Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 11:36 AM EST

PDB ID	:	7TDG
EMDB ID	:	EMD-25828
Title	:	Rabbit RyR1 with AMP-PCP and high Ca2+ embedded in nanodisc in inactivated conformation (Dataset-A)
Authors	:	Nayak, A.R.; Samso, M.
Deposited on	:	2021-12-31
Resolution	:	3.80 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:

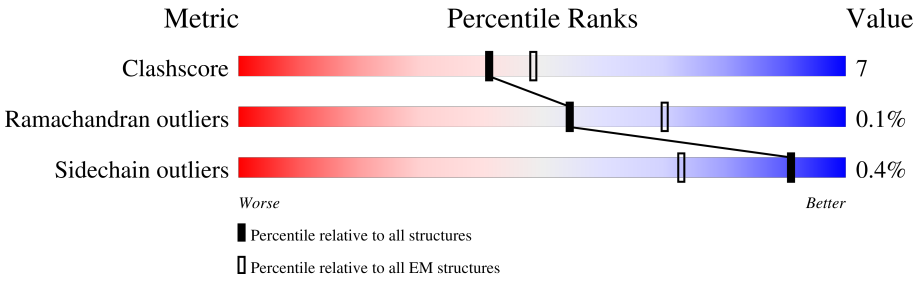
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	71% 11% 18%
1	B	5037	70% 11% 18%
1	C	5037	71% 11% 18%
1	D	5037	71% 11% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 117345 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,RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4134	Total 29247	C 18513	N 5182	O 5395	S 157	0	0
1	C	4134	Total 29244	C 18513	N 5179	O 5395	S 157	0	0
1	D	4134	Total 29228	C 18502	N 5176	O 5393	S 157	0	0
1	B	4134	Total 29246	C 18514	N 5182	O 5393	S 157	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

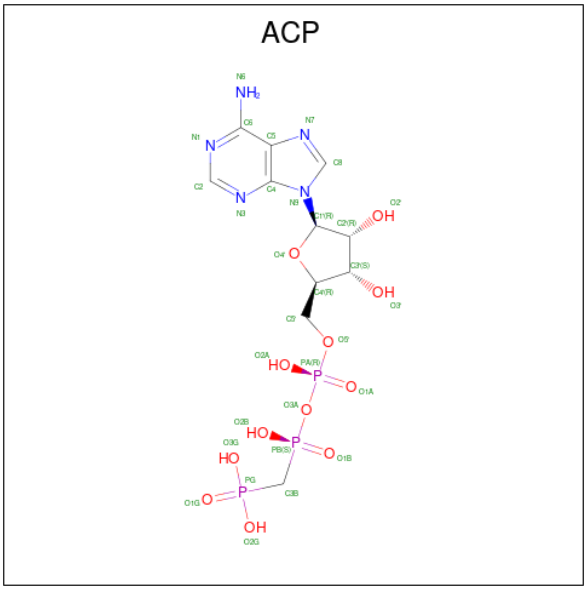
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	Ca 2	0
3	C	2	Total 2	Ca 2	0
3	D	2	Total 2	Ca 2	0
3	B	2	Total 2	Ca 2	0

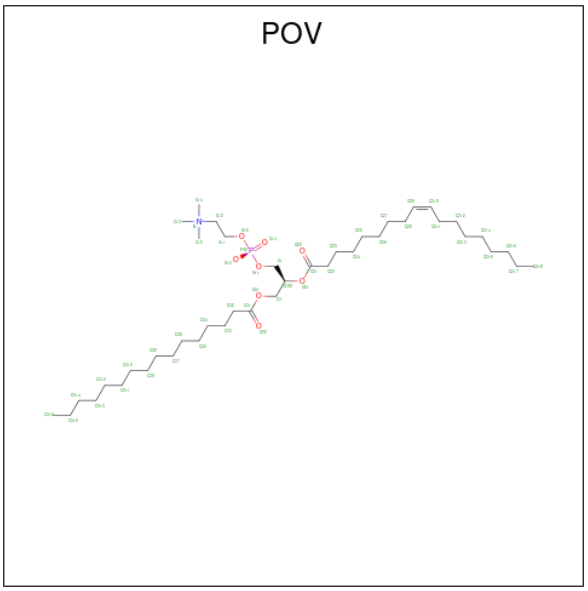
- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-

letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).

