664:LEU:HD13	1.84	0.59
1:B:2128:TYR:CD1	1:B:3673:MET:HE2	2.37	0.59
1:B:4129:ALA:O	1:B:4130:ASN:C	2.40	0.59
1:D:76:ARG:HH22	1:D:174:VAL:HG21	1.68	0.59
1:C:2128:TYR:CD1	1:C:3673:MET:HE2	2.38	0.59
1:D:1483:VAL:HG21	1:D:1575:LEU:HD23	1.74	0.59
1:A:4135:PRO:O	1:A:4139:ILE:HD12	2.02	0.59
1:B:4110:PHE:HD1	1:B:4110:PHE:H	1.51	0.59
1:C:76:ARG:HH22	1:C:174:VAL:HG21	1.68	0.59
1:C:1290:ARG:O	1:C:1291:LEU:HB2	2.02	0.59
1:C:4556:SER:HB3	1:C:4664:LEU:HD13	1.84	0.59
1:D:1291:LEU:HD21	1:D:1580:PHE:CE2	2.38	0.59
1:D:4123:ILE:HG23	1:D:4125:PHE:H	1.68	0.59
1:C:394:GLN:CB	1:C:398:SER:HB3	2.32	0.59
1:D:2128:TYR:O	1:D:3669:PHE:CZ	2.55	0.59
1:A:2128:TYR:CG	1:A:3669:PHE:CE1	2.91	0.59
1:A:3850:GLN:NE2	1:A:3946:GLN:OE1	2.36	0.59
1:A:4637:GLY:O	1:A:4641:PRO:HG2	2.01	0.59
1:B:4556:SER:HB3	1:B:4664:LEU:HD13	1.84	0.59
1:D:4556:SER:HB3	1:D:4664:LEU:HD13	1.84	0.59
1:C:4089:SER:HB3	1:C:4092:ASP:HB2	1.84	0.59
1:A:4087:LEU:O	1:A:4088:ILE:C	2.40	0.59
1:D:2128:TYR:CG	1:D:3669:PHE:CE1	2.89	0.59
1:C:1186:ASP:OD1	1:C:1186:ASP:N	2.36	0.58
1:A:1810:LYS:HG3	1:A:1813:ARG:HH21	1.68	0.58
1:B:4093:PHE:O	1:B:4097:MET:N	2.34	0.58
1:C:1029:GLU:HA	1:C:1032:LYS:HD2	1.86	0.58
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.83	0.58
1:D:2135:LEU:HD22	1:D:3662:ILE:HD13	1.86	0.58
1:B:2286:LEU:C	1:B:2288:LEU:H	2.06	0.58
1:B:517:GLU:N	1:B:517:GLU:OE1	2.34	0.58
1:A:2106:ALA:HB1	1:A:3697:PRO:CB	2.33	0.58
1:A:2135:LEU:HD22	1:A:3662:ILE:HD13	1.86	0.58
1:B:76:ARG:HH22	1:B:174:VAL:HG21	1.68	0.58
1:B:3850:GLN:NE2	1:B:3946:GLN:OE1	2.36	0.58
1:B:4086:GLY:O	1:B:4087:LEU:C	2.40	0.58
1:A:3870:ASN:C	1:A:3872:GLU:N	2.57	0.58
1:B:1186:ASP:OD1	1:B:1186:ASP:N	2.36	0.58
1:C:3850:GLN:NE2	1:C:3946:GLN:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4110:PHE:HD1	1:A:4110:PHE:H	1.52	0.58
1:A:4901:ILE:HG22	1:A:4902:GLU:N	2.19	0.58
1:A:2128:TYR:CB	1:A:3673:MET:HE3	2.31	0.58
1:C:663:TYR:HE1	1:C:745:SER:HB3	1.68	0.58
1:C:2135:LEU:HD22	1:C:3662:ILE:HD13	1.86	0.58
1:D:3850:GLN:NE2	1:D:3946:GLN:OE1	2.36	0.58
1:A:76:ARG:HH22	1:A:174:VAL:HG21	1.68	0.57
1:B:1291:LEU:HD21	1:B:1580:PHE:CE2	2.38	0.57
1:C:2106:ALA:HB1	1:C:3697:PRO:CB	2.34	0.57
1:D:2287:ALA:O	1:D:2288:LEU:HB2	2.04	0.57
1:B:4097:MET:CB	1:B:4108:ILE:HG12	2.34	0.57
1:C:4666:VAL:N	1:C:4667:PRO:CD	2.68	0.57
1:A:2128:TYR:O	1:A:3669:PHE:CZ	2.57	0.57
1:A:4013:LEU:HD12	1:A:4016:LEU:HD22	1.85	0.57
1:B:2135:LEU:HD22	1:B:3662:ILE:HD13	1.86	0.57
1:C:2128:TYR:CB	1:C:3673:MET:HE1	2.30	0.57
1:D:4110:PHE:HD1	1:D:4110:PHE:H	1.51	0.57
1:A:747:CYS:HB2	1:A:756:SER:HB3	1.87	0.57
1:A:2128:TYR:CB	1:A:3669:PHE:HZ	1.96	0.57
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.36	0.57
1:A:41:GLY:O	1:A:45:ARG:NH1	2.38	0.57
1:C:41:GLY:O	1:C:45:ARG:NH1	2.38	0.57
1:B:4076:ALA:HB1	1:B:4080:TYR:CD2	2.39	0.57
1:C:1979:LEU:HG	1:C:1980:LEU:HG	1.87	0.57
1:D:4666:VAL:N	1:D:4667:PRO:CD	2.67	0.57
1:A:1458:HIS:CD2	1:A:1483:VAL:HG21	2.40	0.57
1:B:1812:LEU:HD13	1:B:1862:ILE:HG12	1.86	0.57
1:A:2128:TYR:CB	1:A:3669:PHE:HE1	2.15	0.57
1:C:747:CYS:HB2	1:C:756:SER:HB3	1.87	0.57
1:C:1812:LEU:HD13	1:C:1862:ILE:HG12	1.85	0.57
1:B:3875:MET:O	1:B:3877:ASP:N	2.38	0.57
1:A:4139:ILE:HG22	1:A:4139:ILE:O	2.04	0.56
1:B:747:CYS:HB2	1:B:756:SER:HB3	1.87	0.56
1:B:1290:ARG:O	1:B:1291:LEU:HB2	2.05	0.56
1:D:747:CYS:HB2	1:D:756:SER:HB3	1.87	0.56
1:D:1483:VAL:HG21	1:D:1575:LEU:CD2	2.34	0.56
1:A:394:GLN:CB	1:A:398:SER:HB3	2.35	0.56
1:D:41:GLY:O	1:D:45:ARG:NH1	2.38	0.56
1:D:2128:TYR:CD1	1:D:3673:MET:HE2	2.41	0.56
1:B:41:GLY:O	1:B:45:ARG:NH1	2.38	0.56
1:B:3426:UNK:O	1:B:3430:UNK:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:LEU:HD21	1:A:1578:ALA:HB1	1.86	0.56
1:A:4090:LYS:H	1:A:4120:ASN:HB3	1.69	0.56
1:B:1254:HIS:HB3	1:B:1276:THR:HG21	1.87	0.56
1:D:3426:UNK:O	1:D:3430:UNK:CB	2.54	0.56
1:A:39:ALA:HB1	1:A:137:LEU:HD11	1.88	0.56
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.39	0.56
1:D:39:ALA:HB1	1:D:137:LEU:HD11	1.88	0.56
1:D:1834:VAL:HG13	1:D:1932:PRO:HG3	1.88	0.56
1:D:4093:PHE:O	1:D:4097:MET:N	2.31	0.56
1:A:3803:SER:O	1:A:3806:ASN:ND2	2.39	0.56
1:B:646:PRO:HG2	1:B:779:PRO:HG2	1.88	0.56
1:C:3803:SER:O	1:C:3806:ASN:ND2	2.39	0.56
1:D:1147:ASP:OD1	1:D:1147:ASP:N	2.39	0.56
1:D:3803:SER:O	1:D:3806:ASN:ND2	2.39	0.56
1:A:4110:PHE:HD1	1:A:4110:PHE:N	2.03	0.55
1:C:3871:GLY:O	1:C:3872:GLU:C	2.44	0.55
1:D:4081:VAL:HG22	1:D:4083:ASP:N	2.17	0.55
1:B:1089:TYR:HD1	1:B:1152:MET:HG2	1.72	0.55
1:B:2106:ALA:HB1	1:B:3697:PRO:CB	2.37	0.55
1:C:4068:LEU:HD21	1:C:4111:LEU:HD22	1.87	0.55
1:A:1834:VAL:HG13	1:A:1932:PRO:HG3	1.88	0.55
1:A:4011:GLU:HA	1:A:4014:LYS:HD2	1.88	0.55
1:A:4835:LYS:O	1:A:4839:MET:HG2	2.07	0.55
1:B:1292:SER:O	1:B:1293:LEU:HD23	2.07	0.55
1:D:289:ARG:HB3	1:D:301:VAL:HB	1.89	0.55
1:D:392:ARG:H	1:D:392:ARG:HD3	1.71	0.55
1:B:1439:VAL:HA	1:B:1443:GLN:HG2	1.88	0.55
1:B:4093:PHE:O	1:B:4096:ALA:HB3	2.06	0.55
1:C:3426:UNK:O	1:C:3430:UNK:CB	2.54	0.55
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.39	0.55
1:D:4011:GLU:HA	1:D:4014:LYS:HD2	1.88	0.55
1:B:392:ARG:H	1:B:392:ARG:HD3	1.71	0.55
1:B:2287:ALA:O	1:B:2349:ASN:ND2	2.39	0.55
1:A:3767:GLN:NE2	1:A:3806:ASN:OD1	2.40	0.55
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.39	0.55
1:D:1292:SER:O	1:D:1293:LEU:HD23	2.06	0.55
1:D:1483:VAL:CG1	1:D:1484:HIS:N	2.47	0.55
1:A:1812:LEU:HD13	1:A:1862:ILE:HG12	1.88	0.55
1:B:988:LEU:HA	1:B:991:ASN:ND2	2.22	0.55
1:B:3767:GLN:NE2	1:B:3806:ASN:OD1	2.40	0.55
1:C:2247:GLN:O	1:C:2251:PHE:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2475:GLN:O	1:C:2476:ILE:HG22	2.07	0.55
1:A:1263:THR:OG1	1:A:1265:ASP:O	2.24	0.55
1:C:37:LEU:HD11	1:C:191:VAL:HG11	1.89	0.55
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.89	0.55
1:C:1834:VAL:HG13	1:C:1932:PRO:HG3	1.88	0.55
1:D:3661:TRP:HB3	1:D:3662:ILE:HD12	1.89	0.55
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.89	0.55
1:A:646:PRO:HG2	1:A:779:PRO:HG2	1.89	0.55
1:A:3426:UNK:O	1:A:3430:UNK:CB	2.54	0.55
1:A:4938:ASP:OD1	1:B:4944:ARG:NH1	2.36	0.55
1:B:39:ALA:HB1	1:B:137:LEU:HD11	1.88	0.55
1:B:3803:SER:O	1:B:3806:ASN:ND2	2.39	0.55
1:C:3661:TRP:HB3	1:C:3662:ILE:HD12	1.88	0.55
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.39	0.55
1:D:646:PRO:HG2	1:D:779:PRO:HG2	1.88	0.55
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.36	0.55
1:B:4835:LYS:O	1:B:4839:MET:HG2	2.07	0.55
1:D:1089:TYR:HD1	1:D:1152:MET:HG2	1.72	0.55
1:D:4835:LYS:O	1:D:4839:MET:HG2	2.07	0.55
1:A:2045:GLN:HB2	1:A:2047:GLU:HG2	1.90	0.54
1:B:1147:ASP:OD1	1:B:1147:ASP:N	2.39	0.54
1:B:3839:CYS:HG	1:B:3881:THR:HG1	1.55	0.54
1:B:4011:GLU:HA	1:B:4014:LYS:HD2	1.88	0.54
1:C:1089:TYR:HD1	1:C:1152:MET:HG2	1.72	0.54
1:C:4011:GLU:HA	1:C:4014:LYS:HD2	1.88	0.54
1:D:2247:GLN:O	1:D:2251:PHE:HB2	2.06	0.54
1:A:1147:ASP:OD1	1:A:1147:ASP:N	2.39	0.54
1:B:4082:THR:HG21	1:B:4088:ILE:HG23	1.89	0.54
1:C:3767:GLN:NE2	1:C:3806:ASN:OD1	2.40	0.54
1:D:1290:ARG:O	1:D:1291:LEU:HB2	2.07	0.54
1:D:3767:GLN:NE2	1:D:3806:ASN:OD1	2.40	0.54
1:A:1089:TYR:HD1	1:A:1152:MET:HG2	1.72	0.54
1:B:289:ARG:HB3	1:B:301:VAL:HB	1.89	0.54
1:B:358:THR:OG1	1:B:359:TYR:N	2.40	0.54
1:C:39:ALA:HB1	1:C:137:LEU:HD11	1.88	0.54
1:C:358:THR:OG1	1:C:359:TYR:N	2.40	0.54
1:C:646:PRO:HG2	1:C:779:PRO:HG2	1.88	0.54
1:C:2285:GLU:O	1:C:2286:LEU:CB	2.54	0.54
1:A:1473:THR:O	1:A:1483:VAL:HG12	2.08	0.54
1:B:1834:VAL:HG13	1:B:1932:PRO:HG3	1.88	0.54
1:C:850:ASP:N	1:C:850:ASP:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4835:LYS:O	1:C:4839:MET:HG2	2.06	0.54
1:B:2045:GLN:HB2	1:B:2047:GLU:HG2	1.89	0.54
1:D:1812:LEU:HD13	1:D:1862:ILE:HG12	1.88	0.54
1:A:4110:PHE:N	1:A:4110:PHE:CD1	2.76	0.54
1:B:37:LEU:HD11	1:B:191:VAL:HG11	1.89	0.54
1:B:2247:GLN:O	1:B:2251:PHE:HB2	2.06	0.54
1:D:4065:PHE:CE2	1:D:4131:ARG:HD2	2.41	0.54
1:A:358:THR:OG1	1:A:359:TYR:N	2.40	0.54
1:C:392:ARG:HD3	1:C:392:ARG:H	1.71	0.54
1:D:1263:THR:OG1	1:D:1265:ASP:O	2.24	0.54
1:A:37:LEU:HD11	1:A:191:VAL:HG11	1.89	0.54
1:D:4086:GLY:O	1:D:4087:LEU:C	2.46	0.54
1:A:392:ARG:HD3	1:A:392:ARG:H	1.71	0.54
1:A:4132:PHE:C	1:A:4135:PRO:HD2	2.28	0.54
1:A:2128:TYR:CD1	1:A:3673:MET:HE2	2.41	0.54
1:B:4666:VAL:N	1:B:4667:PRO:CD	2.70	0.54
1:B:4901:ILE:HG22	1:B:4902:GLU:N	2.23	0.54
1:D:4901:ILE:HG22	1:D:4902:GLU:N	2.23	0.53
1:D:708:GLY:H	1:D:713:SER:HB2	1.73	0.53
1:C:708:GLY:H	1:C:713:SER:HB2	1.73	0.53
1:A:850:ASP:OD1	1:A:850:ASP:N	2.41	0.53
1:A:3870:ASN:O	1:A:3872:GLU:N	2.42	0.53
1:B:850:ASP:OD1	1:B:850:ASP:N	2.41	0.53
1:C:666:VAL:HG11	1:C:684:VAL:HG11	1.90	0.53
1:D:13:PHE:O	1:D:15:ARG:NH1	2.42	0.53
1:A:13:PHE:O	1:A:15:ARG:NH1	2.42	0.53
1:A:4075:GLU:HG2	1:A:4076:ALA:N	2.24	0.53
1:B:4586:PRO:HA	1:B:4628:VAL:HG21	1.90	0.53
1:D:358:THR:OG1	1:D:359:TYR:N	2.40	0.53
1:A:575:LEU:HA	1:A:578:ILE:HG12	1.91	0.53
1:B:1263:THR:OG1	1:B:1265:ASP:O	2.24	0.53
1:C:3817:LEU:HD21	1:C:3898:ASP:CB	2.39	0.53
1:A:2121:PHE:CD2	1:A:3701:LEU:HD13	2.44	0.53
1:C:2287:ALA:O	1:C:2288:LEU:HB3	2.09	0.53
1:D:575:LEU:HA	1:D:578:ILE:HG12	1.91	0.53
1:D:745:SER:HB2	1:D:758:ARG:HB3	1.91	0.53
1:D:4083:ASP:N	1:D:4084:PRO:HD3	2.24	0.53
1:A:3817:LEU:HD21	1:A:3898:ASP:CB	2.39	0.53
1:B:591:ASP:OD1	1:B:1594:ARG:NH1	2.42	0.53
1:B:708:GLY:H	1:B:713:SER:HB2	1.73	0.53
1:C:3550:UNK:O	1:C:3554:UNK:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2286:LEU:O	1:D:2287:ALA:C	2.45	0.53
1:A:3550:UNK:O	1:A:3554:UNK:N	2.42	0.53
1:B:666:VAL:HG11	1:B:684:VAL:HG11	1.90	0.53
1:D:591:ASP:OD1	1:D:1594:ARG:NH1	2.42	0.53
1:A:708:GLY:H	1:A:713:SER:HB2	1.73	0.52
1:A:1483:VAL:HG23	1:A:1556:UNK:CB	2.39	0.52
1:B:13:PHE:O	1:B:15:ARG:NH1	2.42	0.52
1:B:3550:UNK:O	1:B:3554:UNK:N	2.42	0.52
1:C:575:LEU:HA	1:C:578:ILE:HG12	1.91	0.52
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.36	0.52
1:D:2121:PHE:CD2	1:D:3701:LEU:HD13	2.43	0.52
1:D:4586:PRO:HA	1:D:4628:VAL:HG21	1.90	0.52
1:B:2128:TYR:HB3	1:B:3669:PHE:CE1	2.36	0.52
1:B:5004:THR:HB	1:B:5007:GLU:HG3	1.91	0.52
1:C:5004:THR:HB	1:C:5007:GLU:HG3	1.91	0.52
1:D:666:VAL:HG11	1:D:684:VAL:HG11	1.90	0.52
1:D:3817:LEU:HD21	1:D:3898:ASP:CB	2.39	0.52
1:B:745:SER:HB2	1:B:758:ARG:HB3	1.91	0.52
1:C:745:SER:HB2	1:C:758:ARG:HB3	1.91	0.52
1:C:1147:ASP:OD1	1:C:1147:ASP:N	2.39	0.52
1:A:666:VAL:HG11	1:A:684:VAL:HG11	1.90	0.52
1:B:645:ARG:HB3	1:B:824:GLU:O	2.10	0.52
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.36	0.52
1:B:3817:LEU:HD21	1:B:3898:ASP:CB	2.39	0.52
1:B:4640:GLU:HB3	1:B:4641:PRO:HD3	1.92	0.52
1:D:37:LEU:HD11	1:D:191:VAL:HG11	1.89	0.52
1:D:1458:HIS:CD2	1:D:1458:HIS:H	2.26	0.52
1:D:2121:PHE:CE2	1:D:3701:LEU:HB2	2.43	0.52
1:D:3550:UNK:O	1:D:3554:UNK:N	2.42	0.52
1:A:1228:ILE:HD12	1:A:1228:ILE:H	1.75	0.52
1:B:4863:TYR:CZ	1:B:4901:ILE:HD11	2.45	0.52
1:C:1261:ASP:OD1	1:C:1262:GLY:N	2.43	0.52
1:C:2128:TYR:HB3	1:C:3673:MET:HE3	1.90	0.52
1:D:4897:ILE:HG13	1:D:4901:ILE:HG13	1.92	0.52
1:B:299:LEU:HG	1:B:357:LEU:HD22	1.91	0.52
1:C:591:ASP:OD1	1:C:1594:ARG:NH1	2.42	0.52
1:C:4863:TYR:CZ	1:C:4901:ILE:HD11	2.45	0.52
1:D:1261:ASP:OD1	1:D:1262:GLY:N	2.43	0.52
1:D:4640:GLU:HB3	1:D:4641:PRO:HD3	1.91	0.52
1:C:2121:PHE:CD2	1:C:3701:LEU:HD13	2.44	0.52
1:C:4901:ILE:HG22	1:C:4902:GLU:N	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:LEU:HA	1:B:578:ILE:HG12	1.91	0.52
1:B:1228:ILE:H	1:B:1228:ILE:HD12	1.75	0.52
1:B:1261:ASP:OD1	1:B:1262:GLY:N	2.43	0.52
1:C:13:PHE:O	1:C:15:ARG:NH1	2.42	0.52
1:D:1228:ILE:HD12	1:D:1228:ILE:H	1.75	0.52
1:B:4897:ILE:HG13	1:B:4901:ILE:HG13	1.92	0.52
1:C:3648:ARG:HH21	1:C:3652:MET:HE1	1.75	0.52
1:D:645:ARG:HB3	1:D:824:GLU:O	2.10	0.52
1:D:2106:ALA:HB3	1:D:3697:PRO:CG	2.38	0.52
1:D:5004:THR:HB	1:D:5007:GLU:HG3	1.92	0.52
1:A:591:ASP:OD1	1:A:1594:ARG:NH1	2.42	0.52
1:C:2106:ALA:HB3	1:C:3697:PRO:CG	2.40	0.52
1:C:4897:ILE:HG13	1:C:4901:ILE:HG13	1.92	0.52
1:D:182:LEU:HD11	1:D:189:LEU:HD12	1.92	0.52
1:D:3817:LEU:HD21	1:D:3898:ASP:HB2	1.93	0.52
1:A:1261:ASP:OD1	1:A:1262:GLY:N	2.43	0.51
1:A:3873:LYS:NZ	1:A:3873:LYS:H	2.08	0.51
1:B:2121:PHE:CD2	1:B:3701:LEU:HD13	2.46	0.51
1:C:1228:ILE:HD12	1:C:1228:ILE:H	1.75	0.51
1:D:672:VAL:HG21	1:D:675:LEU:HG	1.92	0.51
1:D:4863:TYR:CZ	1:D:4901:ILE:HD11	2.45	0.51
1:A:745:SER:HB2	1:A:758:ARG:HB3	1.91	0.51
1:B:2128:TYR:HB3	1:B:3673:MET:HE3	1.93	0.51
1:C:357:LEU:HA	1:C:378:LEU:HA	1.92	0.51
1:C:645:ARG:HB3	1:C:824:GLU:O	2.10	0.51
1:C:3871:GLY:O	1:C:3873:LYS:N	2.44	0.51
1:C:4640:GLU:HB3	1:C:4641:PRO:HD3	1.91	0.51
1:D:3648:ARG:HH21	1:D:3652:MET:HE1	1.75	0.51
1:B:1870:VAL:HG21	1:B:2092:GLN:HA	1.93	0.51
1:D:1076:ARG:HB3	1:D:1191:VAL:HG12	1.92	0.51
1:A:3870:ASN:HD21	1:A:3872:GLU:CG	2.24	0.51
1:A:5004:THR:HB	1:A:5007:GLU:HG3	1.91	0.51
1:C:1263:THR:OG1	1:C:1265:ASP:O	2.24	0.51
1:D:1157:GLU:N	1:D:1157:GLU:OE1	2.44	0.51
1:D:2128:TYR:HB2	1:D:3673:MET:CE	2.36	0.51
1:A:1076:ARG:HB3	1:A:1191:VAL:HG12	1.92	0.51
1:B:684:VAL:HG12	1:B:781:VAL:HG23	1.93	0.51
1:C:684:VAL:HG12	1:C:781:VAL:HG23	1.93	0.51
1:C:4082:THR:O	1:C:4086:GLY:N	2.43	0.51
1:D:1979:LEU:HD23	1:D:1980:LEU:HG	1.93	0.51
1:A:645:ARG:HB3	1:A:824:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3648:ARG:HH21	1:A:3652:MET:HE1	1.75	0.51
1:A:3661:TRP:HB3	1:A:3662:ILE:HD12	1.92	0.51
1:B:2007:ASN:O	1:B:2011:HIS:N	2.44	0.51
1:C:1870:VAL:HG21	1:C:2092:GLN:HA	1.93	0.51
1:D:1812:LEU:HD21	1:D:1861:GLN:HG2	1.93	0.51
1:A:4897:ILE:O	1:A:4901:ILE:HG13	2.11	0.51
1:B:1076:ARG:HB3	1:B:1191:VAL:HG12	1.92	0.51
1:C:1157:GLU:N	1:C:1157:GLU:OE1	2.44	0.51
1:A:3817:LEU:HD21	1:A:3898:ASP:HB2	1.93	0.51
1:A:4863:TYR:CZ	1:A:4901:ILE:HD11	2.46	0.51
1:C:1292:SER:O	1:C:1293:LEU:HD23	2.11	0.51
1:B:1157:GLU:OE1	1:B:1157:GLU:N	2.44	0.50
1:C:672:VAL:HG21	1:C:675:LEU:HG	1.93	0.50
1:A:357:LEU:HA	1:A:378:LEU:HA	1.92	0.50
1:A:2007:ASN:O	1:A:2011:HIS:N	2.44	0.50
1:B:500:ALA:HA	1:B:503:PHE:HB2	1.92	0.50
1:B:1089:TYR:HA	1:B:1151:CYS:O	2.12	0.50
1:C:1076:ARG:HB3	1:C:1191:VAL:HG12	1.92	0.50
1:C:1089:TYR:HA	1:C:1151:CYS:O	2.12	0.50
1:C:2248:ARG:NH2	1:C:2285:GLU:OE2	2.44	0.50
1:C:2642:UNK:O	1:C:2644:UNK:N	2.45	0.50
1:C:3817:LEU:HD21	1:C:3898:ASP:HB2	1.93	0.50
1:D:2642:UNK:O	1:D:2644:UNK:N	2.45	0.50
1:A:1157:GLU:N	1:A:1157:GLU:OE1	2.44	0.50
1:D:684:VAL:HG12	1:D:781:VAL:HG23	1.93	0.50
1:D:4096:ALA:O	1:D:4097:MET:C	2.49	0.50
1:A:500:ALA:HA	1:A:503:PHE:HB2	1.92	0.50
1:A:2106:ALA:HB3	1:A:3697:PRO:CG	2.41	0.50
1:A:1108:GLU:OE1	1:A:1108:GLU:N	2.39	0.50
1:B:1108:GLU:OE1	1:B:1108:GLU:N	2.39	0.50
1:C:500:ALA:HA	1:C:503:PHE:HB2	1.92	0.50
1:D:357:LEU:HA	1:D:378:LEU:HA	1.92	0.50
1:A:1089:TYR:HA	1:A:1151:CYS:O	2.12	0.50
1:A:1870:VAL:HG21	1:A:2092:GLN:HA	1.93	0.50
1:B:2248:ARG:NH2	1:B:2285:GLU:OE2	2.44	0.50
1:C:4182:GLU:HG2	1:C:4192:ARG:HG2	1.92	0.50
1:A:684:VAL:HG12	1:A:781:VAL:HG23	1.93	0.50
1:B:357:LEU:HA	1:B:378:LEU:HA	1.92	0.50
1:B:3817:LEU:HD21	1:B:3898:ASP:HB2	1.93	0.50
1:B:3867:ASN:HA	1:B:3869:GLN:NE2	2.27	0.50
1:D:4065:PHE:HE2	1:D:4131:ARG:CD	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2006:ILE:HD12	1:B:2009:LEU:HD23	1.94	0.50
1:B:2642:UNK:O	1:B:2644:UNK:N	2.44	0.50
1:B:3986:TRP:HA	1:B:3989:VAL:HG22	1.94	0.50
1:C:644:ILE:HG21	1:C:1615:VAL:HG11	1.94	0.50
1:C:1108:GLU:OE1	1:C:1108:GLU:N	2.39	0.50
1:D:4124:ASN:ND2	1:D:4127:GLU:OE1	2.44	0.50
1:A:2006:ILE:HD12	1:A:2009:LEU:HD23	1.94	0.50
1:A:2642:UNK:O	1:A:2644:UNK:N	2.45	0.50
1:C:1220:GLN:NE2	1:D:3527:UNK:O	2.45	0.50
1:C:2006:ILE:HD12	1:C:2009:LEU:HD23	1.94	0.50
1:D:2006:ILE:HD12	1:D:2009:LEU:HD23	1.94	0.50
1:A:672:VAL:HG21	1:A:675:LEU:HG	1.93	0.49
1:A:2283:ASN:HD22	1:A:2286:LEU:HD22	1.77	0.49
1:D:644:ILE:HG21	1:D:1615:VAL:HG11	1.94	0.49
1:D:1870:VAL:HG21	1:D:2092:GLN:HA	1.93	0.49
1:A:2121:PHE:CE2	1:A:3701:LEU:HB2	2.46	0.49
1:A:2038:LEU:HD22	1:A:3661:TRP:CH2	2.48	0.49
1:A:4134:GLU:HB3	1:A:4135:PRO:HD3	1.93	0.49
1:C:1973:GLN:OE1	1:C:3642:TYR:N	2.45	0.49
1:D:500:ALA:HA	1:D:503:PHE:HB2	1.93	0.49
1:D:2248:ARG:NH2	1:D:2285:GLU:OE2	2.44	0.49
1:C:759:ILE:HB	1:C:762:CYS:HB3	1.95	0.49
1:D:2128:TYR:CB	1:D:3673:MET:HE3	2.31	0.49
1:A:129:ASP:OD1	1:A:129:ASP:N	2.46	0.49
1:A:644:ILE:HG21	1:A:1615:VAL:HG11	1.94	0.49
1:A:2442:LEU:HD12	1:A:2443:ILE:HD13	1.95	0.49
1:A:3986:TRP:HA	1:A:3989:VAL:HG22	1.94	0.49
1:B:672:VAL:HG21	1:B:675:LEU:HG	1.94	0.49
1:C:2288:LEU:O	1:C:2288:LEU:HG	2.11	0.49
1:D:850:ASP:OD1	1:D:850:ASP:N	2.41	0.49
1:D:2128:TYR:CD2	1:D:3673:MET:HE2	2.32	0.49
1:A:1973:GLN:OE1	1:A:3642:TYR:N	2.45	0.49
1:B:644:ILE:HG21	1:B:1615:VAL:HG11	1.94	0.49
1:D:3986:TRP:HA	1:D:3989:VAL:HG22	1.94	0.49
1:D:4132:PHE:O	1:D:4135:PRO:HD2	2.12	0.49
1:D:4097:MET:HA	1:D:4108:ILE:HD13	1.95	0.49
1:A:1690:ASP:OD1	1:A:1691:GLN:N	2.46	0.49
1:B:2442:LEU:HD12	1:B:2443:ILE:HD13	1.95	0.49
1:B:4860:ARG:NH2	1:C:4629:TYR:OH	2.45	0.49
1:D:1690:ASP:OD1	1:D:1691:GLN:N	2.46	0.49
1:A:1292:SER:O	1:A:1579:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1458:HIS:NE2	1:A:1483:VAL:HG21	2.28	0.49
1:B:1973:GLN:OE1	1:B:3642:TYR:N	2.46	0.49
1:B:3642:TYR:O	1:B:3643:ASN:HB2	2.13	0.49
1:C:3986:TRP:HA	1:C:3989:VAL:HG22	1.94	0.49
1:C:4132:PHE:HA	1:C:4135:PRO:HD2	1.95	0.49
1:D:4068:LEU:HD13	1:D:4107:GLU:HG3	1.93	0.49
1:A:1810:LYS:HG3	1:A:1813:ARG:NH2	2.28	0.49
1:C:1460:HIS:HB3	1:C:1494:UNK:HA	1.95	0.49
1:C:2023:LEU:O	1:C:2028:ARG:NH1	2.46	0.49
1:C:4108:ILE:HD12	1:C:4111:LEU:HD23	1.94	0.49
1:D:1973:GLN:OE1	1:D:3642:TYR:N	2.45	0.49