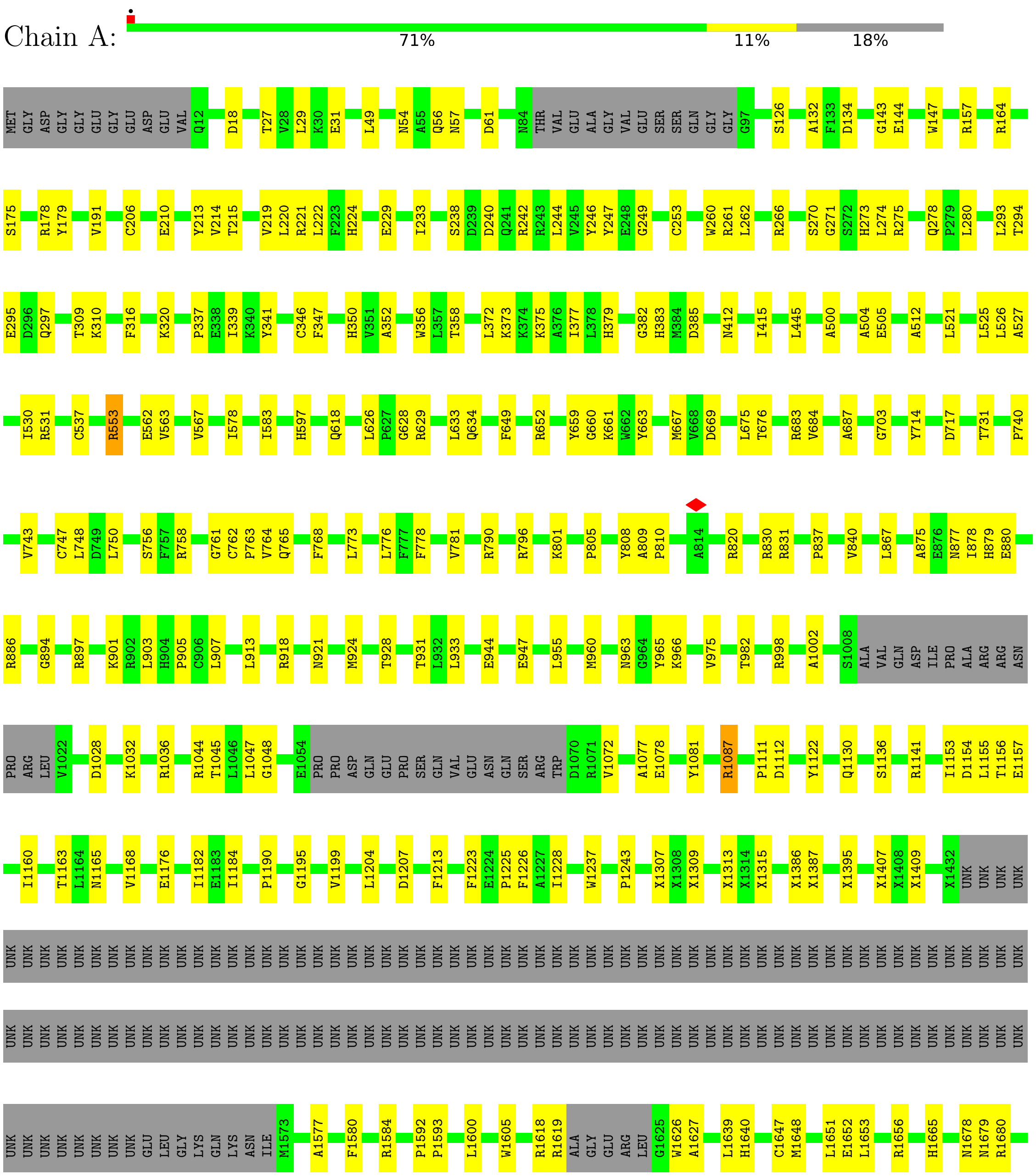


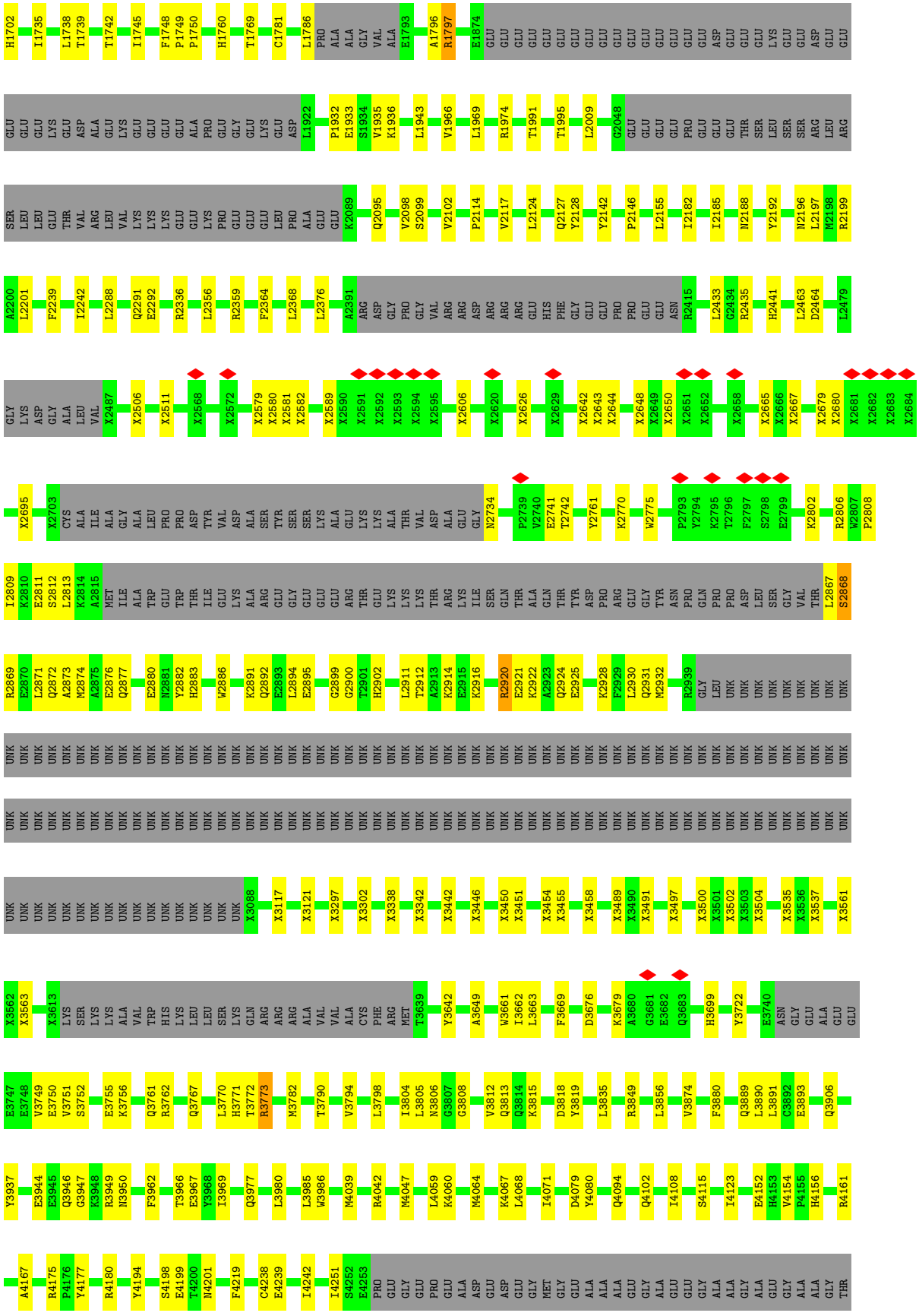
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			61	51	1	8	1	
5	A	1	Total	C	N	O	P	0
			61	51	1	8	1	
5	C	1	Total	C	N	O	P	0
			77	67	1	8	1	
5	C	1	Total	C	N	O	P	0
			77	67	1	8	1	
5	C	1	Total	C	N	O	P	0
			77	67	1	8	1	
5	D	1	Total	C	N	O	P	0
			45	35	1	8	1	
5	B	1	Total	C	N	O	P	0
			61	51	1	8	1	
5	B	1	Total	C	N	O	P	0
			61	51	1	8	1	

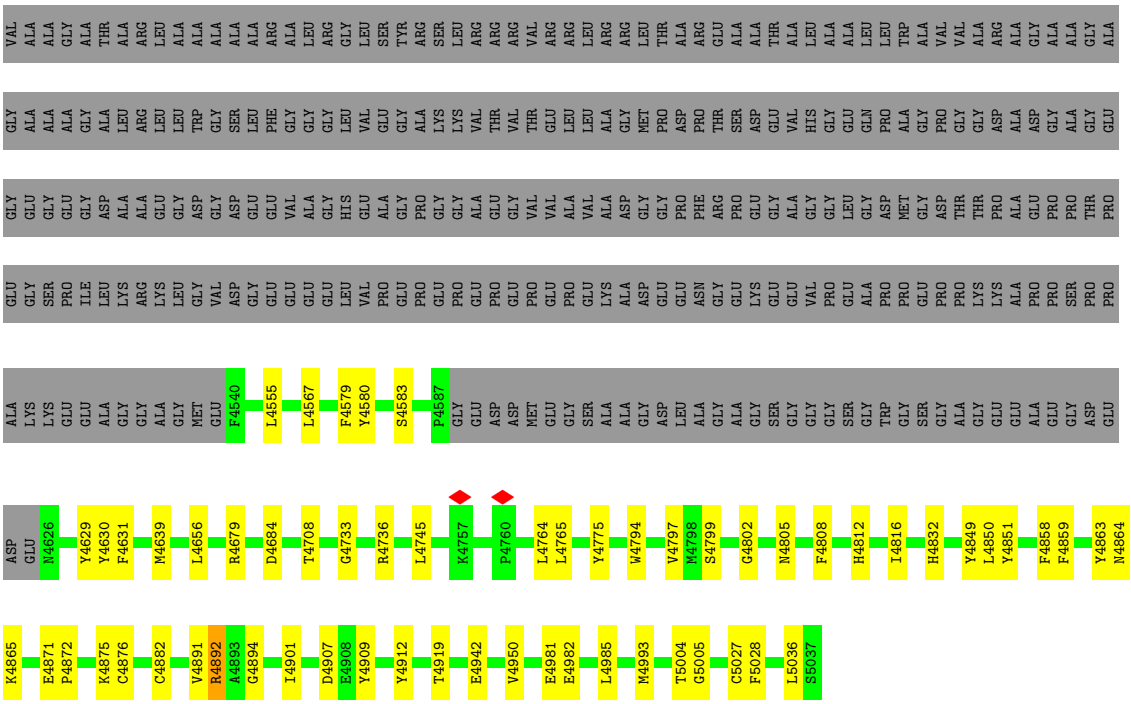
3 Residue-property plots (i)

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,RyR1

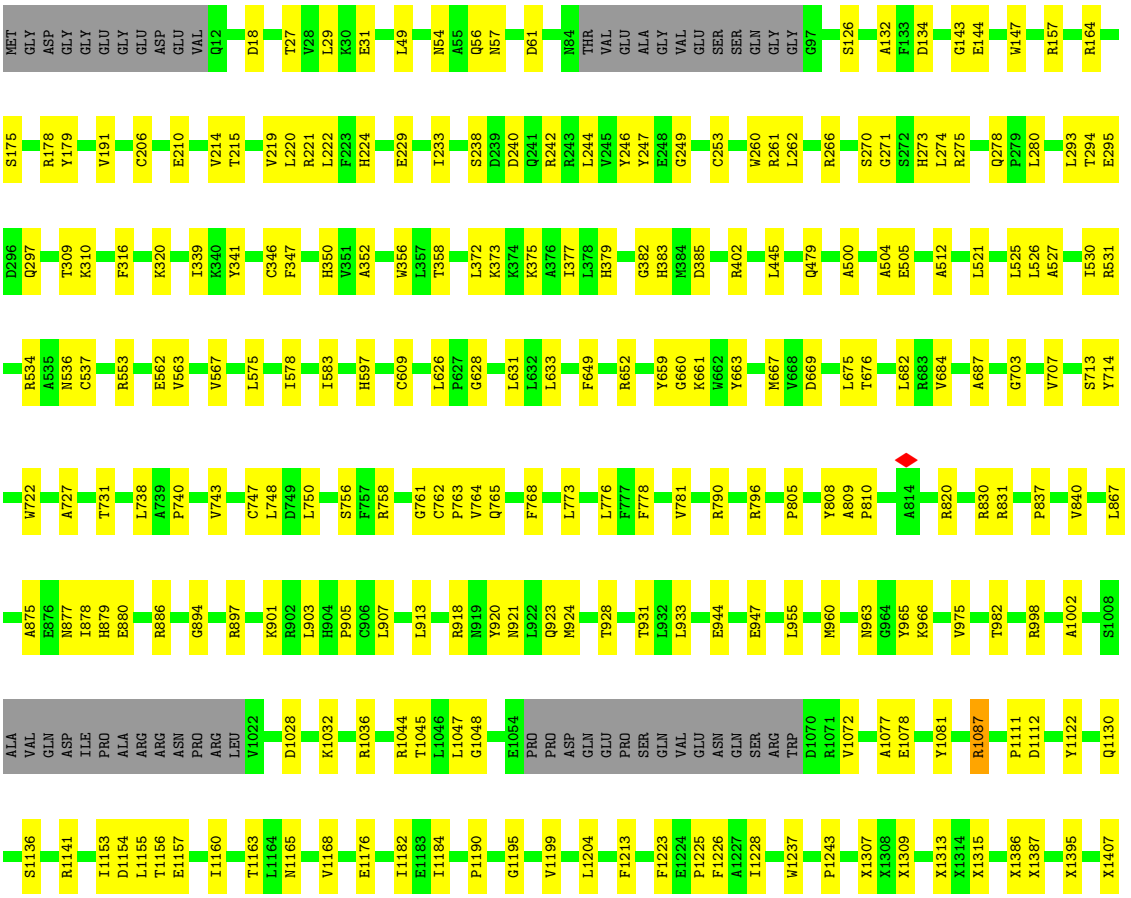


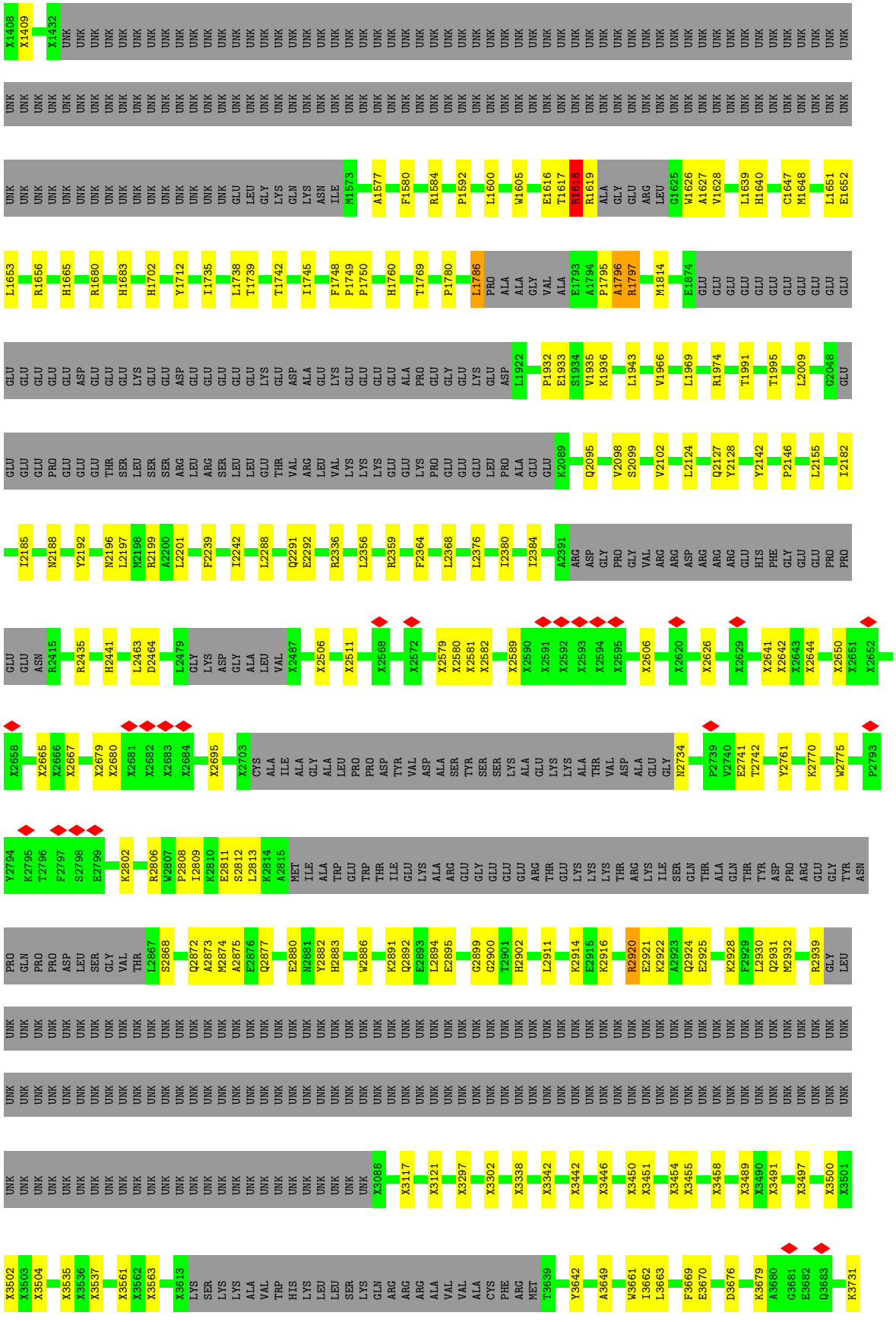


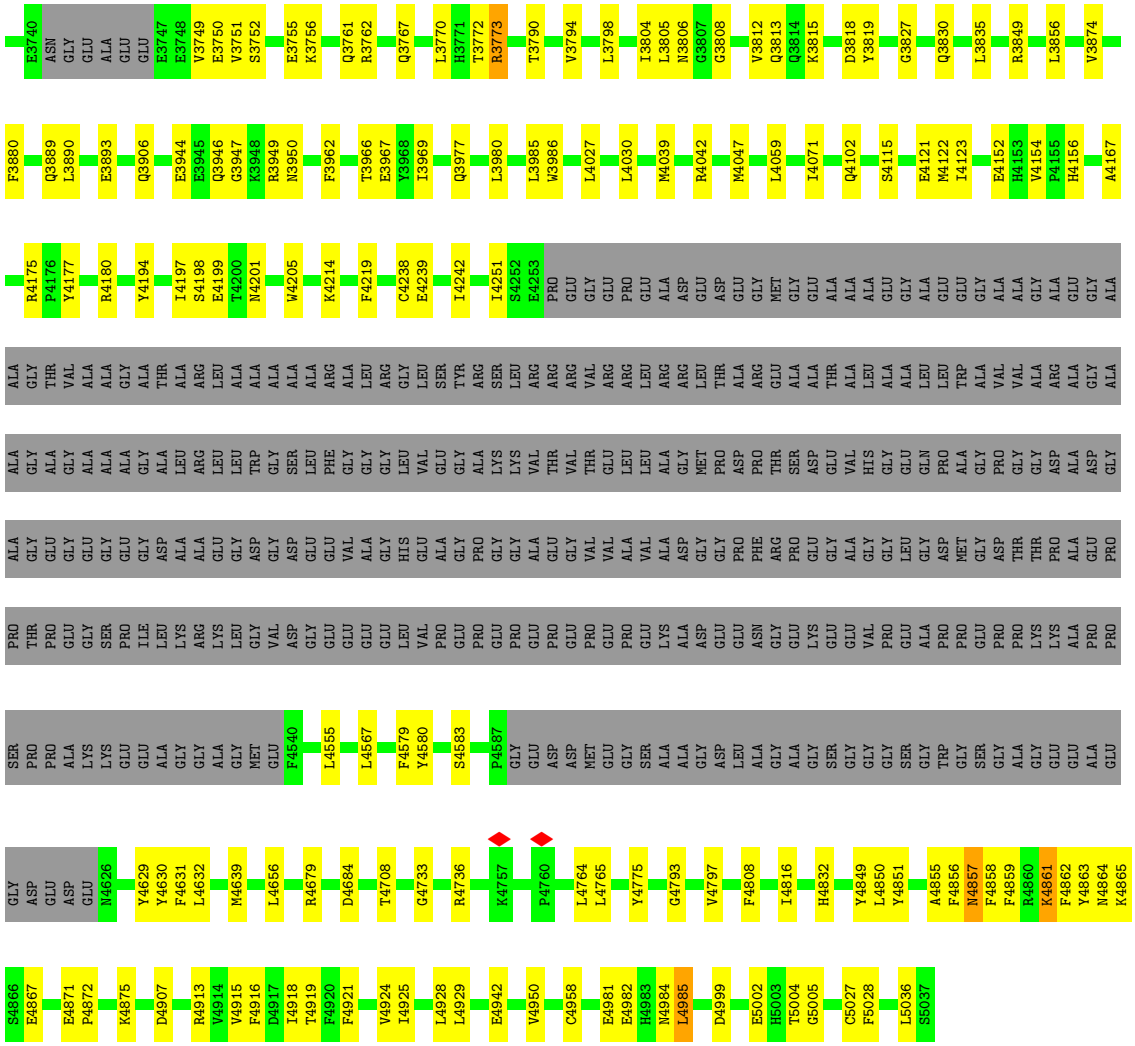


• Molecule 1: Ryanodine receptor 1,RyR1

Chain C:

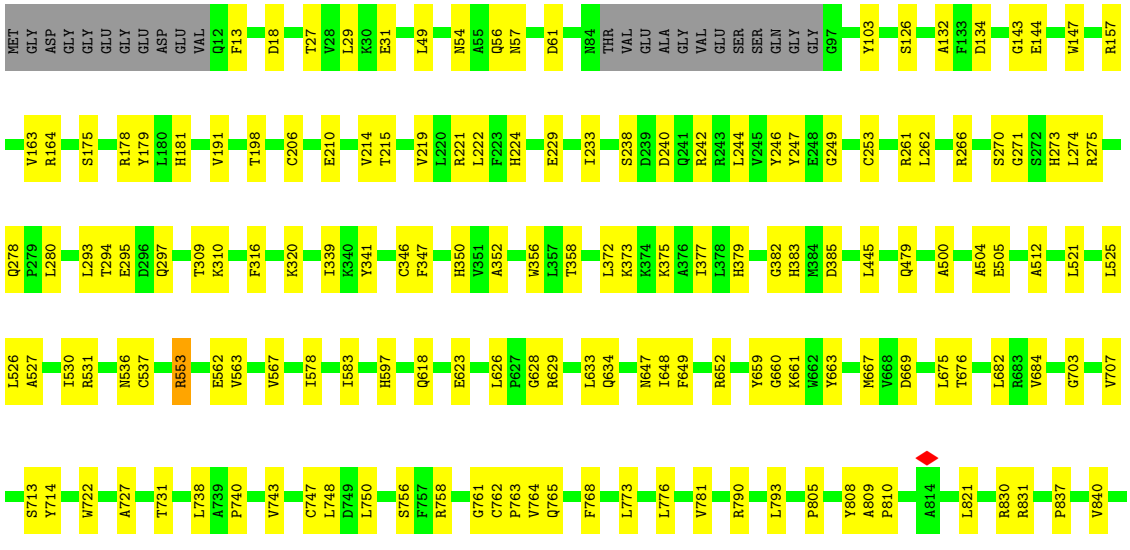


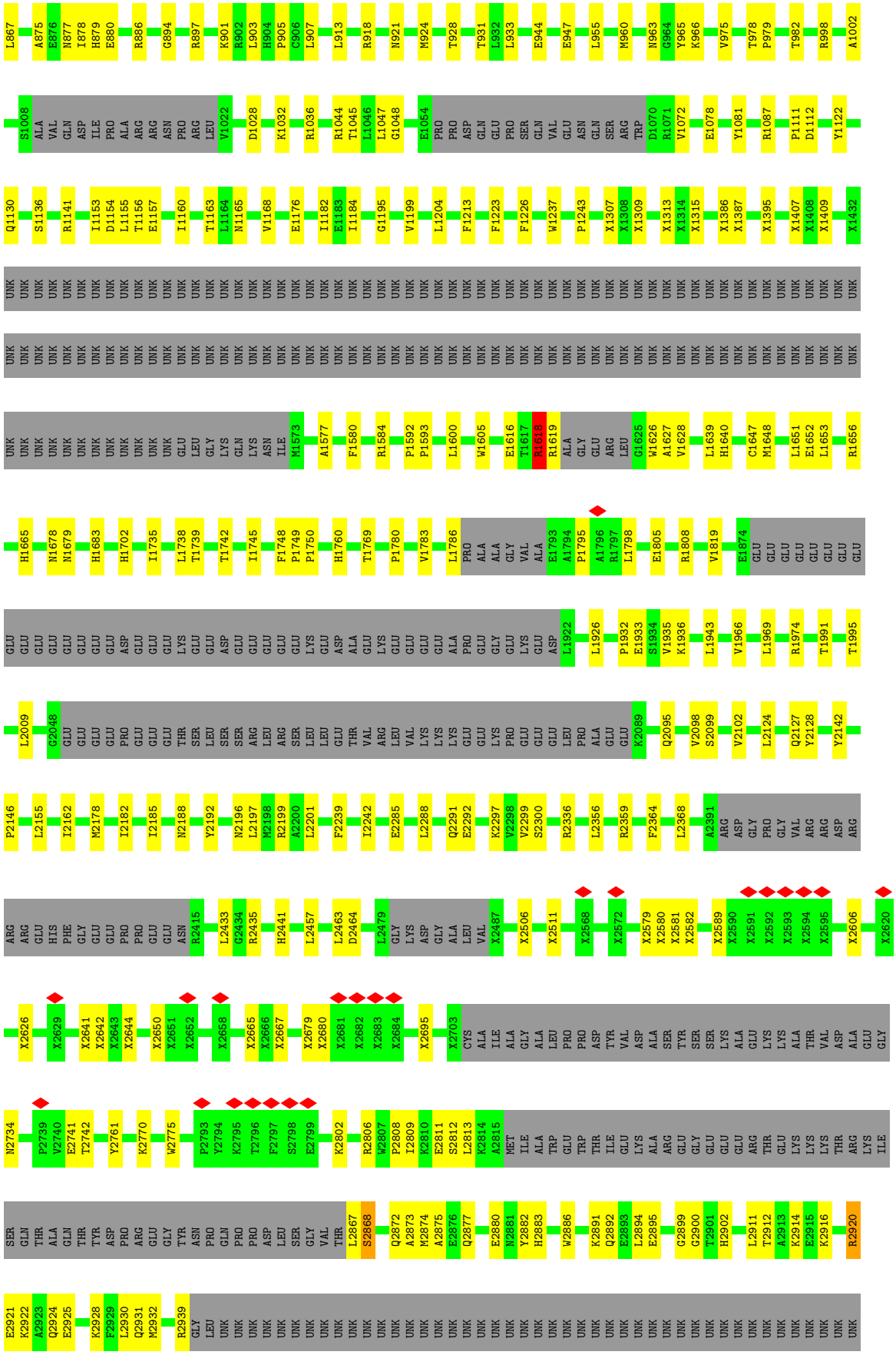


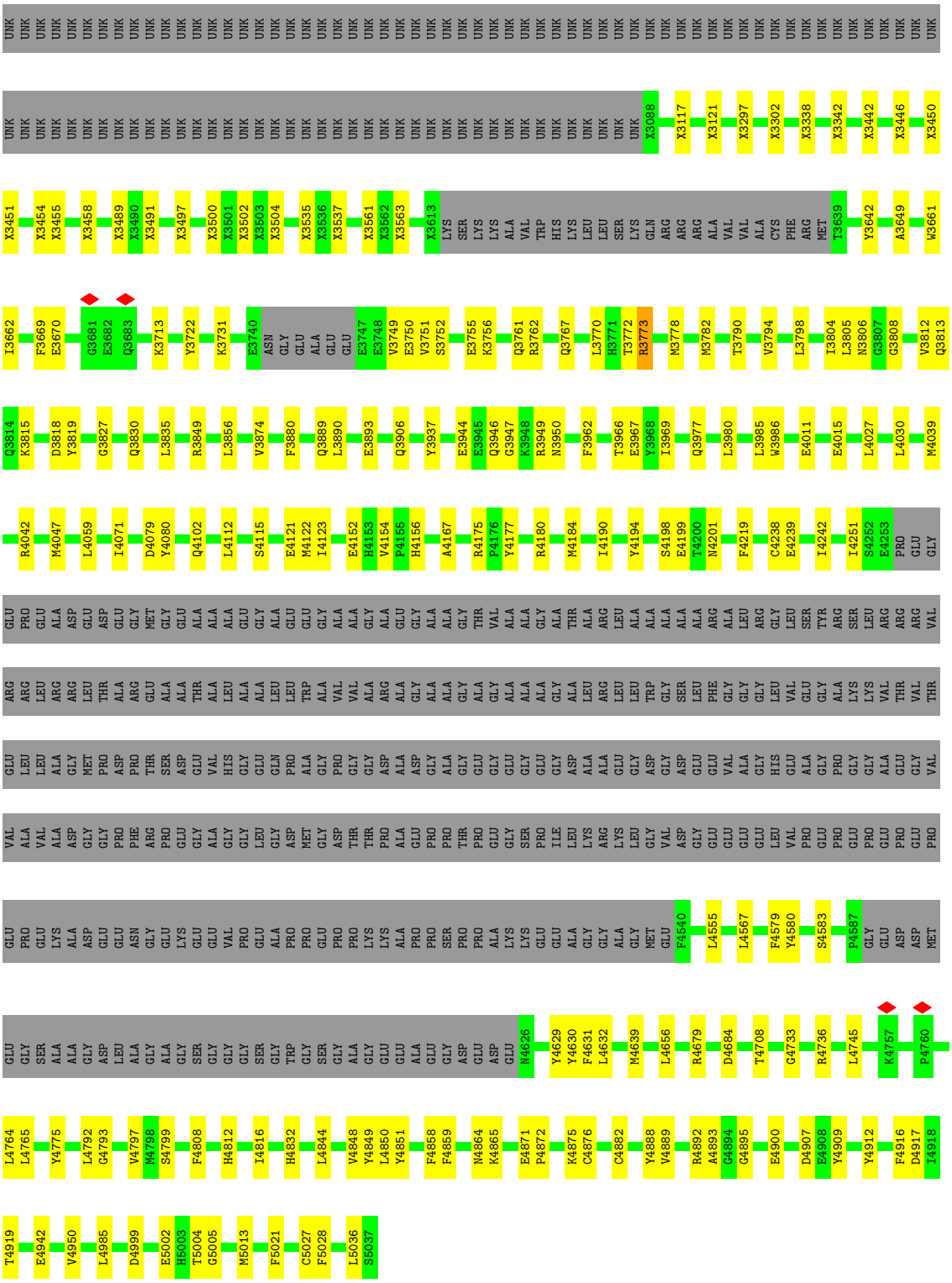


• Molecule 1: Ryanodine receptor 1,RyR1

Chain D:

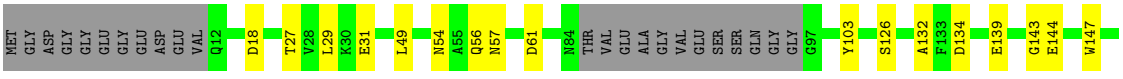


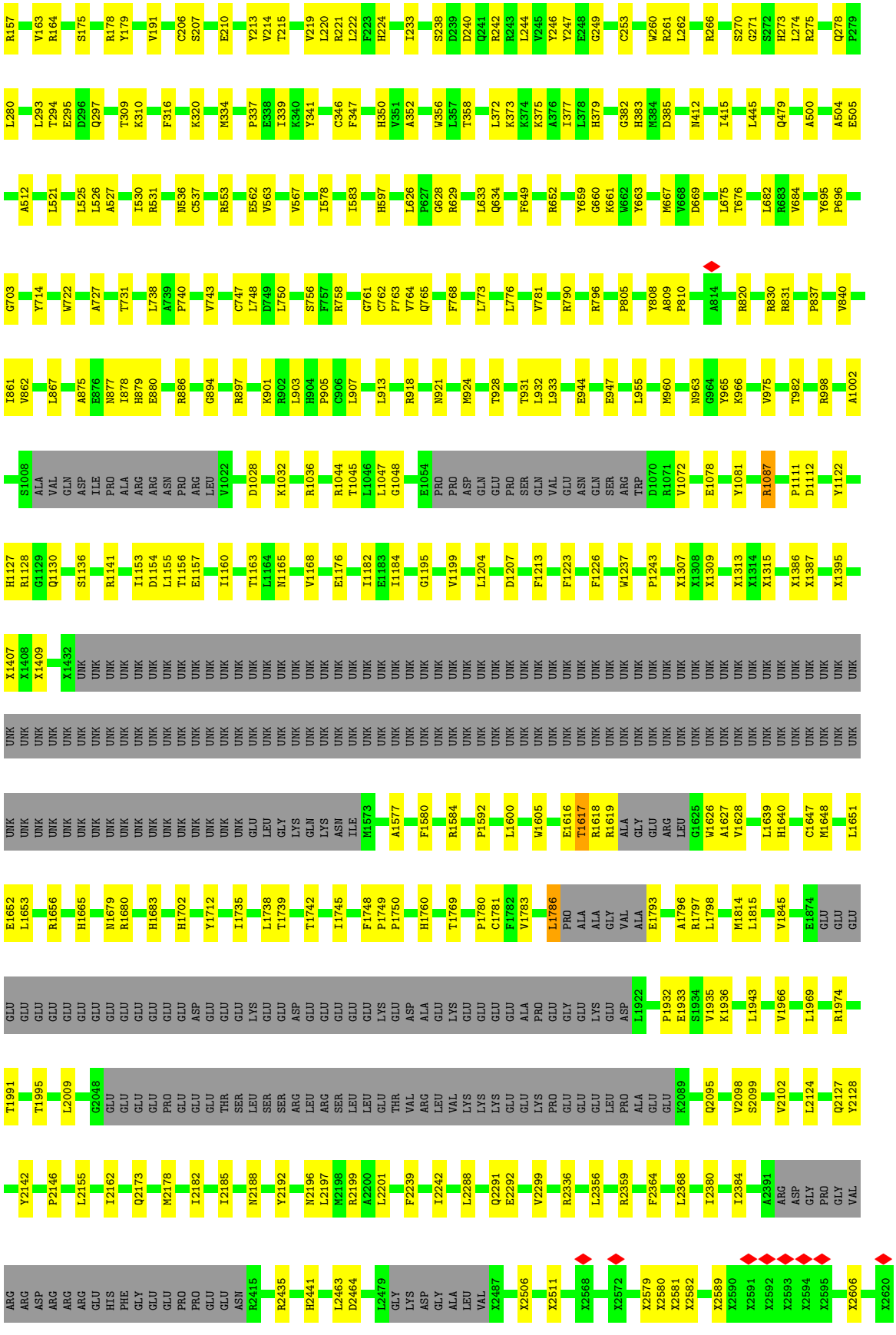


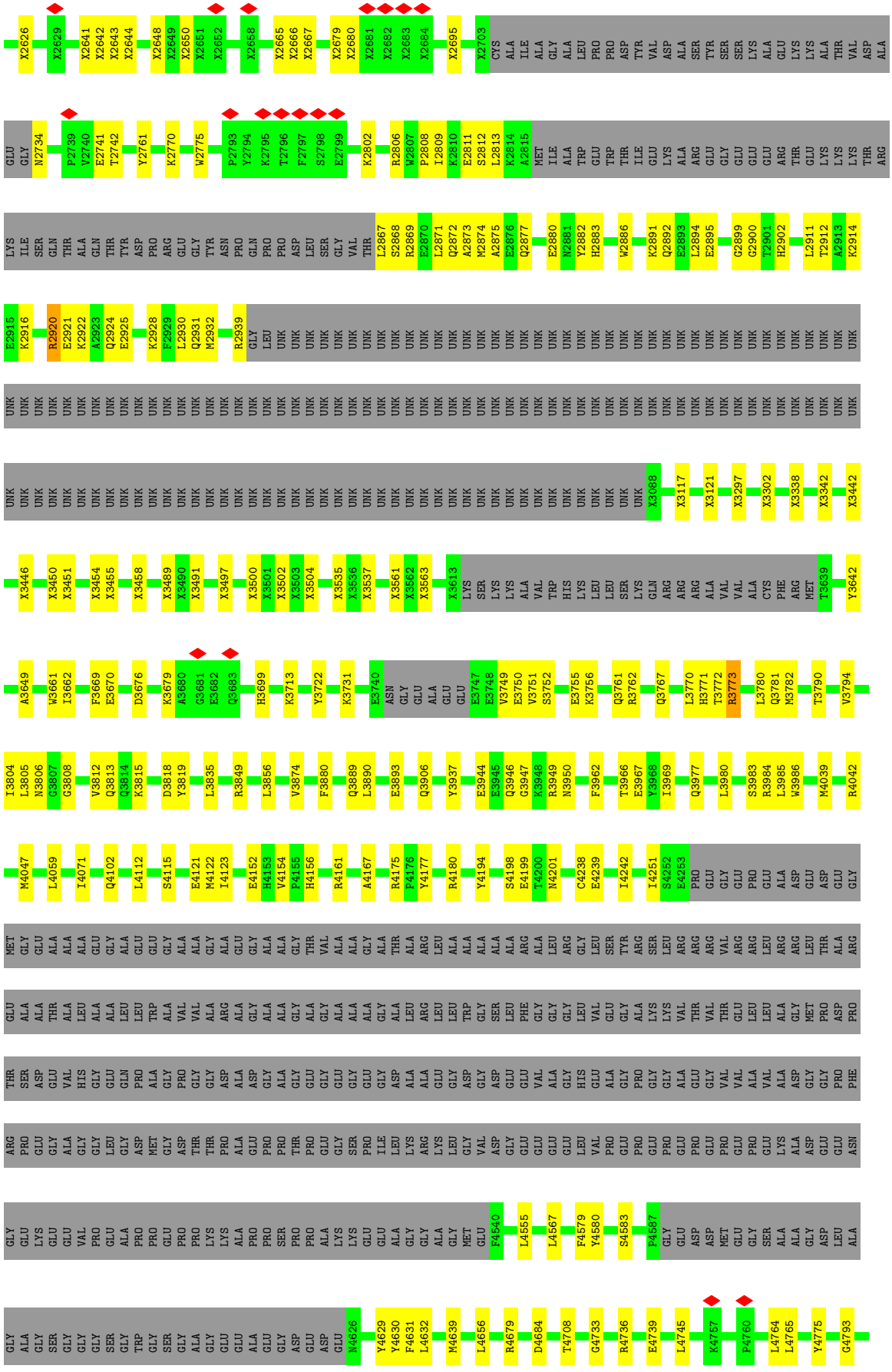


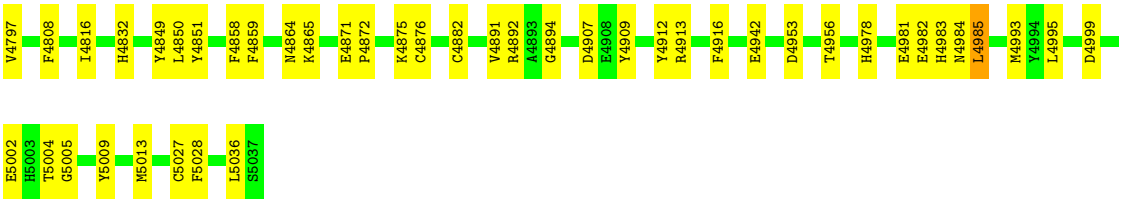
• Molecule 1: Ryanodine receptor 1,RyR1

Chain B:








V4797
F4808
I4816
H4832
Y4849
L4850
Y4851
F4858
F4859
N4864
K4865
E4871
P4872
K4875
C4876
C4882
V4891
R4892
A4893
G4894
D4907
F4908
Y4909
Y4912
R4913
F4916
E4942
D4953
T4956
H4978
E4981
E4982
H4983
N4984
L4985
M4993
Y4994
L4995
D4999
E5002
H5003
T5004
G5005
Y5009
M5013
C5027
F5028
L5036
S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	90530	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 ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	477.36002, 477.36002, 477.36002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/25300	0.49	2/34345 (0.0%)
1	B	0.26	0/25299	0.49	2/34344 (0.0%)
1	C	0.26	0/25297	0.50	3/34342 (0.0%)
1	D	0.26	0/25281	0.50	4/34322 (0.0%)
All	All	0.26	0/101177	0.50	11/137353 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1618	ARG	O-C-N	-13.63	100.89	122.70
1	C	1618	ARG	O-C-N	-5.73	113.53	122.70
1	C	4985	LEU	CA-CB-CG	5.69	128.38	115.30
1	D	4895	GLY	C-N-CA	-5.34	111.09	122.30
1	B	4985	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	4985	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	4985	LEU	CA-CB-CG	5.15	127.15	115.30
1	D	1112	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	1112	ASP	CB-CG-OD1	5.06	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1112	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	1112	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1617	THR	Mainchain
1	C	1618	ARG	Mainchain
1	D	1618	ARG	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29247	0	24751	396	0
1	B	29246	0	24757	415	0
1	C	29244	0	24747	378	0
1	D	29228	0	24714	404	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	31	0	14	1	0
4	B	31	0	14	1	0
4	C	31	0	14	2	0
4	D	31	0	14	1	0
5	A	61	0	85	18	0
5	B	61	0	85	19	0
5	C	77	0	105	17	0
5	D	45	0	65	16	0
All	All	117345	0	99365	1592	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 (1592) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4858:PHE:CE2	5:A:5106:POV:H33A	1.60	1.36
1:B:4858:PHE:CE2	5:B:5106:POV:H33A	1.60	1.36
1:D:4858:PHE:CE2	5:D:5105:POV:H33A	1.59	1.36
1:D:1618:ARG:O	1:D:1626:TRP:HA	1.12	1.29
1:D:1618:ARG:O	1:D:1626:TRP:CA	1.91	1.17
1:A:1680:ARG:HB2	1:A:1796:ALA:HB1	1.29	1.12
1:A:1619:ARG:HA	1:A:1626:TRP:HA	1.31	1.04
1:D:648:ILE:HD11	1:D:821:LEU:HD11	1.40	1.02
1:D:647:ASN:OD1	1:D:821:LEU:HA	1.59	1.01
1:A:4858:PHE:CE2	5:A:5106:POV:C33	2.45	1.00
1:A:3722:TYR:CZ	1:A:3782:MET:CE	2.45	0.99
1:B:4858:PHE:CE2	5:B:5106:POV:C33	2.45	0.99
1:A:3722:TYR:CE2	1:A:3782:MET:HE3	1.96	0.99
1:D:4858:PHE:CE2	5:D:5105:POV:C33	2.44	0.98
1:B:1680:ARG:HB2	1:B:1796:ALA:CB	1.94	0.97
1:B:4858:PHE:CD2	5:B:5106:POV:H33A	2.02	0.95
1:A:4858:PHE:CD2	5:A:5106:POV:H33A	2.02	0.94
5:A:5106:POV:H13A	1:B:4629:TYR:CZ	2.02	0.94
1:A:1619:ARG:C	1:A:1626:TRP:H	1.70	0.94
1:A:4629:TYR:CZ	5:D:5105:POV:H13A	2.03	0.93
1:D:4858:PHE:CD2	5:D:5105:POV:H33A	2.02	0.93
1:C:4629:TYR:CZ	5:B:5106:POV:H13A	2.03	0.92
1:A:1680:ARG:HB2	1:A:1796:ALA:CB	2.01	0.90
1:A:3722:TYR:CE2	1:A:3782:MET:CE	2.54	0.90
1:A:1618:ARG:O	1:A:1627:ALA:N	2.04	0.90
5:C:5106:POV:H13A	1:D:4629:TYR:CZ	2.05	0.89
1:A:3722:TYR:CE1	1:A:3782:MET:HE2	2.08	0.88
1:A:4808:PHE:CE1	5:A:5105:POV:H35	2.08	0.87
1:B:1618:ARG:O	1:B:1626:TRP:HA	1.74	0.87
1:A:2867:LEU:CB	1:A:2872:GLN:OE1	2.22	0.86
1:C:1795:PRO:O	1:C:1797:ARG:N	2.09	0.85
1:A:3722:TYR:CZ	1:A:3782:MET:HE2	2.10	0.84
1:C:1786:LEU:HD23	1:C:1786:LEU:H	1.42	0.83
1:C:4808:PHE:CE1	5:C:5105:POV:H35	2.13	0.82
1:C:633:LEU:HD23	1:C:1639:LEU:HD21	1.62	0.82
1:A:2867:LEU:CB	1:A:2872:GLN:CD	2.48	0.82
1:B:4858:PHE:CD2	5:B:5106:POV:C33	2.63	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:5107:POV:H35	1:D:4808:PHE:CE1	2.15	0.82
1:A:4858:PHE:CD2	5:A:5106:POV:C33	2.63	0.81
1:D:4858:PHE:CD2	5:D:5105:POV:C33	2.63	0.81
1:C:4851:TYR:HE1	5:C:5106:POV:H312	1.46	0.81
1:D:4888:TYR:O	1:D:4892:ARG:NH1	2.13	0.80
1:A:2581:UNK:HA	1:A:2895:GLU:HG3	1.64	0.80
1:C:4858:PHE:CD2	5:C:5106:POV:H33A	2.16	0.80
1:A:4808:PHE:HE1	5:A:5105:POV:H35	1.45	0.80
1:B:2581:UNK:HA	1:B:2895:GLU:HG3	1.64	0.80
1:C:2581:UNK:HA	1:C:2895:GLU:HG3	1.64	0.79
1:D:2581:UNK:HA	1:D:2895:GLU:HG3	1.64	0.79
1:C:2806:ARG:HH21	1:C:2808:PRO:HG3	1.48	0.79
1:D:4865:LYS:H	1:D:4875:LYS:HE2	1.47	0.79
1:B:4808:PHE:CE1	5:B:5105:POV:H35	2.18	0.79
1:A:2806:ARG:HH21	1:A:2808:PRO:HG3	1.48	0.78
1:A:3722:TYR:CZ	1:A:3782:MET:HE3	2.14	0.78
1:A:293:LEU:HD11	1:A:297:GLN:H	1.49	0.78
1:A:1796:ALA:O	1:A:1797:ARG:HB2	1.82	0.78
1:D:2806:ARG:HH21	1:D:2808:PRO:HG3	1.48	0.78
1:B:1619:ARG:HA	1:B:1626:TRP:HA	1.66	0.77
1:B:2874:MET:HA	1:B:2877:GLN:HB3	1.65	0.77
1:B:293:LEU:HD11	1:B:297:GLN:H	1.49	0.77
1:D:293:LEU:HD11	1:D:297:GLN:H	1.49	0.77
1:B:2806:ARG:HH21	1:B:2808:PRO:HG3	1.48	0.77
1:A:2874:MET:HA	1:A:2877:GLN:HB3	1.65	0.77
1:C:293:LEU:HD11	1:C:297:GLN:H	1.49	0.76
1:D:793:LEU:HD13	1:D:821:LEU:HD21	1.67	0.76
1:A:1619:ARG:CA	1:A:1626:TRP:HA	2.14	0.76
1:D:648:ILE:CD1	1:D:821:LEU:HD11	2.17	0.75
5:C:5106:POV:C13	1:D:4629:TYR:CZ	2.68	0.75
1:A:1680:ARG:CB	1:A:1796:ALA:HB1	2.13	0.75
1:B:4858:PHE:HE2	5:B:5106:POV:H33A	1.49	0.75
1:C:4808:PHE:HE1	5:C:5105:POV:H35	1.50	0.74
1:A:2867:LEU:O	1:A:2868:SER:O	2.06	0.73
1:C:1680:ARG:HB2	1:C:1796:ALA:HB1	1.71	0.73
1:B:1781:CYS:SG	1:B:1783:VAL:HG23	2.27	0.73
1:B:3722:TYR:CE2	1:B:3782:MET:CE	2.71	0.73
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.70	0.73
1:C:1078:GLU:OE2	1:C:1237:TRP:NE1	2.21	0.73
1:A:1078:GLU:OE2	1:A:1237:TRP:NE1	2.21	0.73
1:B:3722:TYR:CZ	1:B:3782:MET:HE2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4851:TYR:HE1	5:B:5106:POV:H312	1.52	0.73
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.70	0.72
1:A:894:GLY:HA3	1:A:903:LEU:HB3	1.70	0.72
1:C:4865:LYS:H	1:C:4875:LYS:HE2	1.52	0.72
1:B:2868:SER:O	1:B:2872:GLN:NE2	2.21	0.72
1:C:1616:GLU:O	1:C:1628:VAL:HA	1.90	0.72
1:B:894:GLY:HA3	1:B:903:LEU:HB3	1.70	0.72
1:B:4865:LYS:H	1:B:4875:LYS:HE2	1.54	0.72
1:A:2868:SER:O	1:A:2872:GLN:NE2	2.23	0.72
5:A:5106:POV:C13	1:B:4629:TYR:CZ	2.72	0.72
1:C:1786:LEU:HD23	1:C:1786:LEU:N	2.04	0.72
1:C:4629:TYR:CZ	5:B:5106:POV:C13	2.73	0.72
5:C:5107:POV:H35	1:D:4808:PHE:HE1	1.54	0.71
4:A:5104:ACP:O3G	4:A:5104:ACP:O2B	2.09	0.70
1:B:3722:TYR:CE2	1:B:3782:MET:HE3	2.25	0.70
4:C:5104:ACP:O3G	4:C:5104:ACP:O2B	2.09	0.70