1:B:129:ASP:N	1:B:129:ASP:OD1	2.46	0.48
1:B:1654:SER:HB3	1:B:1704:PRO:HG3	1.95	0.48
1:C:484:LEU:HD21	1:C:540:PHE:HE1	1.78	0.48
1:C:4211:LYS:NZ	2:C:5101:ACP:O1B	2.28	0.48
1:B:951:LYS:HB2	1:B:971:ASP:HB3	1.96	0.48
1:B:1690:ASP:OD1	1:B:1691:GLN:N	2.46	0.48
1:C:2007:ASN:O	1:C:2011:HIS:N	2.44	0.48
1:D:1089:TYR:HA	1:D:1151:CYS:O	2.12	0.48
1:A:1654:SER:HB3	1:A:1704:PRO:HG3	1.95	0.48
1:C:1690:ASP:OD1	1:C:1691:GLN:N	2.46	0.48
1:C:3844:LEU:HD11	1:C:3932:ASP:HB3	1.96	0.48
1:D:484:LEU:HD21	1:D:540:PHE:HE1	1.78	0.48
1:D:2007:ASN:O	1:D:2011:HIS:N	2.44	0.48
1:A:484:LEU:HD21	1:A:540:PHE:HE1	1.78	0.48
1:A:951:LYS:HB2	1:A:971:ASP:HB3	1.96	0.48
1:A:4068:LEU:HD21	1:A:4111:LEU:HD22	1.95	0.48
1:B:3648:ARG:HH21	1:B:3652:MET:HE1	1.78	0.48
1:C:487:VAL:O	1:C:491:ILE:HG13	2.14	0.48
1:C:2442:LEU:HD12	1:C:2443:ILE:HD13	1.95	0.48
1:C:3962:PHE:O	1:C:3966:THR:HG23	2.14	0.48
1:D:2442:LEU:HD12	1:D:2443:ILE:HD13	1.95	0.48
1:D:3844:LEU:HD11	1:D:3932:ASP:HB3	1.96	0.48
1:A:3844:LEU:HD11	1:A:3932:ASP:HB3	1.95	0.48
1:B:3844:LEU:HD11	1:B:3932:ASP:HB3	1.96	0.48
1:C:1654:SER:HB3	1:C:1704:PRO:HG3	1.96	0.48
1:D:1765:VAL:HG12	1:D:1767:VAL:H	1.79	0.48
1:A:1765:VAL:HG12	1:A:1767:VAL:H	1.79	0.48
1:B:2098:VAL:HG11	1:B:2127:GLN:HE21	1.79	0.48
1:D:1654:SER:HB3	1:D:1704:PRO:HG3	1.95	0.48
1:A:487:VAL:O	1:A:491:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2098:VAL:HG11	1:A:2127:GLN:HE21	1.79	0.48
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.14	0.48
1:B:1765:VAL:HG12	1:B:1767:VAL:H	1.79	0.48
1:B:2123:LEU:O	1:B:2127:GLN:HG2	2.14	0.48
1:D:3962:PHE:O	1:D:3966:THR:HG23	2.14	0.48
1:B:487:VAL:O	1:B:491:ILE:HG13	2.14	0.48
1:B:1460:HIS:HB3	1:B:1494:UNK:HA	1.95	0.48
1:B:4181:ILE:HD12	1:B:4991:PHE:HB2	1.95	0.48
1:C:129:ASP:OD1	1:C:129:ASP:N	2.46	0.48
1:D:759:ILE:HB	1:D:762:CYS:HB3	1.95	0.48
1:A:759:ILE:HB	1:A:762:CYS:HB3	1.95	0.48
1:A:4181:ILE:HD12	1:A:4991:PHE:HB2	1.96	0.48
1:B:1289:LEU:HD23	1:B:1458:HIS:CD2	2.49	0.48
1:C:1109:LEU:HD22	1:C:1605:TRP:HZ2	1.79	0.48
1:C:4181:ILE:HD12	1:C:4991:PHE:HB2	1.96	0.48
1:D:951:LYS:HB2	1:D:971:ASP:HB3	1.96	0.48
1:D:3644:LEU:HG	1:D:3645:PRO:O	2.14	0.48
1:D:4132:PHE:C	1:D:4135:PRO:HD2	2.34	0.48
1:A:2123:LEU:O	1:A:2127:GLN:HG2	2.14	0.48
1:C:674:PHE:HE1	1:C:680:THR:H	1.61	0.48
1:A:674:PHE:HE1	1:A:680:THR:H	1.62	0.47
1:A:1460:HIS:HB3	1:A:1494:UNK:HA	1.95	0.47
1:C:2123:LEU:O	1:C:2127:GLN:HG2	2.14	0.47
1:A:3866:ILE:O	1:A:3870:ASN:HB3	2.13	0.47
1:A:3966:THR:HA	1:A:3969:ILE:HG12	1.96	0.47
1:A:4128:PHE:O	1:A:4128:PHE:CD1	2.67	0.47
1:C:3817:LEU:CD2	1:C:3898:ASP:HB2	2.44	0.47
1:D:3817:LEU:CD2	1:D:3898:ASP:HB2	2.44	0.47
1:B:484:LEU:HD21	1:B:540:PHE:HE1	1.78	0.47
1:C:951:LYS:HB2	1:C:971:ASP:HB3	1.96	0.47
1:C:4580:TYR:HE1	1:C:4629:TYR:HB3	1.79	0.47
1:A:3817:LEU:CD2	1:A:3898:ASP:HB2	2.44	0.47
1:B:2367:ALA:HA	1:B:2373:GLY:HA3	1.96	0.47
1:C:3966:THR:HA	1:C:3969:ILE:HG12	1.96	0.47
1:D:1460:HIS:HB3	1:D:1494:UNK:HA	1.95	0.47
1:A:500:ALA:HB1	1:A:504:ALA:HB2	1.96	0.47
1:A:1109:LEU:HD22	1:A:1605:TRP:HZ2	1.79	0.47
1:A:2247:GLN:NE2	1:A:2278:ALA:O	2.45	0.47
1:A:3843:ASP:HB3	1:A:3846:ALA:HB3	1.97	0.47
1:A:3878:ASP:OD1	1:A:3879:GLU:N	2.48	0.47
1:B:3962:PHE:O	1:B:3966:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1780:PRO:O	1:C:1782:PHE:HD2	1.98	0.47
1:D:487:VAL:O	1:D:491:ILE:HG13	2.14	0.47
1:A:1479:GLU:C	1:A:1481:GLY:H	2.17	0.47
1:A:4666:VAL:N	1:A:4667:PRO:HD2	2.30	0.47
1:B:1109:LEU:HD22	1:B:1605:TRP:HZ2	1.79	0.47
1:B:2106:ALA:HB3	1:B:3697:PRO:CG	2.40	0.47
1:B:3878:ASP:OD1	1:B:3879:GLU:N	2.48	0.47
1:D:2128:TYR:C	1:D:3669:PHE:CE1	2.88	0.47
1:D:4106:PRO:HB2	1:D:4109:GLN:HG2	1.95	0.47
1:A:4069:LYS:HG2	1:A:4130:ASN:ND2	2.24	0.47
1:B:674:PHE:HE1	1:B:680:THR:H	1.63	0.47
1:B:759:ILE:HB	1:B:762:CYS:HB3	1.95	0.47
1:B:4061:PHE:HZ	1:B:4131:ARG:HH21	1.61	0.47
1:C:1765:VAL:HG12	1:C:1767:VAL:H	1.79	0.47
1:C:2474:LEU:HG	1:C:2494:UNK:CB	2.44	0.47
1:C:2476:ILE:HG23	1:C:2476:ILE:O	2.15	0.47
1:C:4090:LYS:HA	1:C:4123:ILE:CG1	2.30	0.47
1:D:500:ALA:HB1	1:D:504:ALA:HB2	1.96	0.47
1:D:1480:GLN:HA	1:D:1573:MET:HA	1.96	0.47
1:D:2123:LEU:O	1:D:2127:GLN:HG2	2.14	0.47
1:A:3667:HIS:O	1:A:3669:PHE:N	2.48	0.47
1:B:500:ALA:HB1	1:B:504:ALA:HB2	1.96	0.47
1:B:1480:GLN:HA	1:B:1573:MET:HA	1.96	0.47
1:B:3843:ASP:HB3	1:B:3846:ALA:HB3	1.97	0.47
1:D:2106:ALA:HB1	1:D:3697:PRO:HB3	1.97	0.47
1:D:4088:ILE:HG23	1:D:4092:ASP:HB2	1.97	0.47
1:A:2285:GLU:O	1:A:2286:LEU:CB	2.62	0.47
1:B:348:VAL:HG13	1:B:349:GLN:H	1.79	0.47
1:B:3966:THR:HA	1:B:3969:ILE:HG12	1.96	0.47
1:B:4938:ASP:OD1	1:C:4944:ARG:NH1	2.38	0.47
1:C:1214:PHE:CD1	1:C:1218:GLY:HA3	2.50	0.47
1:C:2098:VAL:HG11	1:C:2127:GLN:HE21	1.79	0.47
1:A:2240:CYS:SG	1:A:2250:MET:HG3	2.55	0.47
1:A:2367:ALA:HA	1:A:2373:GLY:HA3	1.96	0.47
1:A:4901:ILE:CG2	1:A:4902:GLU:N	2.78	0.47
1:B:3817:LEU:CD2	1:B:3898:ASP:HB2	2.45	0.47
1:C:2257:LEU:O	1:C:2261:SER:OG	2.24	0.47
1:D:4112:LEU:CD2	1:D:4123:ILE:HD11	2.42	0.47
1:A:2474:LEU:HG	1:A:2494:UNK:CB	2.44	0.46
1:A:3870:ASN:CG	1:A:3872:GLU:H	2.19	0.46
1:B:659:TYR:HB3	1:B:660:GLY:H	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:ASP:OD1	1:D:129:ASP:N	2.46	0.46
1:D:1214:PHE:CD1	1:D:1218:GLY:HA3	2.50	0.46
1:D:2367:ALA:HA	1:D:2373:GLY:HA3	1.96	0.46
1:D:3966:THR:HA	1:D:3969:ILE:HG12	1.96	0.46
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.29	0.46
1:A:4836:GLN:O	1:A:4840:THR:OG1	2.28	0.46
1:C:348:VAL:HG13	1:C:349:GLN:H	1.79	0.46
1:C:1480:GLN:HA	1:C:1573:MET:HA	1.96	0.46
1:D:2098:VAL:HG11	1:D:2127:GLN:HE21	1.79	0.46
1:D:3843:ASP:HB3	1:D:3846:ALA:HB3	1.97	0.46
1:D:4123:ILE:HD12	1:D:4123:ILE:HA	1.58	0.46
1:C:3951:PHE:HB3	1:C:4012:LEU:HD11	1.97	0.46
1:D:3557:UNK:O	1:D:3561:UNK:N	2.49	0.46
1:D:4081:VAL:HG11	1:D:4088:ILE:HG13	1.97	0.46
1:A:3557:UNK:O	1:A:3561:UNK:N	2.49	0.46
1:B:1863:LEU:O	1:B:1871:PHE:HE2	1.98	0.46
1:B:3666:ASP:O	1:B:3667:HIS:HB3	2.16	0.46
1:C:2367:ALA:HA	1:C:2373:GLY:HA3	1.96	0.46
1:C:3015:UNK:O	1:C:3017:UNK:N	2.48	0.46
1:D:3015:UNK:O	1:D:3017:UNK:N	2.49	0.46
1:B:4939:ALA:O	1:B:4943:LEU:HG	2.16	0.46
1:C:2288:LEU:HD13	1:C:2346:VAL:HB	1.98	0.46
1:D:348:VAL:HG13	1:D:349:GLN:H	1.79	0.46
1:D:2106:ALA:HB3	1:D:3697:PRO:HG2	1.98	0.46
1:D:3951:PHE:HB3	1:D:4012:LEU:HD11	1.98	0.46
1:A:3527:UNK:O	1:D:1220:GLN:NE2	2.48	0.46
1:B:1275:ARG:HB2	1:B:1275:ARG:CZ	2.44	0.46
1:B:1979:LEU:HG	1:B:1980:LEU:H	1.80	0.46
1:B:4642:ALA:O	1:B:4644:TRP:N	2.49	0.46
1:A:348:VAL:HG13	1:A:349:GLN:H	1.80	0.46
1:C:4836:GLN:O	1:C:4840:THR:OG1	2.28	0.46
1:D:4123:ILE:HG23	1:D:4125:PHE:N	2.30	0.46
1:B:2121:PHE:CE2	1:B:3701:LEU:HB2	2.46	0.46
1:B:4642:ALA:O	1:B:4645:CYS:N	2.49	0.46
1:C:20:VAL:HG22	1:C:204:PRO:HB3	1.98	0.46
1:C:3658:LYS:HE2	1:C:3658:LYS:HB3	1.65	0.46
1:D:138:GLN:NE2	1:D:140:ASP:O	2.49	0.46
1:D:1109:LEU:HD22	1:D:1605:TRP:HZ2	1.79	0.46
1:D:2172:PRO:HA	1:D:2175:GLU:HG2	1.98	0.46
1:D:4181:ILE:HD12	1:D:4991:PHE:HB2	1.97	0.46
1:A:1214:PHE:CD1	1:A:1218:GLY:HA3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3644:LEU:HD23	1:A:3649:ALA:HB2	1.97	0.45
1:A:3699:HIS:O	1:A:3703:LEU:HG	2.16	0.45
1:B:20:VAL:HG22	1:B:204:PRO:HB3	1.98	0.45
1:B:1252:HIS:CD2	1:B:1253:PRO:HD2	2.51	0.45
1:B:2476:ILE:HG23	1:B:2476:ILE:O	2.16	0.45
1:B:3951:PHE:HB3	1:B:4012:LEU:HD11	1.98	0.45
1:C:138:GLN:NE2	1:C:140:ASP:O	2.49	0.45
1:C:3557:UNK:O	1:C:3561:UNK:N	2.49	0.45
1:C:3699:HIS:O	1:C:3703:LEU:HG	2.16	0.45
1:C:3843:ASP:HB3	1:C:3846:ALA:HB3	1.97	0.45
1:D:1186:ASP:OD1	1:D:1186:ASP:N	2.36	0.45
1:A:138:GLN:NE2	1:A:140:ASP:O	2.49	0.45
1:A:3015:UNK:O	1:A:3017:UNK:N	2.48	0.45
1:B:3557:UNK:O	1:B:3561:UNK:N	2.49	0.45
1:B:4070:ASP:OD1	1:B:4071:ILE:N	2.49	0.45
1:C:500:ALA:HB1	1:C:504:ALA:HB2	1.96	0.45
1:C:2172:PRO:HA	1:C:2175:GLU:HG2	1.98	0.45
1:D:394:GLN:CB	1:D:398:SER:HB3	2.45	0.45
1:A:2257:LEU:O	1:A:2261:SER:OG	2.24	0.45
1:A:3839:CYS:SG	1:A:3881:THR:OG1	2.69	0.45
1:B:138:GLN:NE2	1:B:140:ASP:O	2.49	0.45
1:B:3875:MET:C	1:B:3877:ASP:N	2.70	0.45
1:C:2121:PHE:CE2	1:C:3701:LEU:HB2	2.46	0.45
1:D:1473:THR:O	1:D:1483:VAL:HG13	2.16	0.45
1:D:2382:GLU:O	1:D:2386:ILE:HG12	2.17	0.45
1:D:3871:GLY:O	1:D:3872:GLU:HB3	2.17	0.45
1:A:1483:VAL:HG22	1:A:1575:LEU:CD2	2.43	0.45
1:B:3015:UNK:O	1:B:3017:UNK:N	2.49	0.45
1:B:3699:HIS:O	1:B:3703:LEU:HG	2.16	0.45
1:B:4750:ILE:HG22	1:B:4752:ALA:H	1.82	0.45
1:C:661:LYS:HA	1:C:661:LYS:HD3	1.80	0.45
1:C:4123:ILE:HG22	1:C:4125:PHE:N	2.31	0.45
1:D:4094:GLN:O	1:D:4094:GLN:NE2	2.49	0.45
1:A:3951:PHE:HB3	1:A:4012:LEU:HD11	1.97	0.45
1:B:1780:PRO:O	1:B:1782:PHE:HD2	2.00	0.45
1:C:2382:GLU:O	1:C:2386:ILE:HG12	2.17	0.45
1:C:3757:GLU:HG3	1:C:4719:PHE:HZ	1.81	0.45
1:A:20:VAL:HG22	1:A:204:PRO:HB3	1.98	0.45
1:A:395:GLN:HE21	1:A:395:GLN:HB2	1.50	0.45
1:B:1214:PHE:CD1	1:B:1218:GLY:HA3	2.50	0.45
1:B:4642:ALA:C	1:B:4644:TRP:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:HIS:CD2	1:C:1253:PRO:HD2	2.51	0.45
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.29	0.45
1:D:4088:ILE:HG23	1:D:4092:ASP:CB	2.46	0.45
1:A:663:TYR:CE1	1:A:745:SER:HB3	2.52	0.45
1:A:4102:GLN:OE1	1:A:4102:GLN:N	2.49	0.45
1:A:4750:ILE:HG22	1:A:4752:ALA:H	1.82	0.45
1:B:1810:LYS:HD3	1:B:1813:ARG:NH2	2.32	0.45
1:B:4836:GLN:O	1:B:4840:THR:OG1	2.28	0.45
1:C:2106:ALA:HB1	1:C:3697:PRO:HB3	1.98	0.45
1:D:2107:GLN:NE2	1:D:3680:ALA:O	2.50	0.45
1:A:526:LEU:O	1:A:530:ILE:HG22	2.17	0.45
1:A:2382:GLU:O	1:A:2386:ILE:HG12	2.17	0.45
1:A:4901:ILE:HB	1:A:4913:ARG:HH21	1.82	0.45
1:B:661:LYS:HA	1:B:661:LYS:HD3	1.80	0.45
1:B:4580:TYR:HE1	1:B:4629:TYR:HB3	1.81	0.45
1:B:4791:TYR:OH	1:B:4815:ASP:O	2.34	0.45
1:D:322:LYS:HD2	1:D:322:LYS:HA	1.79	0.45
1:A:1252:HIS:CD2	1:A:1253:PRO:HD2	2.51	0.45
1:A:4139:ILE:O	1:A:4139:ILE:CG2	2.65	0.45
1:B:259:LEU:HD12	1:B:284:HIS:CD2	2.52	0.45
1:C:3848:GLU:O	1:C:3852:LYS:HG2	2.17	0.45
1:D:4750:ILE:HG22	1:D:4752:ALA:H	1.82	0.45
1:B:1607:ARG:NH2	1:B:1610:ASN:OD1	2.50	0.45
1:B:3658:LYS:HB3	1:B:3658:LYS:HE2	1.65	0.45
1:C:322:LYS:HD2	1:C:322:LYS:HA	1.79	0.45
1:D:1044:ARG:HA	1:D:1044:ARG:HD3	1.78	0.45
1:D:1108:GLU:OE1	1:D:1108:GLU:N	2.39	0.45
1:D:3699:HIS:O	1:D:3703:LEU:HG	2.16	0.45
1:D:3852:LYS:HB3	1:D:3852:LYS:HE2	1.69	0.45
1:B:526:LEU:O	1:B:530:ILE:HG22	2.17	0.44
1:B:1280:GLN:H	1:B:1280:GLN:CD	2.21	0.44
1:B:1291:LEU:HD22	1:B:1595:LEU:HG	1.99	0.44
1:B:2172:PRO:HA	1:B:2175:GLU:HG2	1.98	0.44
1:B:2382:GLU:O	1:B:2386:ILE:HG12	2.17	0.44
1:C:299:LEU:O	1:C:375:LYS:NZ	2.51	0.44
1:C:659:TYR:HB3	1:C:660:GLY:H	1.57	0.44
1:D:20:VAL:HG22	1:D:204:PRO:HB3	1.98	0.44
1:D:661:LYS:HA	1:D:661:LYS:HD3	1.80	0.44
1:A:1439:VAL:HA	1:A:1443:GLN:HG2	1.99	0.44
1:A:2106:ALA:HB1	1:A:3697:PRO:HB3	1.97	0.44
1:B:979:PRO:O	1:B:1036:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:LEU:O	1:C:530:ILE:HG22	2.17	0.44
1:D:4985:LEU:O	1:D:4988:TYR:N	2.50	0.44
1:A:2107:GLN:HB2	1:A:3683:GLN:OE1	2.16	0.44
1:A:2284:ASN:O	1:A:2287:ALA:O	2.35	0.44
1:B:603:LEU:HD23	1:B:606:LEU:HD12	2.00	0.44
1:B:1041:GLN:HA	1:B:1044:ARG:HG3	2.00	0.44
1:C:1607:ARG:NH2	1:C:1610:ASN:OD1	2.50	0.44
1:C:2045:GLN:HB2	1:C:2047:GLU:HG2	2.00	0.44
1:C:4059:LEU:HD13	1:C:4167:ALA:HB2	1.99	0.44
1:C:4938:ASP:OD1	1:D:4944:ARG:NH1	2.38	0.44
1:D:526:LEU:O	1:D:530:ILE:HG22	2.17	0.44
1:D:1252:HIS:CD2	1:D:1253:PRO:HD2	2.51	0.44
1:D:4059:LEU:HD13	1:D:4167:ALA:HB2	1.99	0.44
1:A:1969:LEU:HD12	1:A:2009:LEU:HD21	2.00	0.44
1:A:2172:PRO:HA	1:A:2175:GLU:HG2	1.98	0.44
1:B:4813:LEU:HD23	1:B:4813:LEU:HA	1.86	0.44
1:C:4750:ILE:HG22	1:C:4752:ALA:H	1.82	0.44
1:D:299:LEU:O	1:D:375:LYS:NZ	2.51	0.44
1:D:2109:ASP:N	1:D:2109:ASP:OD1	2.51	0.44
1:D:2474:LEU:O	1:D:2475:GLN:CB	2.64	0.44
1:D:4960:ILE:HB	1:D:4983:HIS:CD2	2.53	0.44
1:A:1155:LEU:HD12	1:A:1184:ILE:HG13	2.00	0.44
1:A:1712:TYR:CD2	1:A:1840:PRO:HB2	2.53	0.44
1:B:3757:GLU:HG3	1:B:4719:PHE:HZ	1.81	0.44
1:B:4960:ILE:HB	1:B:4983:HIS:CD2	2.53	0.44
1:A:182:LEU:HD11	1:A:189:LEU:HD12	1.99	0.44
1:A:1186:ASP:OD1	1:A:1186:ASP:N	2.36	0.44
1:A:2002:PRO:HA	1:A:2005:GLN:HB2	2.00	0.44
1:A:3757:GLU:HG3	1:A:4719:PHE:HZ	1.82	0.44
1:B:299:LEU:O	1:B:375:LYS:NZ	2.51	0.44
1:B:4088:ILE:N	1:B:4088:ILE:HD13	2.33	0.44
1:D:3757:GLU:HG3	1:D:4719:PHE:HZ	1.82	0.44
1:A:2158:CYS:O	1:A:2162:ILE:HG13	2.18	0.44
1:A:4127:GLU:O	1:A:4128:PHE:C	2.55	0.44
1:A:4960:ILE:HB	1:A:4983:HIS:CD2	2.52	0.44
1:B:1546:UNK:O	1:B:1548:UNK:N	2.51	0.44
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.51	0.44
1:C:1546:UNK:O	1:C:1548:UNK:N	2.51	0.44
1:C:2093:SER:OG	1:C:2094:LEU:N	2.51	0.44
1:D:1969:LEU:HD12	1:D:2009:LEU:HD21	2.00	0.44
1:D:4580:TYR:HE1	1:D:4629:TYR:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:HB2	1:A:193:ALA:HB3	2.00	0.44
1:A:2121:PHE:CE2	1:A:3701:LEU:HD13	2.53	0.44
1:A:4580:TYR:HE1	1:A:4629:TYR:HB3	1.81	0.44
1:B:196:MET:SD	1:B:196:MET:N	2.91	0.44
1:B:1969:LEU:HD12	1:B:2009:LEU:HD21	2.00	0.44
1:C:694:PRO:HG3	1:C:827:LYS:HB3	2.00	0.44
1:C:1695:LEU:HD23	1:C:1695:LEU:HA	1.90	0.44
1:D:694:PRO:HG3	1:D:827:LYS:HB3	2.00	0.44
1:A:299:LEU:O	1:A:375:LYS:NZ	2.51	0.44
1:A:1778:SER:HB3	1:A:1798:LEU:HB2	2.00	0.44
1:A:1849:LEU:HD23	1:A:1849:LEU:HA	1.87	0.44
1:A:2116:LEU:O	1:A:2120:MET:HG2	2.18	0.44
1:B:4901:ILE:HB	1:B:4913:ARG:HH21	1.83	0.44
1:C:1155:LEU:HD12	1:C:1184:ILE:HG13	2.00	0.44
1:D:133:PHE:HB2	1:D:193:ALA:HB3	2.00	0.44
1:D:2158:CYS:O	1:D:2162:ILE:HG13	2.18	0.44
1:A:1028:ASP:O	1:A:1032:LYS:HG3	2.18	0.43
1:A:2093:SER:OG	1:A:2094:LEU:N	2.51	0.43
1:A:2109:ASP:N	1:A:2109:ASP:OD1	2.51	0.43
1:A:2476:ILE:O	1:A:2476:ILE:CG1	2.66	0.43
1:D:418:LEU:HD13	1:D:421:PHE:CE1	2.51	0.43
1:D:1778:SER:HB3	1:D:1798:LEU:HB2	2.00	0.43
1:A:694:PRO:HG3	1:A:827:LYS:HB3	2.00	0.43
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	2.00	0.43
1:A:4059:LEU:HD13	1:A:4167:ALA:HB2	1.99	0.43
1:B:1712:TYR:CD2	1:B:1840:PRO:HB2	2.53	0.43
1:B:1871:PHE:HD1	1:B:1871:PHE:HA	1.51	0.43
1:B:2158:CYS:O	1:B:2162:ILE:HG13	2.18	0.43
1:B:2258:LEU:HD23	1:B:2258:LEU:HA	1.88	0.43
1:C:1712:TYR:CD2	1:C:1840:PRO:HB2	2.53	0.43
1:C:2294:ASP:O	1:C:2298:VAL:HG23	2.19	0.43
1:D:2093:SER:OG	1:D:2094:LEU:N	2.51	0.43
1:A:603:LEU:HD23	1:A:606:LEU:HD12	2.00	0.43
1:A:1546:UNK:O	1:A:1548:UNK:N	2.51	0.43
1:A:2476:ILE:CD1	1:A:2478:THR:HB	2.47	0.43
1:A:4985:LEU:O	1:A:4988:TYR:N	2.51	0.43
1:B:322:LYS:HA	1:B:322:LYS:HD2	1.79	0.43
1:B:694:PRO:HG3	1:B:827:LYS:HB3	2.00	0.43
1:B:1293:LEU:HD23	1:B:1579:MET:HB3	2.00	0.43
1:B:2093:SER:OG	1:B:2094:LEU:N	2.51	0.43
1:B:2116:LEU:O	1:B:2120:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.29	0.43
1:C:196:MET:SD	1:C:196:MET:N	2.91	0.43
1:C:603:LEU:HD23	1:C:606:LEU:HD12	2.00	0.43
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.51	0.43
1:C:2121:PHE:CE2	1:C:3701:LEU:HD13	2.53	0.43
1:C:3949:ARG:O	1:C:3953:LYS:HG3	2.19	0.43
1:C:4112:LEU:HD22	1:C:4123:ILE:CD1	2.40	0.43
1:D:196:MET:SD	1:D:196:MET:N	2.91	0.43
1:D:336:PRO:HA	1:D:337:PRO:HD3	1.89	0.43
1:D:2002:PRO:HA	1:D:2005:GLN:HB2	2.00	0.43
1:D:3873:LYS:HE3	1:D:3873:LYS:HB3	1.61	0.43
1:A:196:MET:SD	1:A:196:MET:N	2.91	0.43
1:A:2258:LEU:HD23	1:A:2258:LEU:HA	1.88	0.43
1:A:3866:ILE:HA	1:A:3869:GLN:OE1	2.18	0.43
1:A:3949:ARG:O	1:A:3953:LYS:HG3	2.19	0.43
1:A:4629:TYR:OH	1:D:4860:ARG:NH2	2.52	0.43
1:B:336:PRO:HA	1:B:337:PRO:HD3	1.88	0.43
1:B:1254:HIS:HB3	1:B:1276:THR:CG2	2.48	0.43
1:B:2002:PRO:HA	1:B:2005:GLN:HB2	2.00	0.43
1:B:2330:ARG:H	1:B:2330:ARG:HG2	1.59	0.43
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	2.00	0.43
1:B:4573:ILE:HG23	1:B:4643:LEU:HD11	2.00	0.43
1:C:2158:CYS:O	1:C:2162:ILE:HG13	2.18	0.43
1:C:2284:ASN:HB2	1:C:3856:LEU:HD21	2.00	0.43
1:D:1291:LEU:HD21	1:D:1580:PHE:CZ	2.53	0.43
1:D:4088:ILE:HG21	1:D:4125:PHE:HE1	1.82	0.43
1:D:4813:LEU:HD23	1:D:4813:LEU:HA	1.87	0.43
1:A:1607:ARG:NH2	1:A:1610:ASN:OD1	2.50	0.43
1:A:3873:LYS:H	1:A:3873:LYS:HZ1	1.66	0.43
1:B:274:LEU:HD23	1:B:339:ILE:HD12	2.01	0.43
1:B:418:LEU:HD13	1:B:421:PHE:CE1	2.51	0.43
1:B:544:LEU:HD23	1:B:577:ILE:HG13	2.01	0.43
1:B:4059:LEU:HD13	1:B:4167:ALA:HB2	1.99	0.43
1:C:274:LEU:HD23	1:C:339:ILE:HD12	2.01	0.43
1:C:1969:LEU:HD12	1:C:2009:LEU:HD21	2.00	0.43
1:C:4123:ILE:HD13	1:C:4123:ILE:HA	1.81	0.43
1:D:1293:LEU:HD23	1:D:1579:MET:HB3	2.00	0.43
1:D:1546:UNK:O	1:D:1548:UNK:N	2.51	0.43
1:D:4897:ILE:O	1:D:4901:ILE:HG13	2.19	0.43
1:A:771:PHE:HD1	1:A:771:PHE:H	1.66	0.43
1:A:4897:ILE:HG13	1:A:4901:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2294:ASP:O	1:B:2298:VAL:HG23	2.19	0.43
1:C:771:PHE:HD1	1:C:771:PHE:H	1.66	0.43
1:C:2128:TYR:HD2	1:C:3673:MET:HE3	1.68	0.43
1:D:1155:LEU:HD12	1:D:1184:ILE:HG13	2.00	0.43
1:D:1712:TYR:CD2	1:D:1840:PRO:HB2	2.53	0.43
1:A:125:ARG:H	1:A:125:ARG:HG3	1.65	0.43
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.92	0.43
1:A:637:LEU:HD23	1:A:637:LEU:HA	1.91	0.43
1:B:188:GLU:HG2	1:B:189:LEU:H	1.84	0.43
1:B:4855:ALA:HA	1:B:4859:PHE:HD2	1.84	0.43
1:C:2002:PRO:HA	1:C:2005:GLN:HB2	2.00	0.43
1:C:4860:ARG:NH2	1:D:4629:TYR:OH	2.52	0.43
1:C:4897:ILE:O	1:C:4901:ILE:HG13	2.19	0.43
1:D:603:LEU:HD23	1:D:606:LEU:HD12	2.00	0.43
1:A:1727:ARG:HA	1:A:1727:ARG:HD3	1.86	0.43
1:A:4573:ILE:HG23	1:A:4643:LEU:HD11	2.00	0.43
1:B:182:LEU:HD11	1:B:189:LEU:HD12	1.99	0.43
1:B:1291:LEU:HD21	1:B:1580:PHE:CZ	2.54	0.43
1:B:4070:ASP:O	1:B:4073:GLY:N	2.52	0.43
1:C:4075:GLU:H	1:C:4075:GLU:HG3	1.63	0.43
1:D:2294:ASP:O	1:D:2298:VAL:HG23	2.19	0.43
1:D:3949:ARG:O	1:D:3953:LYS:HG3	2.19	0.43
1:D:4901:ILE:HB	1:D:4913:ARG:HH21	1.83	0.43
1:A:3658:LYS:HA	1:A:3661:TRP:CD1	2.54	0.43
1:B:3589:UNK:O	1:B:3591:UNK:N	2.52	0.43
1:B:3839:CYS:SG	1:B:3881:THR:OG1	2.69	0.43
1:D:188:GLU:HG2	1:D:189:LEU:H	1.84	0.43
1:D:763:PRO:O	1:D:765:GLN:NE2	2.52	0.43
1:D:2116:LEU:O	1:D:2120:MET:HG2	2.18	0.43
1:D:3589:UNK:O	1:D:3591:UNK:N	2.52	0.43
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	2.00	0.43
1:A:188:GLU:HG2	1:A:189:LEU:H	1.84	0.43
1:A:544:LEU:HD23	1:A:577:ILE:HG13	2.01	0.43
1:A:2107:GLN:NE2	1:A:3680:ALA:O	2.52	0.43
1:A:2294:ASP:O	1:A:2298:VAL:HG23	2.18	0.43
1:A:4983:HIS:O	1:A:4984:ASN:CB	2.67	0.43
1:B:771:PHE:HD1	1:B:771:PHE:H	1.66	0.43
1:B:1155:LEU:HD12	1:B:1184:ILE:HG13	2.00	0.43
1:B:1220:GLN:NE2	1:C:3527:UNK:O	2.51	0.43
1:B:2377:LEU:HD11	1:B:2468:GLY:HA3	2.01	0.43
1:C:1293:LEU:HD23	1:C:1579:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1747:LEU:HD23	1:C:2037:ASP:OD2	2.18	0.43
1:C:2107:GLN:NE2	1:C:3680:ALA:O	2.52	0.43
1:C:4791:TYR:OH	1:C:4815:ASP:O	2.34	0.43
1:A:2106:ALA:HB3	1:A:3697:PRO:HG2	2.01	0.42
1:A:4085:ARG:O	1:A:4087:LEU:N	2.52	0.42
1:A:4792:LEU:HD23	1:A:4792:LEU:HA	1.88	0.42
1:B:317:ARG:HG3	1:B:349:GLN:HG2	2.01	0.42
1:B:1778:SER:HB3	1:B:1798:LEU:HB2	2.00	0.42
1:B:2038:LEU:HD23	1:B:2038:LEU:HA	1.74	0.42
1:B:3949:ARG:O	1:B:3953:LYS:HG3	2.19	0.42
1:B:4901:ILE:CG2	1:B:4902:GLU:N	2.82	0.42
1:C:317:ARG:HG3	1:C:349:GLN:HG2	2.01	0.42
1:C:787:VAL:H	1:C:1630:CYS:HB2	1.84	0.42
1:C:1778:SER:HB3	1:C:1798:LEU:HB2	2.00	0.42
1:D:771:PHE:HD1	1:D:771:PHE:H	1.66	0.42
1:A:2283:ASN:HB3	1:A:2285:GLU:O	2.20	0.42
1:A:2377:LEU:HD11	1:A:2468:GLY:HA3	2.01	0.42
1:B:133:PHE:HB2	1:B:193:ALA:HB3	2.00	0.42
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.91	0.42
1:B:2228:MET:HE2	1:B:2228:MET:HB3	1.84	0.42
1:B:2352:VAL:O	1:B:2356:LEU:HG	2.20	0.42
1:C:133:PHE:HB2	1:C:193:ALA:HB3	2.00	0.42
1:C:2116:LEU:O	1:C:2120:MET:HG2	2.18	0.42
1:C:4573:ILE:HG23	1:C:4643:LEU:HD11	2.00	0.42
1:C:4901:ILE:CG2	1:C:4902:GLU:N	2.82	0.42
1:D:1607:ARG:NH2	1:D:1610:ASN:OD1	2.50	0.42
1:D:4117:ALA:HB1	1:D:4120:ASN:HA	2.01	0.42
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.19	0.42
1:D:4855:ALA:HA	1:D:4859:PHE:HD2	1.83	0.42
1:A:274:LEU:HD23	1:A:339:ILE:HD12	2.01	0.42
1:A:672:VAL:HG11	1:A:786:GLY:HA3	2.01	0.42
1:B:4089:SER:HB2	1:B:4092:ASP:H	1.84	0.42
1:B:4897:ILE:O	1:B:4901:ILE:HG13	2.19	0.42
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.92	0.42
1:C:2352:VAL:O	1:C:2356:LEU:HG	2.20	0.42
1:C:2607:UNK:O	1:C:2609:UNK:N	2.53	0.42
1:C:3589:UNK:O	1:C:3591:UNK:N	2.52	0.42
1:C:4855:ALA:HA	1:C:4859:PHE:HD2	1.83	0.42
1:D:1212:ARG:H	1:D:1212:ARG:HG2	1.53	0.42
1:D:4901:ILE:CG2	1:D:4902:GLU:N	2.82	0.42
1:A:913:LEU:HD23	1:A:918:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1770:SER:OG	1:A:1771:LEU:N	2.53	0.42
1:A:2352:VAL:O	1:A:2356:LEU:HG	2.19	0.42
1:A:3589:UNK:O	1:A:3591:UNK:N	2.52	0.42
1:A:3667:HIS:C	1:A:3669:PHE:N	2.70	0.42
1:A:3713:LYS:HE3	1:A:3713:LYS:HB2	1.80	0.42
1:A:4666:VAL:N	1:A:4667:PRO:CD	2.82	0.42
1:A:4897:ILE:HG13	1:A:4901:ILE:HD11	2.00	0.42
1:C:4821:LYS:O	1:C:4825:THR:HG23	2.19	0.42
1:D:317:ARG:HG3	1:D:349:GLN:HG2	2.01	0.42
1:D:2352:VAL:O	1:D:2356:LEU:HG	2.20	0.42
1:D:4983:HIS:O	1:D:4984:ASN:CB	2.67	0.42
1:A:787:VAL:H	1:A:1630:CYS:HB2	1.84	0.42
1:A:4855:ALA:HA	1:A:4859:PHE:HD2	1.84	0.42
1:B:1870:VAL:O	1:B:1871:PHE:CG	2.72	0.42
1:B:2430:ILE:HD13	1:B:2430:ILE:HA	1.93	0.42
1:B:2607:UNK:O	1:B:2609:UNK:N	2.53	0.42
1:B:3713:LYS:HE3	1:B:3713:LYS:HB2	1.80	0.42
1:B:4958:CYS:O	2:B:5101:ACP:N1	2.53	0.42
1:C:350:HIS:CE1	1:C:352:ALA:HB3	2.55	0.42
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	2.00	0.42
1:C:4858:PHE:CZ	5:C:5107:LBN:C40	3.02	0.42
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.85	0.42
1:A:763:PRO:O	1:A:765:GLN:NE2	2.52	0.42
1:A:2607:UNK:O	1:A:2609:UNK:N	2.53	0.42
1:A:4958:CYS:O	2:A:5101:ACP:N1	2.52	0.42
1:B:2155:LEU:HB2	1:B:2188:ASN:ND2	2.35	0.42
1:C:2377:LEU:HD11	1:C:2468:GLY:HA3	2.01	0.42
1:D:544:LEU:HD23	1:D:577:ILE:HG13	2.01	0.42
1:D:4573:ILE:HG23	1:D:4643:LEU:HD11	2.00	0.42
1:A:1483:VAL:HG13	1:A:1575:LEU:HD23	2.02	0.42
1:A:1781:CYS:O	1:A:1782:PHE:CG	2.73	0.42
1:A:2155:LEU:HB2	1:A:2188:ASN:ND2	2.35	0.42
1:A:3658:LYS:HB3	1:A:3658:LYS:HE2	1.65	0.42
1:A:4813:LEU:HD23	1:A:4813:LEU:HA	1.86	0.42
1:B:672:VAL:HG11	1:B:786:GLY:HA3	2.02	0.42
1:B:913:LEU:HD23	1:B:918:ARG:HB2	2.02	0.42
1:B:1980:LEU:O	1:B:1981:MET:C	2.57	0.42
1:B:4862:PHE:HB3	1:B:4901:ILE:CG2	2.50	0.42
1:B:4983:HIS:O	1:B:4984:ASN:CB	2.67	0.42
1:C:544:LEU:HD23	1:C:577:ILE:HG13	2.01	0.42
1:C:4862:PHE:HB3	1:C:4901:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4901:ILE:HB	1:C:4913:ARG:HH21	1.84	0.42
1:D:274:LEU:HD23	1:D:339:ILE:HD12	2.01	0.42
1:D:350:HIS:CE1	1:D:352:ALA:HB3	2.55	0.42
1:D:646:PRO:HD2	1:D:779:PRO:O	2.20	0.42
1:D:2121:PHE:CE2	1:D:3701:LEU:HD13	2.54	0.42
1:D:2128:TYR:CA	1:D:3669:PHE:CE1	3.02	0.42
1:D:3713:LYS:HE3	1:D:3713:LYS:HB2	1.80	0.42
1:A:436:LEU:HA	1:A:437:PRO:HD3	1.86	0.42
1:A:4901:ILE:HG22	1:A:4902:GLU:H	1.84	0.42
1:B:394:GLN:O	1:B:397:GLU:HB2	2.19	0.42
1:B:483:MET:O	1:B:487:VAL:HG23	2.20	0.42
1:B:787:VAL:H	1:B:1630:CYS:HB2	1.84	0.42
1:B:1980:LEU:O	1:B:1982:ARG:N	2.53	0.42
1:B:2285:GLU:O	1:B:2286:LEU:HB2	2.20	0.42
1:C:3694:LYS:HD3	1:C:3695:PRO:O	2.20	0.42
1:D:1770:SER:OG	1:D:1771:LEU:N	2.53	0.42
1:D:2377:LEU:HD11	1:D:2468:GLY:HA3	2.01	0.42
1:D:2607:UNK:O	1:D:2609:UNK:N	2.53	0.42
1:A:3667:HIS:CG	1:A:3668:SER:N	2.87	0.42
1:A:4034:ASN:HD21	1:A:4041:ALA:HB2	1.85	0.42
1:B:49:LEU:HD13	1:B:189:LEU:HB3	2.02	0.42
1:B:350:HIS:CE1	1:B:352:ALA:HB3	2.55	0.42
1:B:1279:SER:OG	1:B:1280:GLN:N	2.52	0.42
1:B:2106:ALA:HB1	1:B:3697:PRO:HB3	2.01	0.42
1:B:2106:ALA:HB3	1:B:3697:PRO:HG2	2.02	0.42
1:B:3694:LYS:HG2	1:B:3695:PRO:HD2	2.02	0.42
1:C:646:PRO:HD2	1:C:779:PRO:O	2.20	0.42
1:C:1634:LEU:HD23	1:C:1634:LEU:HA	1.88	0.42
1:C:1810:LYS:HG2	1:C:1814:MET:SD	2.59	0.42
1:C:2224:ARG:HD2	1:C:2224:ARG:HA	1.85	0.42
1:C:3999:MET:O	1:C:4003:LEU:CB	2.68	0.42
1:C:4858:PHE:CE2	5:C:5107:LBN:C40	3.03	0.42
1:D:49:LEU:HD13	1:D:189:LEU:HB3	2.01	0.42
1:A:2128:TYR:C	1:A:3669:PHE:CE1	2.91	0.42
1:A:4821:LYS:O	1:A:4825:THR:HG23	2.19	0.42
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.92	0.42
1:B:1797:ARG:HE	1:B:1797:ARG:HB3	1.74	0.42
1:B:1930:LYS:HE3	1:B:1930:LYS:HB2	1.97	0.42
1:B:4110:PHE:CD1	1:B:4110:PHE:N	2.87	0.42
1:B:4821:LYS:O	1:B:4825:THR:HG23	2.19	0.42
1:C:336:PRO:HA	1:C:337:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2155:LEU:HB2	1:C:2188:ASN:ND2	2.35	0.42
1:C:2430:ILE:HD13	1:C:2430:ILE:HA	1.93	0.42
1:D:2273:LEU:HD23	1:D:2273:LEU:HA	1.86	0.42
1:A:350:HIS:CE1	1:A:352:ALA:HB3	2.55	0.41
1:A:2276:ALA:O	1:A:2279:SER:OG	2.34	0.41
1:A:2295:LEU:O	1:A:2299:VAL:HG12	2.20	0.41
1:A:3694:LYS:HG2	1:A:3695:PRO:HD2	2.02	0.41
1:A:3999:MET:O	1:A:4003:LEU:CB	2.68	0.41
1:A:4124:ASN:HB3	1:A:4128:PHE:CE2	2.55	0.41
1:B:763:PRO:O	1:B:765:GLN:NE2	2.52	0.41
1:B:1595:LEU:HD23	1:B:1595:LEU:HA	1.93	0.41
1:B:1770:SER:OG	1:B:1771:LEU:N	2.53	0.41
1:B:3944:GLU:HG3	1:B:3947:GLY:H	1.85	0.41
1:B:3999:MET:O	1:B:4003:LEU:CB	2.68	0.41
1:C:4034:ASN:HD21	1:C:4041:ALA:HB2	1.85	0.41
1:C:4170:ILE:HD13	1:C:4170:ILE:HA	1.92	0.41
1:D:266:ARG:H	1:D:266:ARG:HG2	1.71	0.41
1:D:587:ILE:HD12	1:D:624:ASN:HB3	2.02	0.41
1:D:1810:LYS:HG2	1:D:1814:MET:SD	2.59	0.41
1:D:1863:LEU:HA	1:D:1866:ILE:HD12	2.02	0.41
1:D:2155:LEU:HB2	1:D:2188:ASN:ND2	2.35	0.41
1:D:2330:ARG:H	1:D:2330:ARG:HG2	1.60	0.41
1:A:438:ILE:HD13	1:A:438:ILE:HA	1.95	0.41
1:A:1863:LEU:HA	1:A:1866:ILE:HD12	2.02	0.41
1:B:1212:ARG:H	1:B:1212:ARG:HG2	1.53	0.41
1:B:1769:THR:OG1	1:B:1769:THR:O	2.37	0.41
1:B:1979:LEU:HG	1:B:1980:LEU:N	2.35	0.41
1:C:188:GLU:HG2	1:C:189:LEU:H	1.84	0.41
1:C:299:LEU:HD23	1:C:299:LEU:HA	1.91	0.41
1:C:587:ILE:HD12	1:C:624:ASN:HB3	2.03	0.41
1:C:613:ALA:HB2	1:C:1676:LEU:HD12	2.03	0.41
1:C:2295:LEU:O	1:C:2299:VAL:HG12	2.20	0.41
1:C:4238:CYS:O	1:C:4242:ILE:HG12	2.20	0.41
1:D:1942:LEU:HD23	1:D:1942:LEU:HA	1.91	0.41
1:D:4034:ASN:HD21	1:D:4041:ALA:HB2	1.85	0.41
1:A:620:LEU:O	1:A:624:ASN:ND2	2.53	0.41
1:A:1769:THR:OG1	1:A:1769:THR:O	2.37	0.41
1:A:4901:ILE:CG2	1:A:4902:GLU:H	2.33	0.41
1:B:587:ILE:HD12	1:B:624:ASN:HB3	2.02	0.41
1:B:840:VAL:HG12	1:B:1199:VAL:HG22	2.02	0.41
1:B:4034:ASN:HD21	1:B:4041:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:MET:O	1:C:487:VAL:HG23	2.20	0.41
1:C:763:PRO:O	1:C:765:GLN:NE2	2.52	0.41
1:C:840:VAL:HG12	1:C:1199:VAL:HG22	2.02	0.41
1:D:787:VAL:H	1:D:1630:CYS:HB2	1.84	0.41
1:D:2276:ALA:O	1:D:2279:SER:OG	2.34	0.41
1:D:4807:PHE:HB2	5:D:5106:LBN:C29	2.51	0.41
1:D:4836:GLN:O	1:D:4840:THR:OG1	2.28	0.41
1:A:674:PHE:HD1	1:A:674:PHE:HA	1.77	0.41
1:A:1668:ARG:HE	1:A:1668:ARG:HB3	1.72	0.41
1:A:2277:ALA:O	1:A:2281:ILE:HG12	2.21	0.41
1:B:1289:LEU:HD23	1:B:1458:HIS:HD2	1.85	0.41
1:C:266:ARG:H	1:C:266:ARG:HG2	1.71	0.41
1:D:269:TRP:O	1:D:272:SER:OG	2.32	0.41
1:D:613:ALA:HB2	1:D:1676:LEU:HD12	2.03	0.41
1:D:2224:ARG:HD2	1:D:2224:ARG:HA	1.85	0.41
1:D:2258:LEU:HD23	1:D:2258:LEU:HA	1.88	0.41
1:A:646:PRO:HD2	1:A:779:PRO:O	2.20	0.41
1:A:1595:LEU:HD23	1:A:1595:LEU:HA	1.93	0.41
1:A:2243:SER:OG	1:A:2244:ARG:N	2.54	0.41
1:A:4640:GLU:N	1:A:4641:PRO:CD	2.84	0.41
1:B:2391:ALA:O	1:B:2392:ARG:C	2.59	0.41
1:B:4238:CYS:O	1:B:4242:ILE:HG12	2.20	0.41
1:B:4642:ALA:C	1:B:4644:TRP:H	2.23	0.41
1:C:635:THR:HA	1:C:1638:ALA:O	2.21	0.41
1:C:1690:ASP:HB3	1:C:1693:GLN:HG3	2.02	0.41
1:C:1943:LEU:HD22	1:C:2098:VAL:HG22	2.03	0.41
1:D:635:THR:HA	1:D:1638:ALA:O	2.21	0.41
1:D:1291:LEU:HD22	1:D:1595:LEU:HG	2.02	0.41
1:D:1690:ASP:HB3	1:D:1693:GLN:HG3	2.02	0.41
1:D:2243:SER:OG	1:D:2244:ARG:N	2.54	0.41
1:D:3696:ASP:OD2	1:D:3773:ARG:NH2	2.52	0.41
1:A:587:ILE:HD12	1:A:624:ASN:HB3	2.02	0.41
1:A:840:VAL:HG12	1:A:1199:VAL:HG22	2.02	0.41
1:A:1087:ARG:HA	1:A:1153:ILE:O	2.21	0.41
1:A:4088:ILE:HD11	1:A:4125:PHE:CE2	2.55	0.41
1:B:1695:LEU:HD23	1:B:1695:LEU:HA	1.89	0.41
1:B:2952:UNK:O	1:B:2956:UNK:CB	2.69	0.41
1:B:4066:LEU:HD11	1:B:4170:ILE:HD13	2.03	0.41
1:C:181:HIS:HB3	1:C:194:SER:HB3	2.03	0.41
1:C:620:LEU:O	1:C:624:ASN:ND2	2.53	0.41
1:C:4090:LYS:CA	1:C:4123:ILE:HG12	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1802:ILE:O	1:D:1804:LEU:HD22	2.21	0.41
1:D:3999:MET:O	1:D:4003:LEU:CB	2.68	0.41
1:D:4862:PHE:HB3	1:D:4901:ILE:CG2	2.50	0.41
1:A:49:LEU:HD13	1:A:189:LEU:HB3	2.02	0.41
1:A:317:ARG:HG3	1:A:349:GLN:HG2	2.01	0.41
1:A:446:GLN:HG3	1:A:521:LEU:HD21	2.03	0.41
1:A:4109:GLN:HE21	1:A:4109:GLN:HA	1.85	0.41
1:A:4862:PHE:HB3	1:A:4901:ILE:CG2	2.51	0.41
1:B:181:HIS:HB3	1:B:194:SER:HB3	2.03	0.41
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.85	0.41
1:B:646:PRO:HD2	1:B:779:PRO:O	2.20	0.41
1:B:2023:LEU:O	1:B:2028:ARG:NH1	2.53	0.41
1:C:1770:SER:OG	1:C:1771:LEU:N	2.53	0.41
1:C:2277:ALA:O	1:C:2281:ILE:HG12	2.21	0.41
1:D:2277:ALA:O	1:D:2281:ILE:HG12	2.21	0.41
1:D:4013:LEU:O	1:D:4017:LEU:HG	2.21	0.41
1:D:4110:PHE:CD1	1:D:4110:PHE:N	2.88	0.41
1:D:4238:CYS:O	1:D:4242:ILE:HG12	2.20	0.41
1:A:181:HIS:HB3	1:A:194:SER:HB3	2.03	0.41
1:A:483:MET:O	1:A:487:VAL:HG23	2.20	0.41
1:A:978:THR:HA	1:A:979:PRO:HD3	1.96	0.41
1:B:486:LEU:HD12	1:B:486:LEU:HA	1.94	0.41
1:B:613:ALA:HB2	1:B:1676:LEU:HD12	2.03	0.41
1:B:1087:ARG:HA	1:B:1153:ILE:O	2.21	0.41
1:C:125:ARG:H	1:C:125:ARG:HG3	1.65	0.41
1:C:3944:GLU:HG3	1:C:3947:GLY:H	1.86	0.41
1:C:4640:GLU:N	1:C:4641:PRO:CD	2.84	0.41
1:C:4792:LEU:HD23	1:C:4792:LEU:HA	1.88	0.41
1:C:5036:LEU:HD12	1:C:5036:LEU:HA	1.92	0.41
1:D:483:MET:O	1:D:487:VAL:HG23	2.20	0.41
1:D:1595:LEU:HD23	1:D:1595:LEU:HA	1.93	0.41
1:D:3999:MET:O	1:D:4003:LEU:HB3	2.21	0.41
1:D:4791:TYR:OH	1:D:4815:ASP:O	2.34	0.41
1:A:613:ALA:HB2	1:A:1676:LEU:HD12	2.03	0.41
1:A:635:THR:HA	1:A:1638:ALA:O	2.21	0.41
1:A:1078:GLU:OE1	1:A:1080:SER:OG	2.35	0.41
1:A:1130:GLN:HG3	1:A:1136:SER:HB2	2.03	0.41
1:A:3944:GLU:HG3	1:A:3947:GLY:H	1.86	0.41
1:A:4238:CYS:O	1:A:4242:ILE:HG12	2.20	0.41
1:B:594:GLY:HA2	1:B:1594:ARG:HD2	2.03	0.41
1:B:683:ARG:HG3	1:B:717:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1286:MET:HA	1:B:1461:ASP:HA	2.03	0.41
1:B:1601:MET:HA	1:B:1602:PRO:HD3	1.89	0.41
1:B:1810:LYS:HD3	1:B:1813:ARG:HH21	1.85	0.41
1:B:1863:LEU:HA	1:B:1866:ILE:HD12	2.02	0.41
1:B:2277:ALA:O	1:B:2281:ILE:HG12	2.21	0.41
1:B:3668:SER:O	1:B:3669:PHE:CB	2.68	0.41
1:B:4013:LEU:O	1:B:4017:LEU:HG	2.21	0.41
1:B:4170:ILE:HD13	1:B:4170:ILE:HA	1.91	0.41
1:B:4638:TYR:C	1:B:4641:PRO:HD2	2.41	0.41
1:C:1797:ARG:HE	1:C:1797:ARG:HB3	1.74	0.41
1:C:1802:ILE:O	1:C:1804:LEU:HD22	2.21	0.41
1:C:2106:ALA:HB3	1:C:3697:PRO:HG2	2.02	0.41
1:C:2236:LEU:HD23	1:C:2236:LEU:HA	1.90	0.41
1:C:2297:LYS:HE3	1:C:2297:LYS:HB2	1.77	0.41
1:C:3713:LYS:HB2	1:C:3713:LYS:HE3	1.80	0.41
1:C:3999:MET:O	1:C:4003:LEU:HB3	2.21	0.41
1:C:4638:TYR:C	1:C:4641:PRO:HD2	2.42	0.41
1:D:2285:GLU:O	1:D:2286:LEU:HB2	2.20	0.41
1:D:4107:GLU:H	1:D:4107:GLU:HG2	1.44	0.41
1:A:1802:ILE:O	1:A:1804:LEU:HD22	2.21	0.41
1:A:2330:ARG:H	1:A:2330:ARG:HG2	1.60	0.41
1:A:4112:LEU:HD22	1:A:4123:ILE:HD11	2.03	0.41
1:B:1130:GLN:HG3	1:B:1136:SER:HB2	2.03	0.41
1:B:2295:LEU:O	1:B:2299:VAL:HG12	2.20	0.41
1:C:674:PHE:CE1	1:C:679:ALA:HA	2.56	0.41
1:C:1087:ARG:HA	1:C:1153:ILE:O	2.21	0.41
1:C:4999:ASP:O	1:C:5002:GLU:O	2.39	0.41
1:D:578:ILE:HD13	1:D:578:ILE:HA	1.89	0.41
1:D:913:LEU:HD23	1:D:918:ARG:HB2	2.02	0.41
1:D:1130:GLN:HG3	1:D:1136:SER:HB2	2.03	0.41
1:D:1769:THR:O	1:D:1769:THR:OG1	2.37	0.41
1:D:2295:LEU:O	1:D:2299:VAL:HG12	2.20	0.41
1:A:1483:VAL:CG2	1:A:1556:UNK:CB	2.99	0.40
1:A:3684:GLU:H	1:A:3684:GLU:HG3	1.43	0.40
1:A:3999:MET:O	1:A:4003:LEU:HB3	2.21	0.40
1:A:4182:GLU:HG2	1:A:4192:ARG:HG2	2.03	0.40
1:A:4897:ILE:HG13	1:A:4901:ILE:HG13	2.03	0.40
1:B:1802:ILE:O	1:B:1804:LEU:HD22	2.21	0.40
1:B:3873:LYS:HA	1:B:3873:LYS:HD2	1.48	0.40
1:C:2179:ILE:HD11	1:C:2228:MET:HB2	2.03	0.40
1:C:2243:SER:OG	1:C:2244:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:GLN:HG3	1:D:521:LEU:HD21	2.03	0.40
1:D:620:LEU:O	1:D:624:ASN:ND2	2.53	0.40
1:D:652:ARG:NH2	1:D:773:LEU:HG	2.36	0.40
1:D:683:ARG:HG3	1:D:717:ASP:HB3	2.03	0.40
1:D:1797:ARG:HE	1:D:1797:ARG:HB3	1.74	0.40
1:D:2236:LEU:HD23	1:D:2236:LEU:HA	1.90	0.40
1:D:2452:ARG:O	1:D:2456:ILE:HG13	2.22	0.40
1:D:4090:LYS:HA	1:D:4123:ILE:HD13	2.03	0.40
1:A:683:ARG:HG3	1:A:717:ASP:HB3	2.03	0.40
1:A:2952:UNK:O	1:A:2956:UNK:CB	2.69	0.40
1:B:1690:ASP:HB3	1:B:1693:GLN:HG3	2.02	0.40
1:B:2243:SER:OG	1:B:2244:ARG:N	2.54	0.40
1:B:3877:ASP:N	1:B:3877:ASP:OD1	2.50	0.40
1:B:3999:MET:O	1:B:4003:LEU:HB3	2.21	0.40
1:C:913:LEU:HD23	1:C:918:ARG:HB2	2.02	0.40
1:D:2952:UNK:O	1:D:2956:UNK:CB	2.69	0.40
1:A:966:LYS:H	1:A:966:LYS:HG3	1.60	0.40
1:A:1286:MET:HA	1:A:1461:ASP:HA	2.03	0.40
1:A:1671:ARG:HG2	1:A:1714:LEU:HD13	2.03	0.40
1:A:2224:ARG:HA	1:A:2224:ARG:HD2	1.85	0.40
1:B:620:LEU:O	1:B:624:ASN:ND2	2.53	0.40
1:B:674:PHE:HD1	1:B:674:PHE:HA	1.76	0.40
1:B:1585:LYS:HD3	1:B:1585:LYS:HA	1.59	0.40
1:B:3644:LEU:O	1:B:3645:PRO:O	2.39	0.40
1:B:4649:LEU:HD12	1:B:4649:LEU:HA	1.92	0.40
1:C:438:ILE:O	1:C:442:ILE:HG13	2.22	0.40
1:C:1078:GLU:OE1	1:C:1080:SER:OG	2.35	0.40
1:C:1699:GLU:H	1:C:1699:GLU:HG2	1.77	0.40
1:C:1863:LEU:HA	1:C:1866:ILE:HD12	2.02	0.40
1:C:2952:UNK:O	1:C:2956:UNK:CB	2.69	0.40
1:C:4666:VAL:O	1:C:4670:ILE:HG12	2.20	0.40
1:D:291:LEU:HA	1:D:291:LEU:HD23	1.85	0.40
1:D:685:GLY:HA3	1:D:714:TYR:O	2.21	0.40
1:D:1087:ARG:HA	1:D:1153:ILE:O	2.21	0.40
1:D:1781:CYS:O	1:D:1783:VAL:N	2.54	0.40
1:D:1849:LEU:HD23	1:D:1849:LEU:HA	1.87	0.40
1:D:2179:ILE:HD11	1:D:2228:MET:HB2	2.03	0.40
1:D:4640:GLU:N	1:D:4641:PRO:CD	2.84	0.40
1:D:4666:VAL:O	1:D:4670:ILE:HG12	2.20	0.40
1:A:1601:MET:HA	1:A:1602:PRO:HD3	1.89	0.40
1:A:2360:LYS:HB2	1:A:2363:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2391:ALA:O	1:A:2392:ARG:C	2.60	0.40
1:B:685:GLY:HA3	1:B:714:TYR:O	2.21	0.40
1:B:1465:ASP:OD2	1:B:1489:CYS:HB3	2.22	0.40
1:B:1727:ARG:HD3	1:B:1727:ARG:HA	1.86	0.40
1:B:2273:LEU:HD23	1:B:2273:LEU:HA	1.86	0.40
1:B:4131:ARG:O	1:B:4131:ARG:HG3	2.21	0.40
1:C:1982:ARG:O	1:C:1983:ALA:C	2.60	0.40
1:C:2391:ALA:O	1:C:2392:ARG:C	2.60	0.40
1:C:3869:GLN:O	1:C:3870:ASN:HB2	2.21	0.40
1:C:4181:ILE:HD11	1:C:4988:TYR:CA	2.42	0.40
1:C:4806:ASN:HD21	5:C:5106:LBN:C1	2.34	0.40
1:D:438:ILE:O	1:D:442:ILE:HG13	2.22	0.40
1:D:1078:GLU:OE1	1:D:1080:SER:OG	2.35	0.40
1:D:1981:MET:O	1:D:1982:ARG:C	2.60	0.40
1:A:1476:MET:HA	1:A:1574:PRO:CA	2.47	0.40
1:A:1982:ARG:O	1:A:1983:ALA:C	2.60	0.40
1:A:4122:MET:CB	1:A:4124:ASN:HB2	2.51	0.40
1:B:438:ILE:O	1:B:442:ILE:HG13	2.22	0.40
1:B:635:THR:HA	1:B:1638:ALA:O	2.21	0.40
1:B:1938:GLN:H	1:B:1938:GLN:HG2	1.76	0.40
1:B:3766:GLN:HG2	1:B:3769:ARG:HH21	1.87	0.40
1:B:4985:LEU:O	1:B:4988:TYR:N	2.53	0.40
1:C:594:GLY:HA2	1:C:1594:ARG:HD2	2.03	0.40
1:C:672:VAL:HG11	1:C:786:GLY:HA3	2.02	0.40
1:C:1698:LEU:HD23	1:C:1698:LEU:HA	1.94	0.40
1:C:1930:LYS:HE3	1:C:1930:LYS:HB2	1.97	0.40
1:C:1981:MET:O	1:C:1982:ARG:C	2.60	0.40
1:D:594:GLY:HA2	1:D:1594:ARG:HD2	2.03	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	3095/5037 (61%)	2890 (93%)	188 (6%)	17 (0%)	29	64
1	B	3095/5037 (61%)	2880 (93%)	188 (6%)	27 (1%)	17	52
1	C	3095/5037 (61%)	2898 (94%)	178 (6%)	19 (1%)	25	59
1	D	3095/5037 (61%)	2895 (94%)	182 (6%)	18 (1%)	25	59
All	All	12380/20148 (61%)	11563 (93%)	736 (6%)	81 (1%)	26	57