1:B:4808:PHE:HE1	5:B:5105:POV:H35	1.56	0.70
1:D:2868:SER:O	1:D:2872:GLN:NE2	2.25	0.70
1:B:982:THR:O	1:B:1036:ARG:NH1	2.25	0.70
1:B:1618:ARG:O	1:B:1626:TRP:CA	2.40	0.70
1:D:982:THR:O	1:D:1036:ARG:NH1	2.25	0.70
4:D:5104:ACP:O3G	4:D:5104:ACP:O2B	2.09	0.70
1:A:982:THR:O	1:A:1036:ARG:NH1	2.25	0.69
1:A:4629:TYR:CZ	5:D:5105:POV:C13	2.73	0.69
1:C:2868:SER:O	1:C:2872:GLN:NE2	2.25	0.69
1:A:840:VAL:HG12	1:A:1199:VAL:HG22	1.74	0.69
1:D:2874:MET:HA	1:D:2877:GLN:HB3	1.74	0.69
1:C:982:THR:O	1:C:1036:ARG:NH1	2.25	0.69
1:A:4858:PHE:HE2	5:A:5106:POV:H33A	1.49	0.69
1:C:2874:MET:HA	1:C:2877:GLN:HB3	1.74	0.69
4:B:5104:ACP:O2B	4:B:5104:ACP:O3G	2.09	0.69
1:D:4851:TYR:HE1	5:D:5105:POV:H312	1.57	0.69
1:B:840:VAL:HG12	1:B:1199:VAL:HG22	1.75	0.69
1:A:3722:TYR:CE1	1:A:3782:MET:CE	2.75	0.69
1:C:4851:TYR:CE1	5:C:5106:POV:H312	2.28	0.69
1:D:647:ASN:OD1	1:D:821:LEU:CA	2.39	0.68
1:D:633:LEU:HD23	1:D:1639:LEU:HD21	1.75	0.68
1:A:1796:ALA:O	1:A:1797:ARG:CB	2.40	0.68
1:B:3722:TYR:CE1	1:B:3782:MET:HE2	2.28	0.68
1:A:633:LEU:HD23	1:A:1639:LEU:HD21	1.76	0.68
1:C:1619:ARG:C	1:C:1626:TRP:HA	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:TYR:O	1:C:373:LYS:NZ	2.27	0.68
1:C:684:VAL:HG12	1:C:781:VAL:HG22	1.76	0.68
1:D:684:VAL:HG12	1:D:781:VAL:HG22	1.76	0.68
1:C:1786:LEU:H	1:C:1786:LEU:CD2	2.06	0.68
1:C:2581:UNK:N	1:C:2899:GLY:O	2.27	0.68
1:D:1078:GLU:OE2	1:D:1237:TRP:NE1	2.27	0.68
1:B:684:VAL:HG12	1:B:781:VAL:HG22	1.76	0.68
1:A:2581:UNK:N	1:A:2899:GLY:O	2.28	0.67
1:C:840:VAL:HG12	1:C:1199:VAL:HG22	1.75	0.67
1:D:623:GLU:CB	1:D:1786:LEU:O	2.43	0.67
1:D:840:VAL:HG12	1:D:1199:VAL:HG22	1.75	0.67
1:D:1679:ASN:CG	1:D:1798:LEU:O	2.32	0.67
1:B:1078:GLU:OE2	1:B:1237:TRP:NE1	2.28	0.67
1:C:4555:LEU:HD22	1:C:4656:LEU:HD11	1.77	0.67
1:A:1619:ARG:C	1:A:1626:TRP:N	2.47	0.66
1:B:3722:TYR:CZ	1:B:3782:MET:CE	2.78	0.66
1:D:2581:UNK:N	1:D:2899:GLY:O	2.28	0.66
1:B:633:LEU:HD23	1:B:1639:LEU:HD21	1.78	0.66
1:B:2581:UNK:N	1:B:2899:GLY:O	2.28	0.66
1:A:537:CYS:HB2	1:A:567:VAL:HG23	1.78	0.66
5:C:5106:POV:H13A	1:D:4629:TYR:CE1	2.29	0.66
1:B:537:CYS:HB2	1:B:567:VAL:HG23	1.78	0.66
1:A:684:VAL:HG12	1:A:781:VAL:HG22	1.78	0.66
1:A:1653:LEU:HD12	1:A:1656:ARG:HG3	1.78	0.66
1:A:4555:LEU:HD22	1:A:4656:LEU:HD11	1.77	0.65
1:B:500:ALA:H	1:B:504:ALA:HB3	1.60	0.65
1:B:2809:ILE:HD12	1:B:2813:LEU:HD11	1.79	0.65
1:C:1653:LEU:HD12	1:C:1656:ARG:HG3	1.78	0.65
1:D:247:TYR:O	1:D:373:LYS:NZ	2.30	0.65
1:D:537:CYS:HB2	1:D:567:VAL:HG23	1.78	0.65
1:C:537:CYS:HB2	1:C:567:VAL:HG23	1.79	0.65
1:A:247:TYR:O	1:A:373:LYS:NZ	2.30	0.64
1:D:2809:ILE:HD12	1:D:2813:LEU:HD11	1.79	0.64
1:C:2809:ILE:HD12	1:C:2813:LEU:HD11	1.79	0.64
1:D:669:ASP:HA	1:D:740:PRO:HA	1.80	0.64
1:B:4555:LEU:HD22	1:B:4656:LEU:HD11	1.80	0.64
1:B:1653:LEU:HD12	1:B:1656:ARG:HG3	1.80	0.64
1:B:1786:LEU:HD13	1:B:1786:LEU:H	1.61	0.64
1:A:1618:ARG:O	1:A:1626:TRP:C	2.36	0.64
1:D:500:ALA:H	1:D:504:ALA:HB3	1.63	0.64
1:D:4858:PHE:HE2	5:D:5105:POV:H33A	1.48	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:ASP:HA	1:B:740:PRO:HA	1.80	0.64
1:A:2582:UNK:O	1:A:2899:GLY:N	2.31	0.64
1:D:1653:LEU:HD12	1:D:1656:ARG:HG3	1.80	0.64
1:A:669:ASP:HA	1:A:740:PRO:HA	1.80	0.64
1:A:4832:HIS:NE2	1:A:4942:GLU:OE1	2.31	0.64
1:A:4851:TYR:HE1	5:A:5106:POV:H312	1.62	0.64
1:C:667:MET:HG3	1:C:790:ARG:HH21	1.63	0.64
1:D:4115:SER:HB2	1:D:4123:ILE:HG21	1.80	0.64
1:B:2928:LYS:O	1:B:2931:GLN:NE2	2.31	0.64
1:A:944:GLU:HA	1:A:947:GLU:HB2	1.80	0.64
1:D:4555:LEU:HD22	1:D:4656:LEU:HD11	1.80	0.64
1:B:206:CYS:HB3	1:B:271:GLY:HA3	1.80	0.64
1:C:669:ASP:HA	1:C:740:PRO:HA	1.80	0.63
1:C:2582:UNK:O	1:C:2899:GLY:N	2.31	0.63
1:C:2928:LYS:O	1:C:2931:GLN:NE2	2.31	0.63
1:C:49:LEU:HD11	1:C:191:VAL:HG13	1.79	0.63
1:C:500:ALA:H	1:C:504:ALA:HB3	1.63	0.63
1:D:2582:UNK:O	1:D:2899:GLY:N	2.31	0.63
1:B:1680:ARG:CB	1:B:1796:ALA:CB	2.75	0.63
1:A:531:ARG:NH2	1:A:562:GLU:OE1	2.32	0.63
1:D:531:ARG:NH2	1:D:562:GLU:OE1	2.31	0.63
1:B:1680:ARG:HB2	1:B:1796:ALA:HB2	1.80	0.63
1:A:2809:ILE:HD12	1:A:2813:LEU:HD11	1.79	0.63
1:D:944:GLU:HA	1:D:947:GLU:HB2	1.80	0.63
1:D:2928:LYS:O	1:D:2931:GLN:NE2	2.31	0.63
1:A:4115:SER:HB2	1:A:4123:ILE:HG21	1.81	0.63
1:B:4832:HIS:NE2	1:B:4942:GLU:OE1	2.31	0.63
1:A:49:LEU:HD11	1:A:191:VAL:HG13	1.80	0.63
1:A:2928:LYS:O	1:A:2931:GLN:NE2	2.31	0.63
1:A:206:CYS:HB3	1:A:271:GLY:HA3	1.81	0.63
1:B:531:ARG:NH2	1:B:562:GLU:OE1	2.32	0.63
1:A:4629:TYR:OH	5:D:5105:POV:H13A	1.98	0.63
1:C:531:ARG:NH2	1:C:562:GLU:OE1	2.31	0.63
1:C:3770:LEU:HD22	1:C:3804:ILE:HD11	1.80	0.62
1:C:4832:HIS:NE2	1:C:4942:GLU:OE1	2.31	0.62
1:D:667:MET:HG3	1:D:790:ARG:HH21	1.63	0.62
1:D:4832:HIS:NE2	1:D:4942:GLU:OE1	2.32	0.62
1:B:667:MET:HG3	1:B:790:ARG:HH21	1.62	0.62
1:B:4892:ARG:HH21	1:B:4892:ARG:HG3	1.63	0.62
1:B:247:TYR:O	1:B:373:LYS:NZ	2.30	0.62
1:B:4115:SER:HB2	1:B:4123:ILE:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3770:LEU:HD22	1:A:3804:ILE:HD11	1.80	0.62
1:C:4925:ILE:O	1:C:4929:LEU:HB2	2.00	0.62
1:D:3770:LEU:HD22	1:D:3804:ILE:HD11	1.80	0.62
1:B:3770:LEU:HD22	1:B:3804:ILE:HD11	1.80	0.62
1:A:500:ALA:H	1:A:504:ALA:HB3	1.63	0.62
1:A:527:ALA:HB2	1:A:563:VAL:HG22	1.82	0.62
1:D:49:LEU:HD11	1:D:191:VAL:HG13	1.79	0.62
1:D:1618:ARG:CB	1:D:1627:ALA:O	2.48	0.62
1:C:944:GLU:HA	1:C:947:GLU:HB2	1.80	0.62
1:D:527:ALA:HB2	1:D:563:VAL:HG22	1.82	0.62
5:A:5106:POV:H13A	1:B:4629:TYR:OH	1.99	0.62
1:C:4629:TYR:CE1	5:B:5106:POV:H13A	2.34	0.62
1:B:49:LEU:HD11	1:B:191:VAL:HG13	1.81	0.62
1:C:206:CYS:HB3	1:C:271:GLY:HA3	1.82	0.62
1:C:358:THR:HG21	1:C:383:HIS:HB2	1.82	0.62
1:B:2582:UNK:O	1:B:2899:GLY:N	2.32	0.62
1:A:4238:CYS:O	1:A:4242:ILE:HG12	2.00	0.61
1:D:206:CYS:HB3	1:D:271:GLY:HA3	1.81	0.61
1:A:280:LEU:HD11	1:A:316:PHE:HE1	1.65	0.61
1:A:1163:THR:HG22	1:A:1168:VAL:HA	1.82	0.61
1:D:358:THR:HG21	1:D:383:HIS:HB2	1.82	0.61
1:B:652:ARG:HD3	1:B:750:LEU:HD13	1.82	0.61
1:C:652:ARG:HD3	1:C:750:LEU:HD13	1.82	0.61
1:C:280:LEU:HD11	1:C:316:PHE:HE1	1.64	0.61
1:D:4889:VAL:O	1:D:4893:ALA:HB2	2.01	0.61
1:B:1163:THR:HG22	1:B:1168:VAL:HA	1.83	0.61
1:A:358:THR:HG21	1:A:383:HIS:HB2	1.83	0.60
1:C:527:ALA:HB2	1:C:563:VAL:HG22	1.82	0.60
1:D:1163:THR:HG22	1:D:1168:VAL:HA	1.83	0.60
1:B:280:LEU:HD11	1:B:316:PHE:HE1	1.65	0.60
1:A:652:ARG:HD3	1:A:750:LEU:HD13	1.82	0.60
1:D:280:LEU:HD11	1:D:316:PHE:HE1	1.65	0.60