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	674	PHE
1	A	1440	PHE
1	A	1489	CYS
1	A	2476	ILE
1	A	3970	GLN
1	A	3971	GLY
1	B	395	GLN
1	B	674	PHE
1	B	1290	ARG
1	B	1440	PHE
1	B	1489	CYS
1	B	2287	ALA
1	B	3645	PRO
1	B	3876	ALA
1	B	3970	GLN
1	B	3971	GLY
1	C	674	PHE
1	C	1440	PHE
1	C	1489	CYS
1	C	2286	LEU
1	C	3970	GLN
1	C	3971	GLY
1	D	674	PHE
1	D	1290	ARG
1	D	1440	PHE
1	D	1489	CYS
1	D	2288	LEU
1	D	3872	GLU
1	D	3970	GLN
1	D	3971	GLY
1	D	4097	MET
1	A	2286	LEU
1	A	3871	GLY

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Mol	Chain	Res	Type
1	A	4130	ASN
1	A	4985	LEU
1	B	3669	PHE
1	B	3852	LYS
1	B	3875	MET
1	B	5004	THR
1	C	395	GLN
1	D	4985	LEU
1	A	3852	LYS
1	B	1981	MET
1	B	4074	SER
1	B	4102	GLN
1	B	4131	ARG
1	B	4643	LEU
1	B	4985	LEU
1	C	1981	MET
1	C	3669	PHE
1	C	3871	GLY
1	C	3872	GLU
1	C	4074	SER
1	C	4985	LEU
1	C	5004	THR
1	D	1981	MET
1	D	2286	LEU
1	D	5004	THR
1	A	1470	ARG
1	A	1978	ALA
1	B	1470	ARG
1	B	1481	GLY
1	B	1782	PHE
1	B	5003	HIS
1	C	1470	ARG
1	C	1481	GLY
1	C	2476	ILE
1	D	1470	ARG
1	D	1481	GLY
1	D	1782	PHE
1	D	2475	GLN
1	A	3872	GLU
1	B	2286	LEU
1	C	1983	ALA
1	A	1981	MET

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Mol	Chain	Res	Type
1	A	1983	ALA
1	A	2288	LEU
1	B	4067	LYS
1	B	1474	VAL
1	C	1474	VAL
1	D	1474	VAL

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	2435/3579 (68%)	2317 (95%)	118 (5%)	25	58
1	B	2444/3579 (68%)	2328 (95%)	116 (5%)	26	59
1	C	2412/3579 (67%)	2318 (96%)	94 (4%)	32	65
1	D	2418/3579 (68%)	2319 (96%)	99 (4%)	30	64
All	All	9709/14316 (68%)	9282 (96%)	427 (4%)	32	61

All (427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	29	LEU
1	A	61	ASP
1	A	66	CYS
1	A	81	MET
1	A	137	LEU
1	A	168	ASP
1	A	189	LEU
1	A	199	LEU
1	A	262	LEU
1	A	266	ARG
1	A	278	GLN
1	A	308	HIS
1	A	346	CYS
1	A	392	ARG

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Mol	Chain	Res	Type
1	A	395	GLN
1	A	397	GLU
1	A	510	GLU
1	A	545	ASP
1	A	552	ASP
1	A	554	LEU
1	A	585	SER
1	A	616	SER
1	A	629	ARG
1	A	659	TYR
1	A	669	ASP
1	A	672	VAL
1	A	674	PHE
1	A	705	ASN
1	A	735	GLN
1	A	757	PHE
1	A	771	PHE
1	A	772	ASN
1	A	778	PHE
1	A	791	PHE
1	A	811	CYS
1	A	813	GLU
1	A	843	SER
1	A	954	LYS
1	A	966	LYS
1	A	1147	ASP
1	A	1186	ASP
1	A	1217	CYS
1	A	1269	CYS
1	A	1283	LEU
1	A	1286	MET
1	A	1288	PHE
1	A	1289	LEU
1	A	1443	GLN
1	A	1444	GLU
1	A	1462	MET
1	A	1476	MET
1	A	1483	VAL
1	A	1579	MET
1	A	1580	PHE
1	A	1640	HIS
1	A	1700	ASP

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Mol	Chain	Res	Type
1	A	1728	ARG
1	A	1772	ARG
1	A	1778	SER
1	A	1812	LEU
1	A	1838	PHE
1	A	1979	LEU
1	A	2045	GLN
1	A	2189	LYS
1	A	2191	PHE
1	A	2199	ARG
1	A	2249	SER
1	A	2260	ASN
1	A	2284	ASN
1	A	2285	GLU
1	A	2286	LEU
1	A	2288	LEU
1	A	2330	ARG
1	A	2336	ARG
1	A	2364	PHE
1	A	2417	HIS
1	A	2440	MET
1	A	2464	ASP
1	A	2476	ILE
1	A	3661	TRP
1	A	3667	HIS
1	A	3682	GLU
1	A	3684	GLU
1	A	3694	LYS
1	A	3732	SER
1	A	3816	MET
1	A	3824	LYS
1	A	3852	LYS
1	A	3867	ASN
1	A	3869	GLN
1	A	3870	ASN
1	A	3872	GLU
1	A	3873	LYS
1	A	3875	MET
1	A	3898	ASP
1	A	3931	SER
1	A	3970	GLN
1	A	4016	LEU

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Mol	Chain	Res	Type
1	A	4018	ASP
1	A	4021	LYS
1	A	4069	LYS
1	A	4072	VAL
1	A	4104	THR
1	A	4108	ILE
1	A	4109	GLN
1	A	4110	PHE
1	A	4113	SER
1	A	4123	ILE
1	A	4127	GLU
1	A	4131	ARG
1	A	4180	ARG
1	A	4181	ILE
1	A	4640	GLU
1	A	4696	ASP
1	A	4966	ASP
1	A	5002	GLU
1	A	5035	GLN
1	B	17	ASP
1	B	29	LEU
1	B	61	ASP
1	B	66	CYS
1	B	81	MET
1	B	137	LEU
1	B	168	ASP
1	B	189	LEU
1	B	199	LEU
1	B	259	LEU
1	B	262	LEU
1	B	266	ARG
1	B	278	GLN
1	B	308	HIS
1	B	346	CYS
1	B	392	ARG
1	B	395	GLN
1	B	397	GLU
1	B	510	GLU
1	B	545	ASP
1	B	552	ASP
1	B	585	SER
1	B	616	SER

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Mol	Chain	Res	Type
1	B	629	ARG
1	B	659	TYR
1	B	663	TYR
1	B	669	ASP
1	B	672	VAL
1	B	674	PHE
1	B	705	ASN
1	B	735	GLN
1	B	757	PHE
1	B	771	PHE
1	B	772	ASN
1	B	791	PHE
1	B	811	CYS
1	B	843	SER
1	B	879	HIS
1	B	954	LYS
1	B	966	LYS
1	B	991	ASN
1	B	993	HIS
1	B	1032	LYS
1	B	1036	ARG
1	B	1037	ASP
1	B	1047	LEU
1	B	1147	ASP
1	B	1186	ASP
1	B	1217	CYS
1	B	1269	CYS
1	B	1275	ARG
1	B	1283	LEU
1	B	1286	MET
1	B	1288	PHE
1	B	1443	GLN
1	B	1458	HIS
1	B	1462	MET
1	B	1465	ASP
1	B	1579	MET
1	B	1580	PHE
1	B	1585	LYS
1	B	1640	HIS
1	B	1700	ASP
1	B	1728	ARG
1	B	1759	ARG

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Mol	Chain	Res	Type
1	B	1772	ARG
1	B	1778	SER
1	B	1810	LYS
1	B	1812	LEU
1	B	1838	PHE
1	B	2038	LEU
1	B	2045	GLN
1	B	2189	LYS
1	B	2191	PHE
1	B	2199	ARG
1	B	2260	ASN
1	B	2330	ARG
1	B	2336	ARG
1	B	2364	PHE
1	B	2417	HIS
1	B	2464	ASP
1	B	2474	LEU
1	B	2476	ILE
1	B	3667	HIS
1	B	3668	SER
1	B	3669	PHE
1	B	3694	LYS
1	B	3732	SER
1	B	3816	MET
1	B	3824	LYS
1	B	3856	LEU
1	B	3873	LYS
1	B	3874	VAL
1	B	3875	MET
1	B	3898	ASP
1	B	3931	SER
1	B	3970	GLN
1	B	4018	ASP
1	B	4075	GLU
1	B	4080	TYR
1	B	4092	ASP
1	B	4108	ILE
1	B	4110	PHE
1	B	4113	SER
1	B	4124	ASN
1	B	4127	GLU
1	B	4128	PHE

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Mol	Chain	Res	Type
1	B	4131	ARG
1	B	4180	ARG
1	B	4181	ILE
1	B	4665	LYS
1	B	4695	ASP
1	B	4697	VAL
1	B	4966	ASP
1	B	5002	GLU
1	B	5035	GLN
1	C	17	ASP
1	C	29	LEU
1	C	61	ASP
1	C	81	MET
1	C	137	LEU
1	C	168	ASP
1	C	199	LEU
1	C	262	LEU
1	C	266	ARG
1	C	308	HIS
1	C	346	CYS
1	C	392	ARG
1	C	395	GLN
1	C	397	GLU
1	C	545	ASP
1	C	552	ASP
1	C	585	SER
1	C	616	SER
1	C	629	ARG
1	C	652	ARG
1	C	659	TYR
1	C	663	TYR
1	C	669	ASP
1	C	672	VAL
1	C	674	PHE
1	C	705	ASN
1	C	757	PHE
1	C	771	PHE
1	C	772	ASN
1	C	778	PHE
1	C	791	PHE
1	C	811	CYS
1	C	813	GLU

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Mol	Chain	Res	Type
1	C	843	SER
1	C	954	LYS
1	C	966	LYS
1	C	1147	ASP
1	C	1186	ASP
1	C	1217	CYS
1	C	1269	CYS
1	C	1283	LEU
1	C	1286	MET
1	C	1288	PHE
1	C	1291	LEU
1	C	1443	GLN
1	C	1444	GLU
1	C	1462	MET
1	C	1579	MET
1	C	1580	PHE
1	C	1584	ARG
1	C	1640	HIS
1	C	1700	ASP
1	C	1728	ARG
1	C	1772	ARG
1	C	1778	SER
1	C	1812	LEU
1	C	1838	PHE
1	C	1980	LEU
1	C	2037	ASP
1	C	2045	GLN
1	C	2189	LYS
1	C	2191	PHE
1	C	2260	ASN
1	C	2330	ARG
1	C	2336	ARG
1	C	2364	PHE
1	C	2417	HIS
1	C	2440	MET
1	C	2464	ASP
1	C	2476	ILE
1	C	3661	TRP
1	C	3669	PHE
1	C	3694	LYS
1	C	3732	SER
1	C	3816	MET

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Mol	Chain	Res	Type
1	C	3824	LYS
1	C	3873	LYS
1	C	3874	VAL
1	C	3875	MET
1	C	3898	ASP
1	C	3931	SER
1	C	3970	GLN
1	C	4018	ASP
1	C	4069	LYS
1	C	4075	GLU
1	C	4087	LEU
1	C	4098	ASP
1	C	4180	ARG
1	C	4181	ILE
1	C	4696	ASP
1	C	4966	ASP
1	C	4983	HIS
1	C	5002	GLU
1	C	5035	GLN
1	D	17	ASP
1	D	28	VAL
1	D	29	LEU
1	D	61	ASP
1	D	66	CYS
1	D	81	MET
1	D	137	LEU
1	D	168	ASP
1	D	189	LEU
1	D	199	LEU
1	D	262	LEU
1	D	266	ARG
1	D	308	HIS
1	D	346	CYS
1	D	392	ARG
1	D	395	GLN
1	D	397	GLU
1	D	545	ASP
1	D	552	ASP
1	D	554	LEU
1	D	585	SER
1	D	616	SER
1	D	629	ARG

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Mol	Chain	Res	Type
1	D	652	ARG
1	D	669	ASP
1	D	672	VAL
1	D	674	PHE
1	D	705	ASN
1	D	757	PHE
1	D	771	PHE
1	D	772	ASN
1	D	791	PHE
1	D	811	CYS
1	D	843	SER
1	D	954	LYS
1	D	1044	ARG
1	D	1046	LEU
1	D	1112	ASP
1	D	1147	ASP
1	D	1186	ASP
1	D	1217	CYS
1	D	1269	CYS
1	D	1283	LEU
1	D	1286	MET
1	D	1288	PHE
1	D	1458	HIS
1	D	1462	MET
1	D	1579	MET
1	D	1580	PHE
1	D	1640	HIS
1	D	1700	ASP
1	D	1728	ARG
1	D	1772	ARG
1	D	1778	SER
1	D	1838	PHE
1	D	1979	LEU
1	D	2038	LEU
1	D	2189	LYS
1	D	2191	PHE
1	D	2199	ARG
1	D	2260	ASN
1	D	2330	ARG
1	D	2336	ARG
1	D	2364	PHE
1	D	2417	HIS

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Mol	Chain	Res	Type
1	D	2464	ASP
1	D	3644	LEU
1	D	3661	TRP
1	D	3668	SER
1	D	3694	LYS
1	D	3732	SER
1	D	3816	MET
1	D	3852	LYS
1	D	3856	LEU
1	D	3870	ASN
1	D	3872	GLU
1	D	3873	LYS
1	D	3874	VAL
1	D	3875	MET
1	D	3878	ASP
1	D	3898	ASP
1	D	3931	SER
1	D	3970	GLN
1	D	4018	ASP
1	D	4083	ASP
1	D	4110	PHE
1	D	4113	SER
1	D	4119	GLU
1	D	4123	ILE
1	D	4127	GLU
1	D	4128	PHE
1	D	4131	ARG
1	D	4180	ARG
1	D	4181	ILE
1	D	4696	ASP
1	D	4942	GLU
1	D	4966	ASP
1	D	5002	GLU
1	D	5035	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	395	GLN
1	A	735	GLN
1	A	1220	GLN

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Mol	Chain	Res	Type
1	A	3767	GLN
1	A	3850	GLN
1	A	3867	ASN
1	A	3870	ASN
1	A	3946	GLN
1	A	3994	HIS
1	A	4109	GLN
1	A	4130	ASN
1	A	4806	ASN
1	A	4832	HIS
1	B	395	GLN
1	B	735	GLN
1	B	991	ASN
1	B	1220	GLN
1	B	1458	HIS
1	B	3767	GLN
1	B	3850	GLN
1	B	3869	GLN
1	B	3870	ASN
1	B	3946	GLN
1	B	3994	HIS
1	B	4109	GLN
1	B	4124	ASN
1	B	4806	ASN
1	C	138	GLN
1	C	1220	GLN
1	C	1443	GLN
1	C	3767	GLN
1	C	3850	GLN
1	C	3946	GLN
1	C	3994	HIS
1	C	4034	ASN
1	C	4806	ASN
1	D	395	GLN
1	D	1220	GLN
1	D	3767	GLN
1	D	3850	GLN
1	D	3946	GLN
1	D	3994	HIS
1	D	4094	GLN
1	D	4109	GLN
1	D	4806	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 17 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	LBN	A	5108	-	45,45,51	0.32	0	50,53,59	0.31	0
5	LBN	C	5106	-	46,46,51	0.32	0	52,54,59	0.34	0
5	LBN	D	5106	-	46,46,51	0.32	0	52,54,59	0.34	0
5	LBN	A	5107	-	46,46,51	0.32	0	52,54,59	0.34	0
5	LBN	B	5106	-	45,45,51	0.32	0	50,53,59	0.31	0
5	LBN	D	5107	-	45,45,51	0.32	0	50,53,59	0.31	0
2	ACP	B	5101	4	27,33,33	1.67	7 (25%)	32,52,52	2.56	8 (25%)
2	ACP	A	5101	4	27,33,33	1.61	5 (18%)	32,52,52	2.31	5 (15%)
2	ACP	D	5101	4	27,33,33	0.92	1 (3%)	32,52,52	0.85	2 (6%)
2	ACP	C	5101	4	27,33,33	0.89	1 (3%)	32,52,52	0.80	2 (6%)
5	LBN	C	5107	-	45,45,51	0.32	0	50,53,59	0.31	0
5	LBN	B	5107	-	46,46,51	0.33	0	52,54,59	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LBN	A	5108	-	-	24/49/49/55	-
5	LBN	C	5106	-	-	31/50/50/55	-
5	LBN	D	5106	-	-	23/50/50/55	-
5	LBN	A	5107	-	-	35/50/50/55	-
5	LBN	B	5106	-	-	19/49/49/55	-
5	LBN	D	5107	-	-	19/49/49/55	-
2	ACP	B	5101	4	-	8/15/38/38	0/3/3/3
2	ACP	A	5101	4	-	6/15/38/38	0/3/3/3
2	ACP	D	5101	4	-	5/15/38/38	0/3/3/3
2	ACP	C	5101	4	-	3/15/38/38	0/3/3/3
5	LBN	C	5107	-	-	30/49/49/55	-
5	LBN	B	5107	-	-	33/50/50/55	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	PB-O3A	4.25	1.63	1.58
2	B	5101	ACP	PB-O3A	4.02	1.62	1.58
2	A	5101	ACP	PG-O3G	2.79	1.61	1.54
2	B	5101	ACP	PG-O2G	2.78	1.61	1.54
2	B	5101	ACP	PG-O3G	2.77	1.61	1.54
2	A	5101	ACP	PG-O2G	2.67	1.61	1.54
2	B	5101	ACP	C2-N3	-2.61	1.27	1.32
2	B	5101	ACP	C2'-C1'	-2.51	1.50	1.53
2	A	5101	ACP	C2-N3	-2.45	1.28	1.32
2	D	5101	ACP	PB-O2B	-2.41	1.50	1.56
2	C	5101	ACP	PB-O2B	-2.40	1.50	1.56
2	B	5101	ACP	C5-N7	-2.19	1.31	1.39
2	A	5101	ACP	C5-N7	-2.09	1.32	1.39
2	B	5101	ACP	C5-C4	2.05	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5101	ACP	C2-N1-C6	8.11	132.62	118.75
2	A	5101	ACP	C2-N1-C6	7.39	131.39	118.75
2	B	5101	ACP	N3-C2-N1	-6.82	118.02	128.68
2	A	5101	ACP	N3-C2-N1	-6.51	118.50	128.68
2	B	5101	ACP	C1'-N9-C4	-6.03	116.04	126.64
2	A	5101	ACP	C1'-N9-C4	-5.57	116.86	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5101	ACP	C5-C6-N1	-3.25	112.98	120.35
2	B	5101	ACP	C5-C6-N6	3.15	125.14	120.35
2	A	5101	ACP	C5-C6-N6	3.11	125.08	120.35
2	A	5101	ACP	C5-C6-N1	-3.03	113.48	120.35
2	B	5101	ACP	PB-O3A-PA	-2.80	123.69	132.56
2	D	5101	ACP	C5-C6-N6	2.49	124.13	120.35
2	C	5101	ACP	C5-C6-N6	2.25	123.78	120.35
2	D	5101	ACP	O1G-PG-C3B	-2.22	106.45	111.24
2	B	5101	ACP	C3'-C2'-C1'	2.16	104.22	100.98
2	C	5101	ACP	O1G-PG-C3B	-2.10	106.71	111.24
2	B	5101	ACP	C2'-C3'-C4'	2.04	106.60	102.64

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5101	ACP	C5'-O5'-PA-O3A
2	A	5101	ACP	O4'-C4'-C5'-O5'
2	A	5101	ACP	C3'-C4'-C5'-O5'
2	B	5101	ACP	PB-C3B-PG-O2G
2	B	5101	ACP	C5'-O5'-PA-O3A
2	C	5101	ACP	C5'-O5'-PA-O1A
2	C	5101	ACP	C5'-O5'-PA-O3A
2	C	5101	ACP	C4'-C5'-O5'-PA
2	D	5101	ACP	C5'-O5'-PA-O3A
2	D	5101	ACP	C4'-C5'-O5'-PA
5	A	5107	LBN	C1-O1-P1-O2
5	A	5107	LBN	C1-O1-P1-O3
5	A	5107	LBN	C1-O1-P1-O4
5	A	5107	LBN	C9-O2-P1-O3
5	A	5107	LBN	C9-O2-P1-O4
5	A	5107	LBN	C41-C42-C5-C8
5	A	5107	LBN	C35-C34-O7-C2
5	A	5107	LBN	O8-C34-O7-C2
5	A	5108	LBN	N1-C6-C9-O2
5	A	5108	LBN	C35-C34-O7-C2
5	B	5106	LBN	N1-C6-C9-O2
5	B	5106	LBN	C35-C34-O7-C2
5	B	5107	LBN	C1-O1-P1-O4
5	B	5107	LBN	N1-C6-C9-O2
5	B	5107	LBN	C26-C25-O5-C3
5	B	5107	LBN	O6-C25-O5-C3

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Mol	Chain	Res	Type	Atoms
5	B	5107	LBN	O8-C34-O7-C2
5	C	5106	LBN	C9-O2-P1-O3
5	C	5106	LBN	N1-C6-C9-O2
5	C	5106	LBN	C35-C34-O7-C2
5	C	5106	LBN	O8-C34-O7-C2
5	C	5107	LBN	C1-O1-P1-O2
5	C	5107	LBN	C9-O2-P1-O4
5	C	5107	LBN	N1-C6-C9-O2
5	C	5107	LBN	C35-C34-O7-C2
5	D	5106	LBN	C9-O2-P1-O3
5	D	5106	LBN	N1-C6-C9-O2
5	D	5106	LBN	C35-C34-O7-C2
5	D	5106	LBN	O8-C34-O7-C2
5	D	5107	LBN	N1-C6-C9-O2
5	D	5107	LBN	C35-C34-O7-C2
5	A	5107	LBN	O6-C25-O5-C3
5	C	5106	LBN	O6-C25-O5-C3
5	A	5108	LBN	O8-C34-O7-C2
5	C	5107	LBN	O8-C34-O7-C2
5	A	5107	LBN	C26-C25-O5-C3
5	B	5107	LBN	C35-C34-O7-C2
5	C	5106	LBN	C26-C25-O5-C3
5	C	5106	LBN	C41-C42-C5-C8
5	A	5107	LBN	C11-C14-C17-C20
5	C	5106	LBN	C29-C30-C31-C32
5	D	5106	LBN	C27-C28-C29-C30
5	B	5106	LBN	O8-C34-O7-C2
5	D	5107	LBN	O8-C34-O7-C2
5	A	5107	LBN	C29-C30-C31-C32
5	B	5107	LBN	C29-C30-C31-C32
5	B	5107	LBN	C14-C17-C20-C22
5	B	5107	LBN	C31-C32-C33-C4
5	D	5106	LBN	C14-C17-C20-C22
2	B	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	C3'-C4'-C5'-O5'
5	D	5106	LBN	C31-C32-C33-C4
5	A	5108	LBN	C9-C6-N1-C18
5	C	5107	LBN	C9-C6-N1-C18
5	D	5106	LBN	C29-C30-C31-C32
5	A	5108	LBN	C34-C35-C36-C37
5	C	5106	LBN	C35-C36-C37-C38
5	B	5106	LBN	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
5	D	5107	LBN	C34-C35-C36-C37
5	B	5106	LBN	C35-C36-C37-C38
5	D	5107	LBN	C35-C36-C37-C38
5	B	5107	LBN	C9-C6-N1-C15
5	C	5107	LBN	C34-C35-C36-C37
5	A	5107	LBN	C31-C32-C33-C4
5	C	5107	LBN	C41-C42-C5-C8
5	C	5106	LBN	C31-C32-C33-C4
5	D	5106	LBN	C38-C39-C40-C41
5	A	5107	LBN	C9-O2-P1-O1
5	B	5107	LBN	C9-O2-P1-O1
5	C	5106	LBN	C1-O1-P1-O2
5	C	5106	LBN	C9-O2-P1-O1
5	C	5107	LBN	C9-O2-P1-O1
5	D	5106	LBN	C9-O2-P1-O1
5	A	5108	LBN	C9-C6-N1-C15
5	B	5107	LBN	C9-C6-N1-C12
5	C	5107	LBN	C9-C6-N1-C12
5	C	5106	LBN	C8-C11-C14-C17
5	C	5106	LBN	C28-C29-C30-C31
5	A	5108	LBN	C38-C39-C40-C41
5	C	5106	LBN	C36-C37-C38-C39
5	D	5106	LBN	C32-C33-C4-C7
5	B	5107	LBN	C11-C14-C17-C20
5	A	5108	LBN	C36-C37-C38-C39
5	A	5107	LBN	C28-C29-C30-C31
5	C	5106	LBN	C30-C31-C32-C33
5	A	5107	LBN	C30-C31-C32-C33
5	A	5107	LBN	C37-C38-C39-C40
5	B	5106	LBN	C36-C37-C38-C39
5	D	5107	LBN	C36-C37-C38-C39
5	A	5107	LBN	C8-C11-C14-C17
5	A	5107	LBN	C26-C27-C28-C29
5	A	5107	LBN	C36-C37-C38-C39
5	B	5107	LBN	C26-C27-C28-C29
5	C	5107	LBN	C38-C39-C40-C41
5	B	5107	LBN	C9-C6-N1-C18
5	C	5107	LBN	C9-C6-N1-C15
5	A	5108	LBN	C13-C10-C7-C4
5	C	5106	LBN	C26-C27-C28-C29
5	C	5107	LBN	C13-C10-C7-C4
5	B	5106	LBN	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
5	D	5107	LBN	C38-C39-C40-C41
5	A	5108	LBN	C27-C28-C29-C30
5	B	5107	LBN	C32-C33-C4-C7
5	A	5108	LBN	C29-C30-C31-C32
5	C	5107	LBN	C26-C25-O5-C3
5	D	5106	LBN	C39-C40-C41-C42
5	B	5107	LBN	C28-C29-C30-C31
5	C	5106	LBN	C37-C38-C39-C40
5	D	5107	LBN	C29-C30-C31-C32
5	B	5106	LBN	C29-C30-C31-C32
5	B	5107	LBN	C30-C31-C32-C33
5	A	5108	LBN	C9-C6-N1-C12
5	C	5107	LBN	O6-C25-O5-C3
5	A	5107	LBN	C17-C20-C22-C23
5	A	5107	LBN	C27-C28-C29-C30
5	C	5107	LBN	C27-C28-C29-C30
5	B	5107	LBN	C36-C37-C38-C39
5	B	5106	LBN	C39-C40-C41-C42
5	D	5107	LBN	C39-C40-C41-C42
5	B	5106	LBN	C10-C13-C16-C19
5	D	5107	LBN	C10-C13-C16-C19
5	C	5107	LBN	C29-C30-C31-C32
5	D	5106	LBN	C40-C41-C42-C5
5	A	5107	LBN	O1-C1-C2-C3
5	C	5106	LBN	C27-C28-C29-C30
5	B	5106	LBN	C32-C33-C4-C7
5	D	5107	LBN	C32-C33-C4-C7
5	A	5107	LBN	C1-C2-C3-O5
5	C	5106	LBN	C1-C2-C3-O5
5	B	5107	LBN	C8-C11-C14-C17
5	C	5106	LBN	C39-C40-C41-C42
5	C	5106	LBN	C33-C4-C7-C10
5	A	5107	LBN	C33-C4-C7-C10
5	A	5107	LBN	C38-C39-C40-C41
5	B	5106	LBN	C27-C28-C29-C30
5	D	5106	LBN	C17-C20-C22-C23
5	D	5107	LBN	C27-C28-C29-C30
5	C	5107	LBN	C10-C13-C16-C19
5	D	5106	LBN	C8-C11-C14-C17
5	A	5108	LBN	C10-C13-C16-C19
5	A	5108	LBN	C13-C16-C19-C21
5	D	5106	LBN	C11-C14-C17-C20

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Mol	Chain	Res	Type	Atoms
5	A	5107	LBN	C40-C41-C42-C5
5	B	5107	LBN	C17-C20-C22-C23
5	C	5107	LBN	C13-C16-C19-C21
5	C	5107	LBN	C1-C2-C3-O5
5	D	5106	LBN	C1-O1-P1-O2
5	A	5107	LBN	O1-C1-C2-O7
5	A	5108	LBN	C39-C40-C41-C42
5	A	5107	LBN	O7-C2-C3-O5
5	B	5107	LBN	O7-C2-C3-O5
2	B	5101	ACP	C4'-C5'-O5'-PA
5	B	5107	LBN	C27-C28-C29-C30
5	A	5108	LBN	C40-C41-C42-C5
5	B	5107	LBN	C35-C36-C37-C38
5	A	5108	LBN	C42-C5-C8-C11
5	C	5106	LBN	O1-C1-C2-C3
5	B	5106	LBN	C2-C1-O1-P1
5	D	5107	LBN	C2-C1-O1-P1
5	C	5106	LBN	O1-C1-C2-O7
5	C	5107	LBN	O7-C2-C3-O5
5	C	5107	LBN	C28-C29-C30-C31
5	B	5107	LBN	C1-O1-P1-O2
5	C	5107	LBN	C2-C1-O1-P1
2	A	5101	ACP	C5'-O5'-PA-O1A
2	B	5101	ACP	C5'-O5'-PA-O1A
2	D	5101	ACP	C5'-O5'-PA-O1A
5	B	5107	LBN	C9-O2-P1-O4
5	C	5106	LBN	C1-O1-P1-O3
5	C	5107	LBN	C1-O1-P1-O3
5	C	5107	LBN	C9-O2-P1-O3
5	D	5106	LBN	C28-C29-C30-C31
5	B	5106	LBN	C28-C29-C30-C31
5	D	5107	LBN	C28-C29-C30-C31
5	A	5107	LBN	C6-C9-O2-P1
5	B	5107	LBN	C6-C9-O2-P1
5	C	5106	LBN	C17-C20-C22-C23
5	A	5107	LBN	C39-C40-C41-C42
5	C	5107	LBN	C40-C41-C42-C5
2	B	5101	ACP	PB-C3B-PG-O3G
2	D	5101	ACP	PG-C3B-PB-O2B
5	A	5107	LBN	N1-C6-C9-O2
5	B	5107	LBN	C1-C2-C3-O5
5	C	5106	LBN	O7-C2-C3-O5

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Mol	Chain	Res	Type	Atoms
5	A	5107	LBN	C32-C33-C4-C7
5	D	5107	LBN	C13-C10-C7-C4
5	B	5106	LBN	C13-C10-C7-C4
5	B	5106	LBN	C7-C10-C13-C16
5	D	5107	LBN	C7-C10-C13-C16
5	A	5108	LBN	C30-C31-C32-C33
5	B	5107	LBN	C1-C2-O7-C34
5	C	5107	LBN	C33-C4-C7-C10
5	B	5107	LBN	C39-C40-C41-C42
5	A	5108	LBN	C1-O1-P1-O2
5	B	5106	LBN	C1-O1-P1-O2
5	D	5107	LBN	C1-O1-P1-O2
2	A	5101	ACP	C4'-C5'-O5'-PA
5	D	5106	LBN	C42-C5-C8-C11
5	C	5106	LBN	C34-C35-C36-C37
5	A	5108	LBN	C28-C29-C30-C31
5	D	5106	LBN	C26-C27-C28-C29
5	A	5108	LBN	C33-C4-C7-C10
5	C	5107	LBN	C30-C31-C32-C33
5	A	5108	LBN	C2-C1-O1-P1
5	A	5108	LBN	C37-C38-C39-C40
2	A	5101	ACP	PG-C3B-PB-O1B
2	B	5101	ACP	PG-C3B-PB-O1B
2	D	5101	ACP	PG-C3B-PB-O1B
5	C	5106	LBN	C32-C33-C4-C7
5	B	5107	LBN	C38-C39-C40-C41
5	B	5106	LBN	C40-C41-C42-C5
5	D	5107	LBN	C40-C41-C42-C5
5	D	5106	LBN	C36-C37-C38-C39
5	B	5107	LBN	C14-C11-C8-C5
5	C	5106	LBN	O7-C34-C35-C36
5	C	5107	LBN	C26-C27-C28-C29
5	D	5107	LBN	C33-C4-C7-C10
5	B	5106	LBN	C33-C4-C7-C10
5	A	5107	LBN	O7-C34-C35-C36
5	A	5108	LBN	C35-C36-C37-C38
5	D	5106	LBN	C1-O1-P1-O4
5	C	5106	LBN	O8-C34-C35-C36
5	A	5107	LBN	O8-C34-C35-C36
5	C	5107	LBN	C6-C9-O2-P1
5	D	5106	LBN	O7-C34-C35-C36
5	B	5107	LBN	O5-C25-C26-C27

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5106	LBN	1	0
5	D	5106	LBN	1	0
2	B	5101	ACP	1	0
2	A	5101	ACP	1	0
2	C	5101	ACP	1	0
5	C	5107	LBN	2	0

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

Ligand LBN A 5108

Bond lengths　　　　Bond angles

Torsions　　　　Rings

Ligand LBN C 5106

Bond lengths

Bond angles

Torsions

Rings

Ligand LBN D 5106

Bond lengths

Bond angles

Torsions

Rings

Ligand LBN A 5107

Bond lengths

Bond angles

Torsions

Rings

Ligand LBN B 5106

Bond lengths

Bond angles

Torsions

Rings

Ligand LBN D 5107

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP B 5101

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP A 5101

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP D 5101

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP C 5101

Bond lengths

Bond angles

Torsions

Rings

Ligand LBN C 5107

Bond lengths

Bond angles

Torsions

Rings

Ligand LBN B 5107

Bond lengths

Bond angles

Torsions

Rings

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-26610. 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
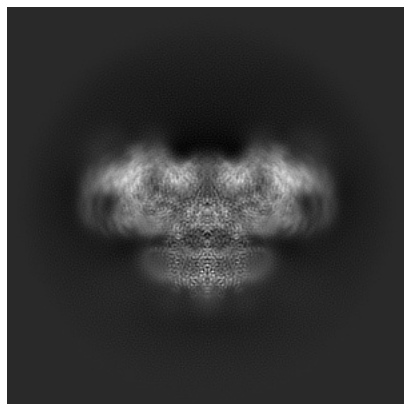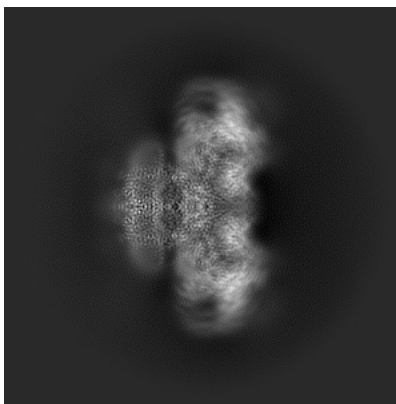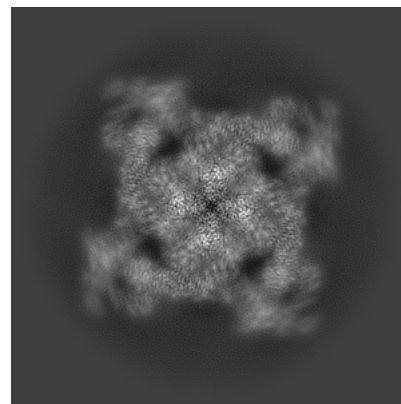
X   Y   Z

6.1.2   Raw map

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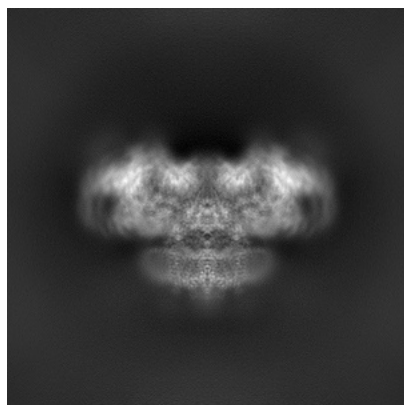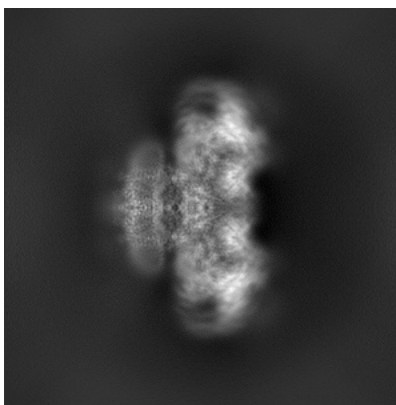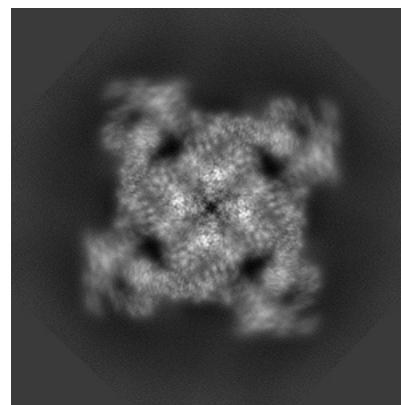
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
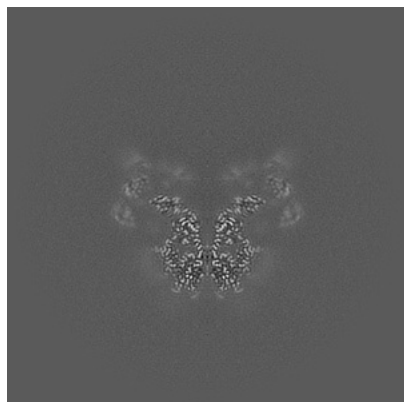
6.2.1 Primary map
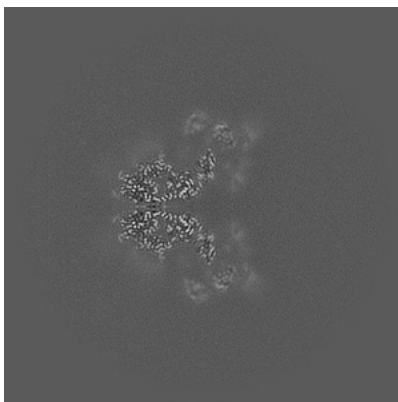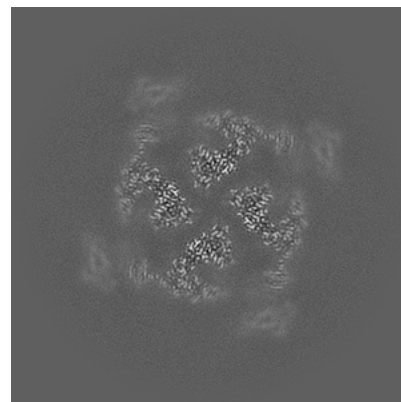
X Index: 276	Y Index: 276	Z Index: 276

6.2.2 Raw map
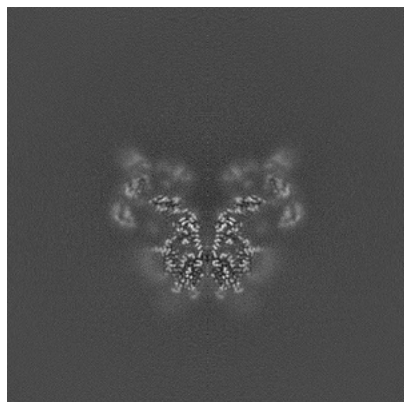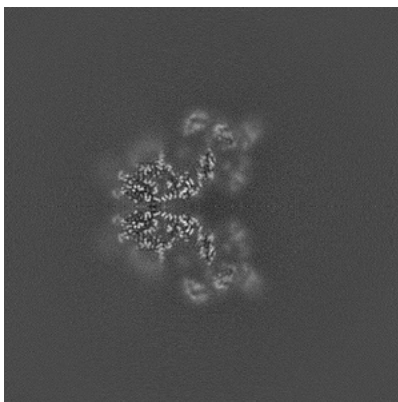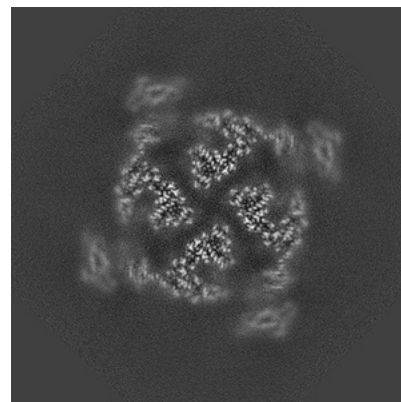
X Index: 276	Y Index: 276	Z Index: 276

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
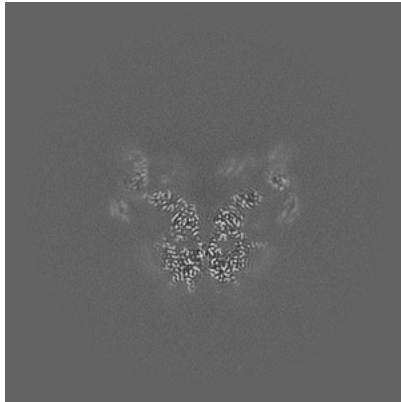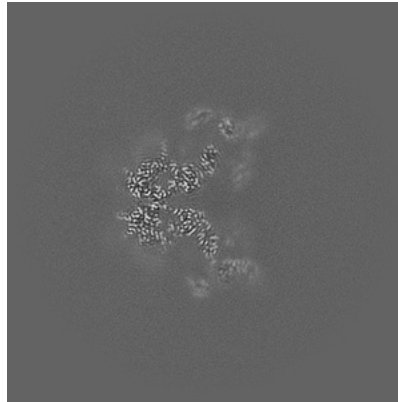
X Index: 280   Y Index: 272   Z Index: 275
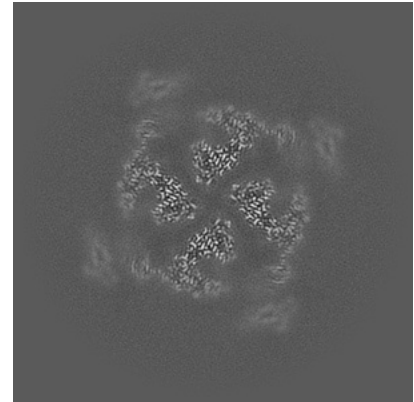
6.3.2 Raw map
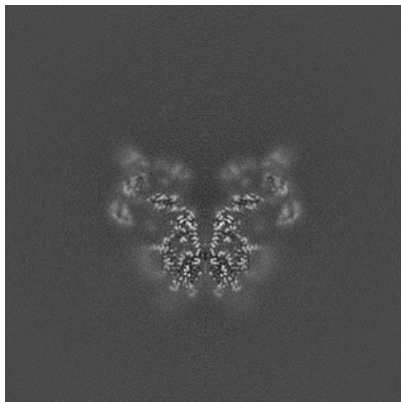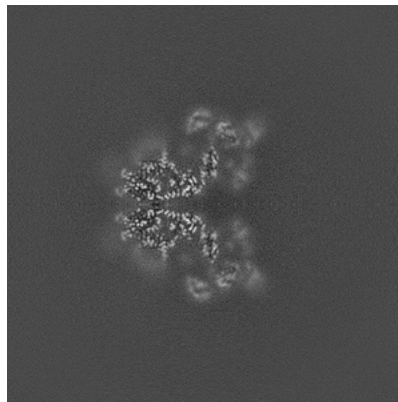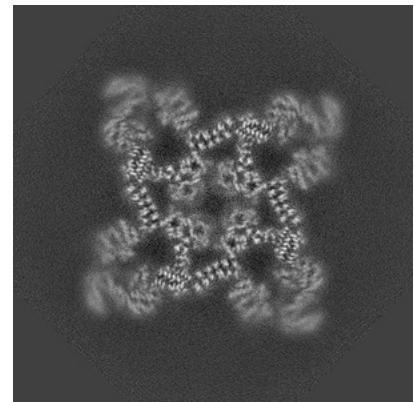
X Index: 276   Y Index: 276   Z Index: 311

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

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

6.4.1　Primary map
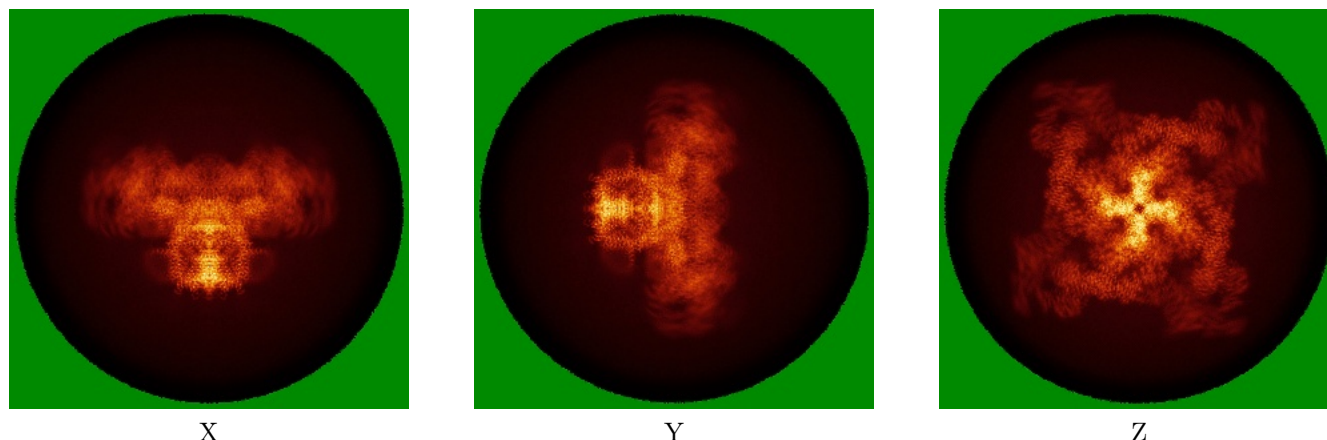
6.4.2　Raw map
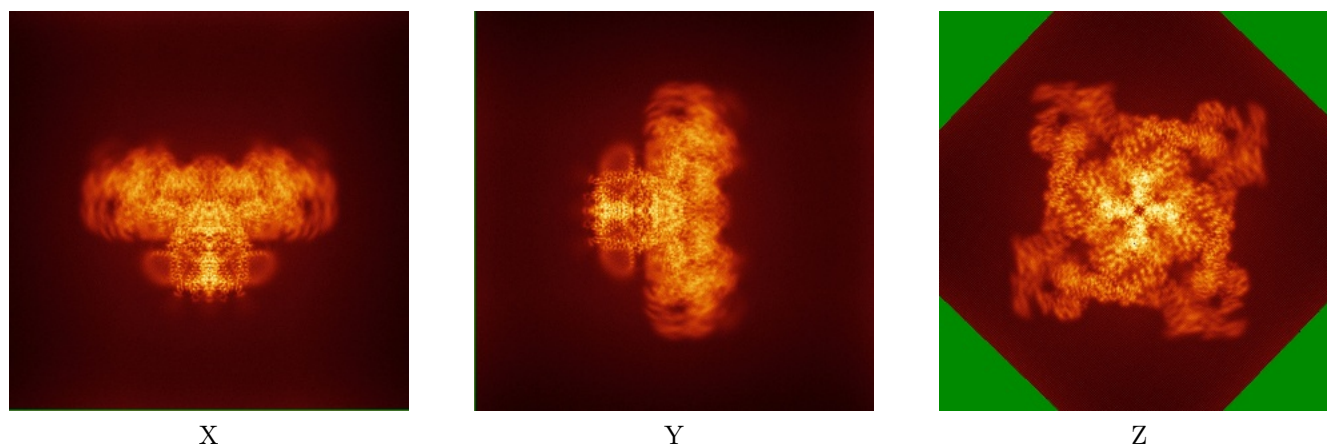
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
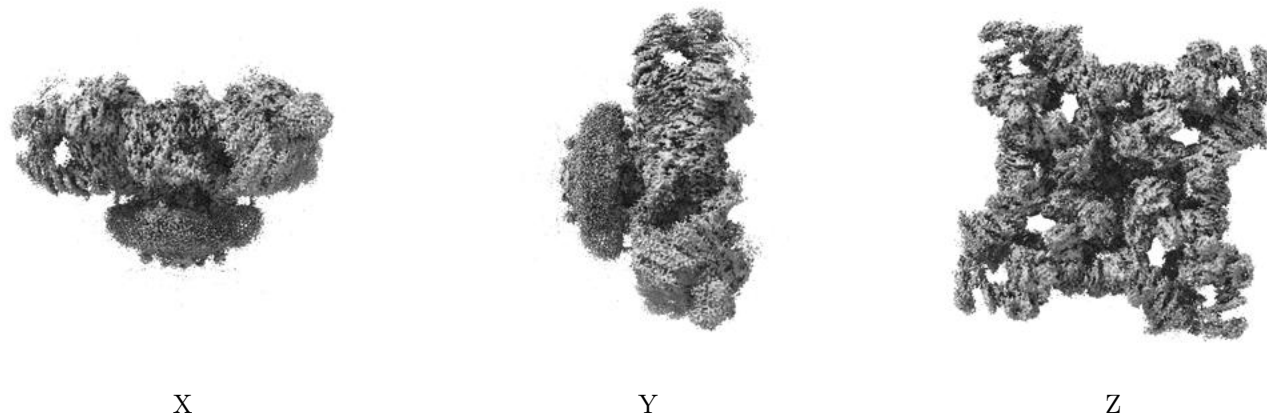
The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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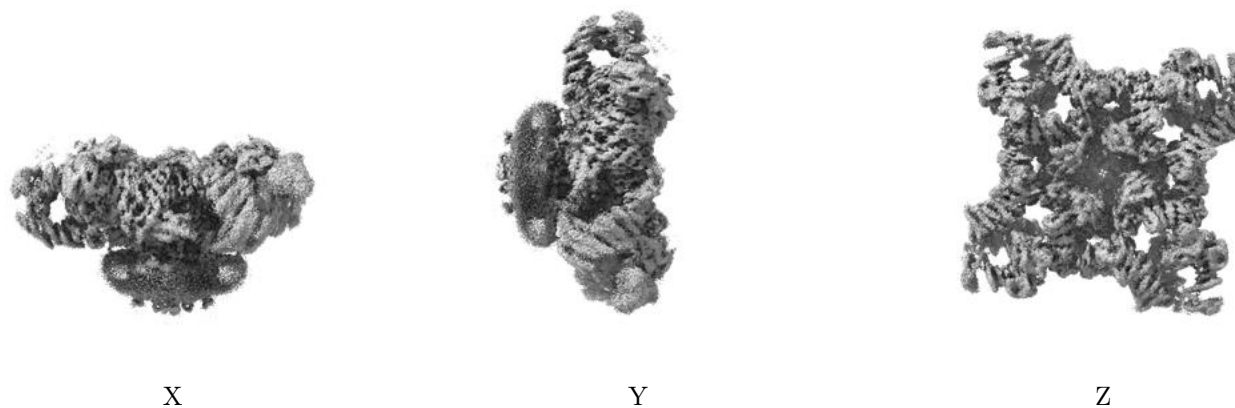
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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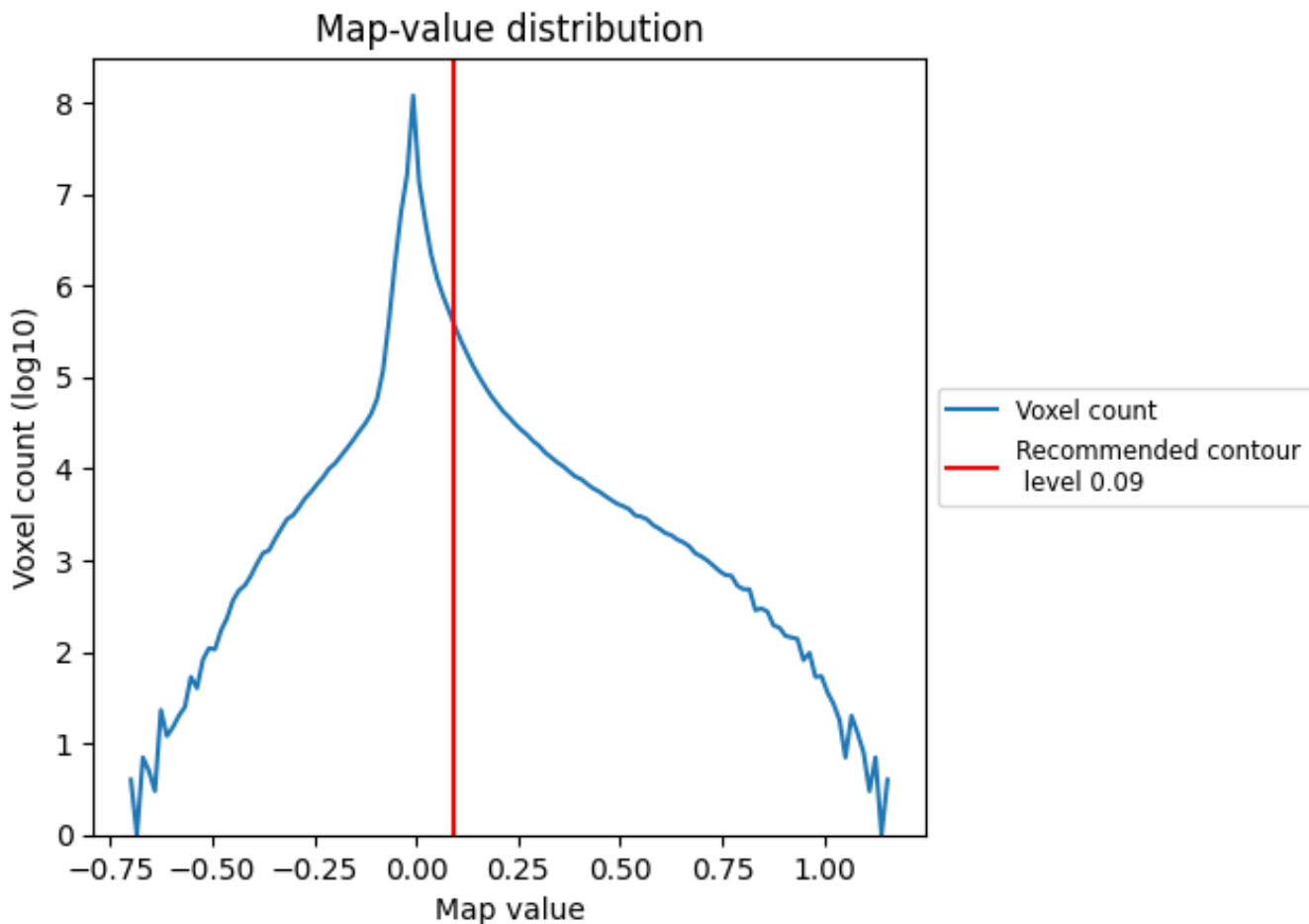
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
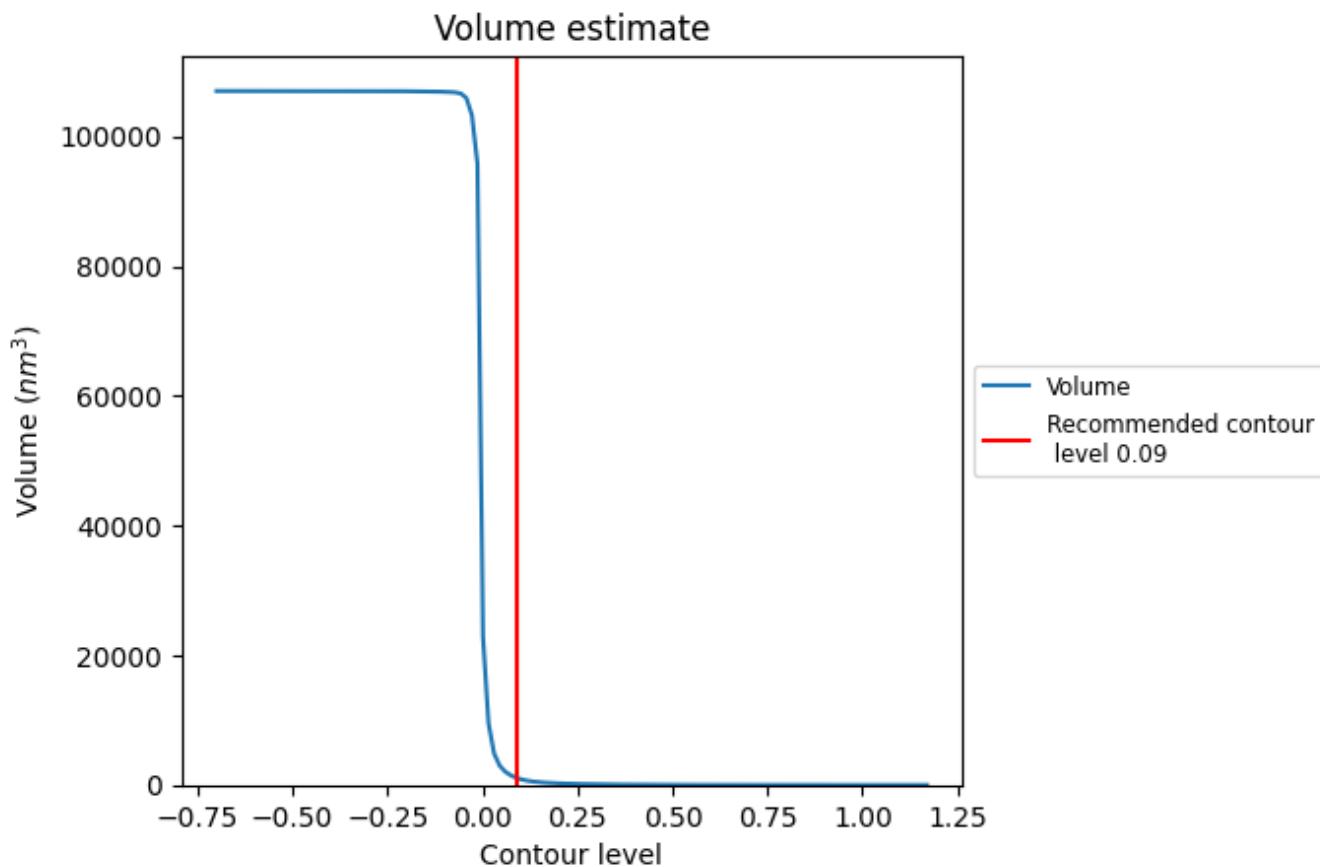
The volume at the recommended contour level is 1086 nm^3; this corresponds to an approximate mass of 981 kDa.

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

7.3 Rotationally averaged power spectrum (i)
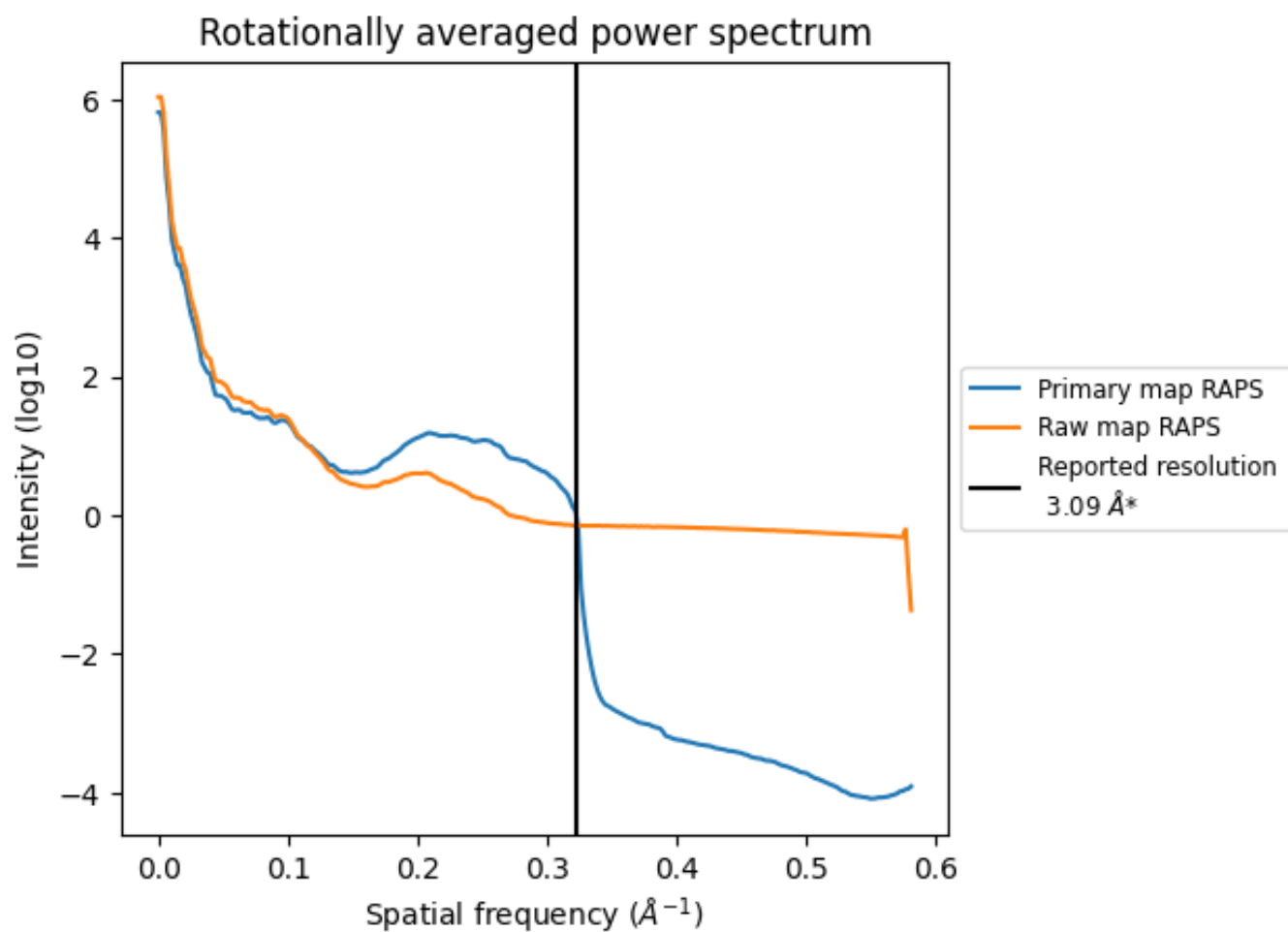
*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ
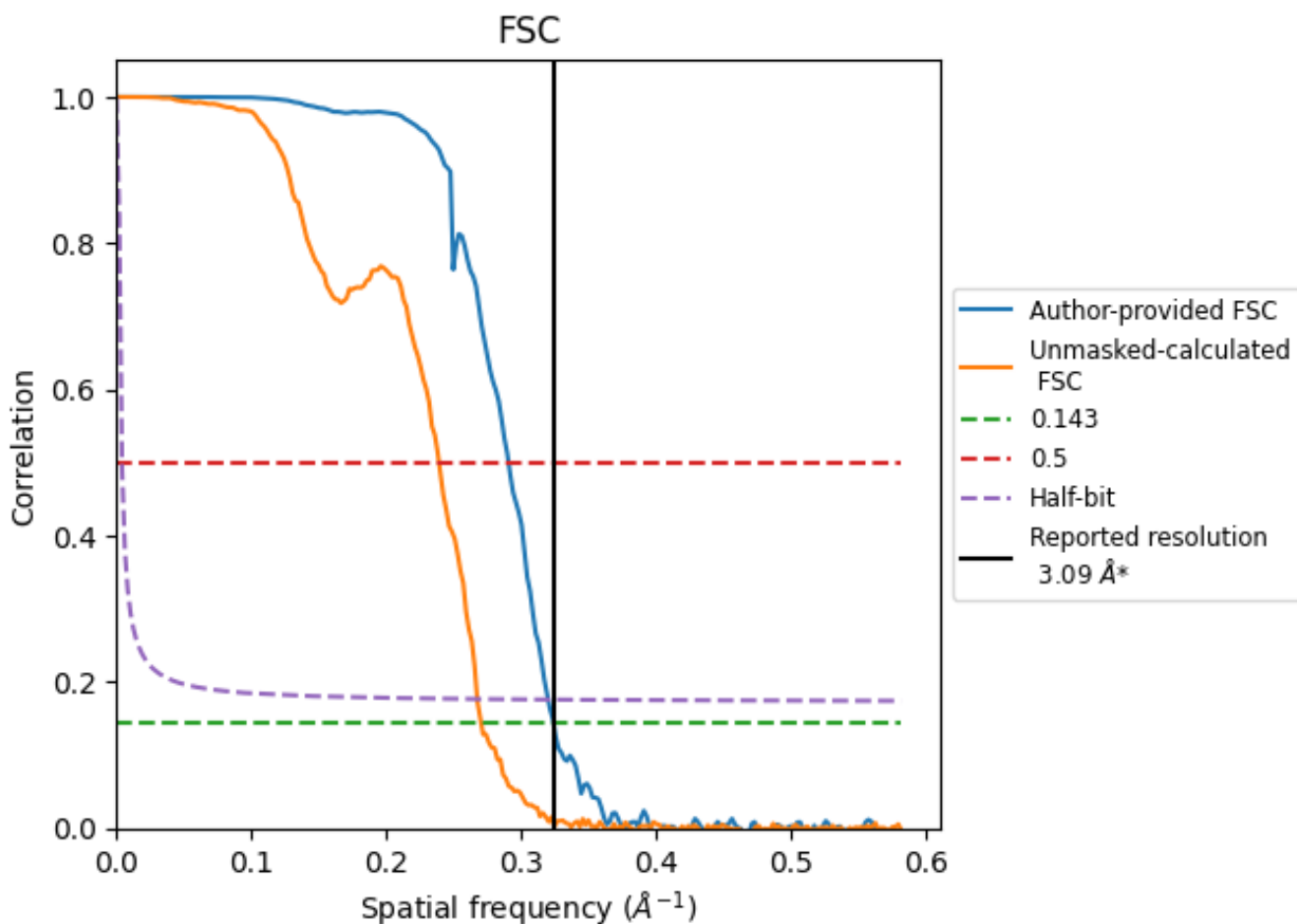
*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

8.2　Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.44	3.13
Unmasked-calculated*	3.70	4.18	3.74

*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 3.70 differs from the reported value 3.09 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-26610 and PDB model 7UMZ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

X	Y	Z
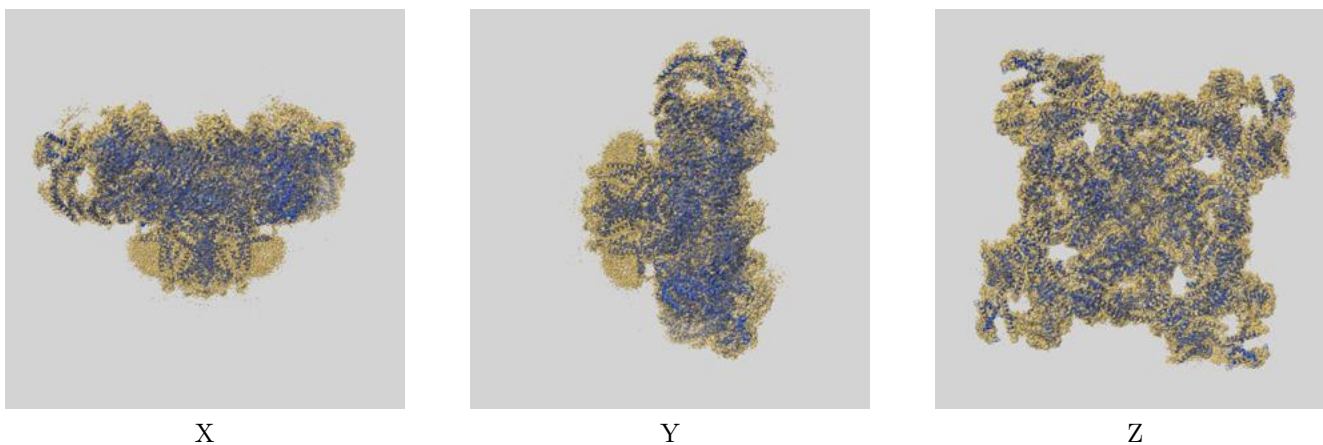
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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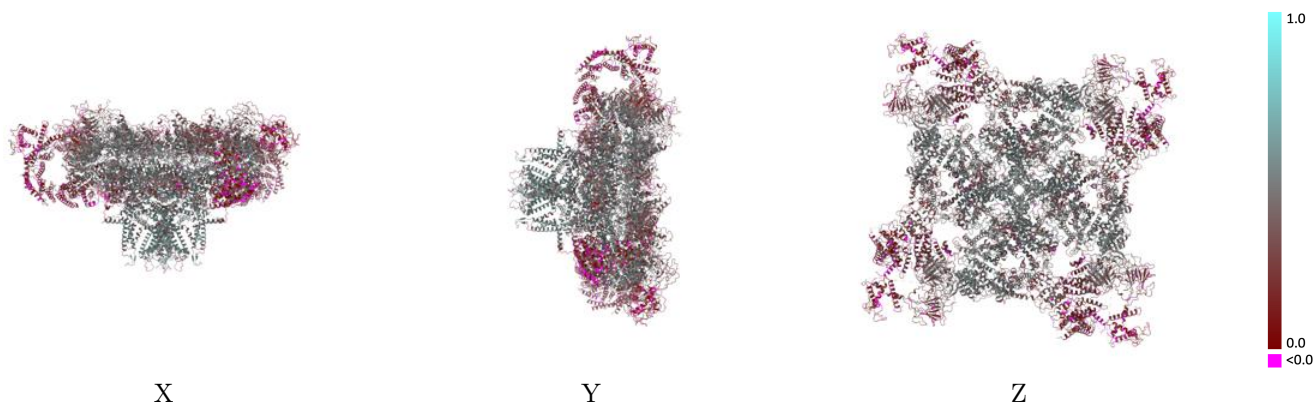
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
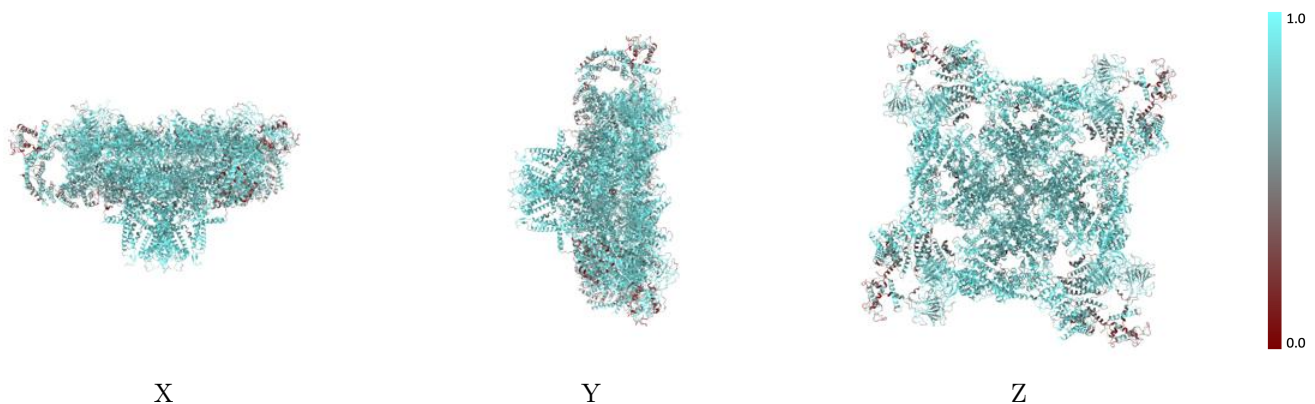
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4　Atom inclusion　ⓘ
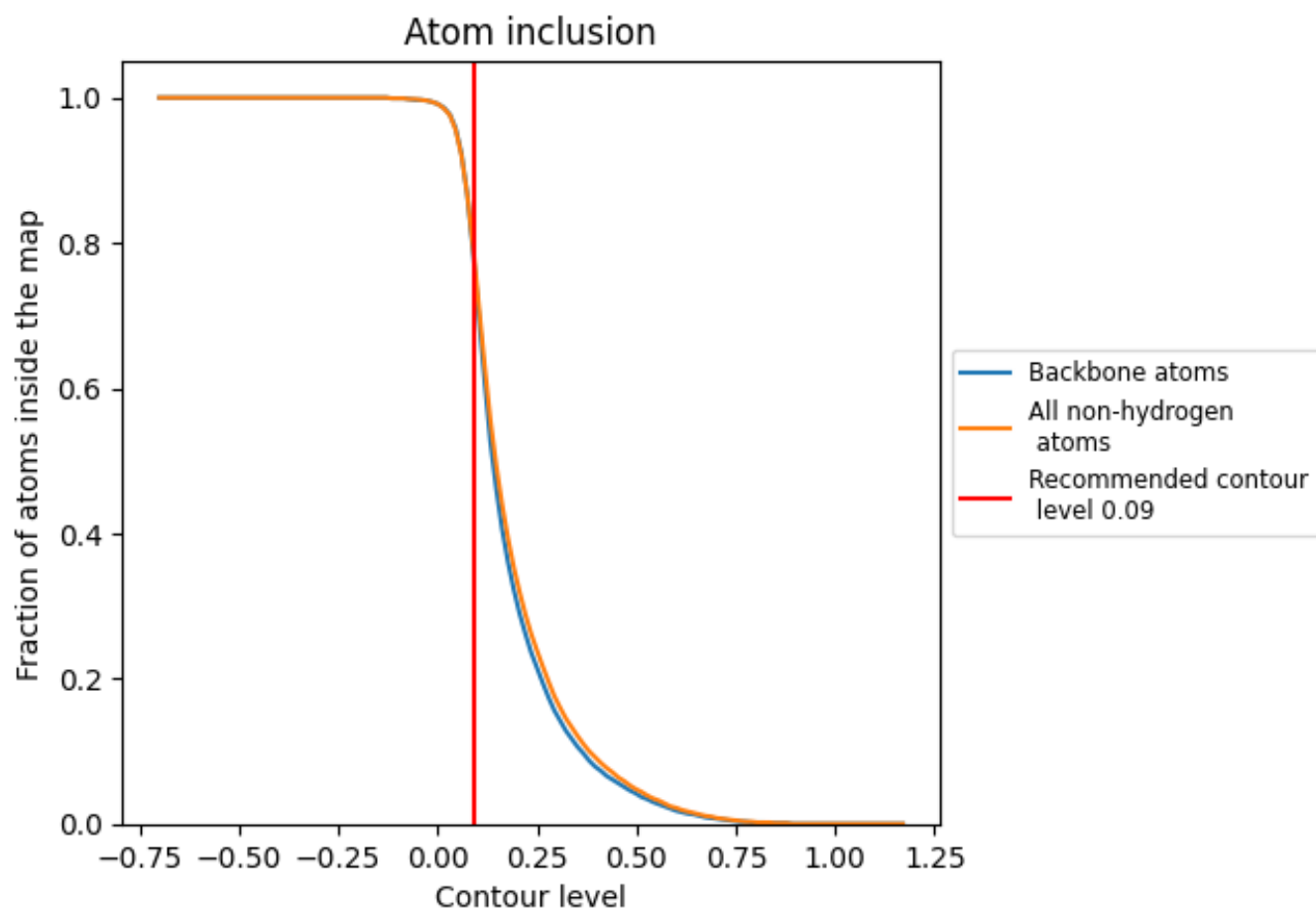
At the recommended contour level, 78% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.3840
A	0.7930	0.3840
B	0.7910	0.3840
C	0.7920	0.3830
D	0.7940	0.3840

1.0

0.0

<0.0