1:D:652:ARG:HD3	1:D:750:LEU:HD13	1.82	0.60
1:C:1163:THR:HG22	1:C:1168:VAL:HA	1.83	0.60
1:C:4857:ASN:ND2	5:C:5106:POV:H14B	2.15	0.60
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.84	0.60
1:B:527:ALA:HB2	1:B:563:VAL:HG22	1.82	0.60
1:D:2192:TYR:HA	1:D:2242:ILE:HD11	1.84	0.60
1:C:731:THR:OG1	1:C:765:GLN:NE2	2.35	0.60
1:C:2192:TYR:HA	1:C:2242:ILE:HD11	1.83	0.60
1:B:358:THR:HG21	1:B:383:HIS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2192:TYR:HA	1:A:2242:ILE:HD11	1.83	0.60
1:D:244:LEU:HD12	1:D:375:LYS:HE2	1.83	0.60
1:C:4629:TYR:OH	5:B:5106:POV:H13A	2.01	0.60
1:D:1739:THR:HG23	1:D:1742:THR:H	1.67	0.60
1:A:1739:THR:HG23	1:A:1742:THR:H	1.67	0.60
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.84	0.60
1:C:2155:LEU:HB2	1:C:2188:ASN:HD21	1.67	0.60
1:D:1619:ARG:C	1:D:1626:TRP:H	2.05	0.60
1:A:1028:ASP:OD2	1:A:1032:LYS:N	2.35	0.59
5:A:5106:POV:H13A	1:B:4629:TYR:CE1	2.36	0.59
1:C:4915:VAL:HA	1:C:4918:ILE:HG22	1.84	0.59
1:B:244:LEU:HD12	1:B:375:LYS:HE2	1.83	0.59
1:B:2695:UNK:H	1:B:2761:TYR:HH	1.50	0.59
1:A:897:ARG:HG2	1:A:905:PRO:HD2	1.84	0.59
1:A:1619:ARG:HA	1:A:1626:TRP:CA	2.20	0.59
1:C:294:THR:HG23	1:C:295:GLU:H	1.68	0.59
1:C:1748:PHE:O	1:C:1750:PRO:HD3	2.02	0.59
1:D:3772:THR:HG23	1:D:3812:VAL:HG22	1.84	0.59
1:B:3772:THR:HG23	1:B:3812:VAL:HG22	1.84	0.59
1:A:1943:LEU:HD21	1:A:2098:VAL:HG22	1.84	0.59
1:A:4629:TYR:CE2	5:D:5105:POV:H13A	2.37	0.59
1:C:244:LEU:HD12	1:C:375:LYS:HE2	1.84	0.59
1:D:731:THR:OG1	1:D:765:GLN:NE2	2.35	0.59
1:B:1748:PHE:O	1:B:1750:PRO:HD3	2.02	0.59
1:D:897:ARG:HG2	1:D:905:PRO:HD2	1.84	0.59
1:B:1943:LEU:HD21	1:B:2098:VAL:HG22	1.85	0.59
1:B:4239:GLU:OE2	1:B:4679:ARG:NH2	2.34	0.59
1:A:3772:THR:HG23	1:A:3812:VAL:HG22	1.84	0.59
1:A:4198:SER:OG	1:A:4201:ASN:ND2	2.35	0.59
1:C:4579:PHE:HB2	1:C:4639:MET:SD	2.42	0.59
1:B:1028:ASP:OD2	1:B:1032:LYS:N	2.35	0.59
1:A:1748:PHE:O	1:A:1750:PRO:HD3	2.02	0.59
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.84	0.59
1:B:897:ARG:HG2	1:B:905:PRO:HD2	1.85	0.59
1:D:1616:GLU:O	1:D:1628:VAL:HA	2.02	0.59
1:C:4708:THR:HG21	1:C:4775:TYR:HB2	1.85	0.59
1:C:4858:PHE:CE2	5:C:5106:POV:H33A	2.38	0.59
1:D:294:THR:HG23	1:D:295:GLU:H	1.68	0.59
1:D:1072:VAL:HG12	1:D:1195:GLY:HA2	1.85	0.59
1:D:4708:THR:HG21	1:D:4775:TYR:HB2	1.85	0.59
1:B:294:THR:HG23	1:B:295:GLU:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1739:THR:HG23	1:B:1742:THR:H	1.67	0.59
1:B:2192:TYR:HA	1:B:2242:ILE:HD11	1.84	0.59
1:C:1739:THR:HG23	1:C:1742:THR:H	1.67	0.59
1:C:2359:ARG:NH2	1:B:179:TYR:OH	2.36	0.59
1:D:2155:LEU:HB2	1:D:2188:ASN:HD21	1.68	0.59
1:D:2770:LYS:HD2	1:D:2775:TRP:HB2	1.85	0.59
1:A:244:LEU:HD12	1:A:375:LYS:HE2	1.84	0.59
1:A:731:THR:OG1	1:A:765:GLN:NE2	2.34	0.59
1:A:4865:LYS:HG2	1:A:4875:LYS:HE3	1.84	0.59
1:A:4892:ARG:NH1	1:D:4917:ASP:OD2	2.36	0.59
1:C:29:LEU:HG	1:C:31:GLU:H	1.68	0.59
1:B:2155:LEU:HB2	1:B:2188:ASN:HD21	1.68	0.59
1:A:294:THR:HG23	1:A:295:GLU:H	1.68	0.58
1:A:4067:LYS:HD3	1:A:4102:GLN:HG3	1.84	0.58
1:C:4239:GLU:OE2	1:C:4679:ARG:NH2	2.34	0.58
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.84	0.58
1:C:2196:ASN:OD1	1:C:2199:ARG:NH2	2.37	0.58
1:D:1748:PHE:O	1:D:1750:PRO:HD3	2.02	0.58
1:B:2770:LYS:HD2	1:B:2775:TRP:HB2	1.85	0.58
1:C:897:ARG:HG2	1:C:905:PRO:HD2	1.84	0.58
1:D:1028:ASP:OD2	1:D:1032:LYS:N	2.36	0.58
1:C:1943:LEU:HD21	1:C:2098:VAL:HG22	1.84	0.58
1:B:731:THR:OG1	1:B:765:GLN:NE2	2.35	0.58
1:B:1786:LEU:H	1:B:1786:LEU:CD1	2.16	0.58
1:A:1072:VAL:HG12	1:A:1195:GLY:HA2	1.86	0.58
1:C:3772:THR:HG23	1:C:3812:VAL:HG22	1.84	0.58
1:B:4978:HIS:CE1	1:B:4983:HIS:NE2	2.71	0.58
1:A:29:LEU:HG	1:A:31:GLU:H	1.69	0.58
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.36	0.58
1:A:2770:LYS:HD2	1:A:2775:TRP:HB2	1.85	0.58
1:A:4799:SER:HB2	1:A:4812:HIS:HE1	1.68	0.58
1:C:4115:SER:HB2	1:C:4123:ILE:HG21	1.85	0.58
1:B:29:LEU:HG	1:B:31:GLU:H	1.69	0.58
1:A:667:MET:HG3	1:A:790:ARG:HH21	1.67	0.58
1:C:3874:VAL:HG11	1:C:3950:ASN:ND2	2.19	0.58
1:D:1243:PRO:HB2	1:D:1600:LEU:HD11	1.86	0.58
1:D:4799:SER:HB2	1:D:4812:HIS:HE1	1.67	0.58
1:D:4858:PHE:HE2	5:D:5105:POV:C33	2.10	0.58
1:B:224:HIS:NE2	1:B:385:ASP:O	2.37	0.58
1:B:1786:LEU:C	1:B:1786:LEU:HD22	2.23	0.58
1:A:179:TYR:OH	1:B:2359:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3770:LEU:HD23	1:C:3770:LEU:O	2.04	0.58
1:A:3874:VAL:HG11	1:A:3950:ASN:ND2	2.19	0.58
1:A:4239:GLU:OE2	1:A:4679:ARG:NH2	2.34	0.58
1:C:1028:ASP:OD2	1:C:1032:LYS:N	2.36	0.58
1:C:1619:ARG:C	1:C:1626:TRP:CA	2.72	0.58
1:B:1072:VAL:HG12	1:B:1195:GLY:HA2	1.85	0.58
1:B:4198:SER:OG	1:B:4201:ASN:ND2	2.37	0.58
1:A:4708:THR:HG21	1:A:4775:TYR:HB2	1.85	0.58
1:D:29:LEU:HG	1:D:31:GLU:H	1.69	0.58
1:D:1943:LEU:HD21	1:D:2098:VAL:HG22	1.84	0.58
1:D:4239:GLU:OE2	1:D:4679:ARG:NH2	2.33	0.58
1:D:4864:ASN:OD1	1:D:4875:LYS:NZ	2.33	0.58
1:B:56:GLN:O	1:B:309:THR:OG1	2.22	0.58
1:B:4708:THR:HG21	1:B:4775:TYR:HB2	1.85	0.58
1:A:830:ARG:HH21	1:A:837:PRO:HB3	1.69	0.57
1:A:2155:LEU:HB2	1:A:2188:ASN:HD21	1.69	0.57
1:A:2589:UNK:O	1:A:2734:ASN:ND2	2.37	0.57
1:C:179:TYR:OH	1:D:2359:ARG:NH2	2.36	0.57
1:D:2589:UNK:O	1:D:2734:ASN:ND2	2.37	0.57
1:D:4859:PHE:HE1	1:D:4909:TYR:HD2	1.52	0.57
1:A:3770:LEU:HD23	1:A:3770:LEU:O	2.04	0.57
1:A:4865:LYS:H	1:A:4875:LYS:HE2	1.69	0.57
1:B:663:TYR:HB3	1:B:809:ALA:HB2	1.86	0.57
1:A:2506:UNK:O	1:A:2511:UNK:N	2.38	0.57
1:C:1243:PRO:HB2	1:C:1600:LEU:HD11	1.86	0.57
1:C:2589:UNK:O	1:C:2734:ASN:ND2	2.37	0.57
1:C:2770:LYS:HD2	1:C:2775:TRP:HB2	1.85	0.57
1:D:1044:ARG:HA	1:D:1047:LEU:HD22	1.86	0.57
1:D:3874:VAL:HG11	1:D:3950:ASN:ND2	2.19	0.57
1:D:4184:MET:HB3	1:D:4190:ILE:HD13	1.85	0.57
1:B:861:ILE:HG23	1:B:862:VAL:HG13	1.85	0.57
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.37	0.57
1:B:3874:VAL:HG11	1:B:3950:ASN:ND2	2.20	0.57
1:A:663:TYR:HB3	1:A:809:ALA:HB2	1.86	0.57
1:C:2506:UNK:O	1:C:2511:UNK:N	2.38	0.57
1:D:2506:UNK:O	1:D:2511:UNK:N	2.38	0.57
1:B:1781:CYS:SG	1:B:1783:VAL:CG2	2.92	0.57
1:B:2642:UNK:N	1:B:2872:GLN:HB2	2.19	0.57
1:B:2644:UNK:H	1:B:2872:GLN:HA	1.69	0.57
1:B:2916:LYS:HG3	1:B:2920:ARG:HE	1.70	0.57
1:A:1044:ARG:HA	1:A:1047:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2291:GLN:O	1:A:2292:GLU:HG3	2.05	0.57
1:D:224:HIS:NE2	1:D:385:ASP:O	2.37	0.57
1:B:2589:UNK:O	1:B:2734:ASN:ND2	2.37	0.57
1:B:3806:ASN:HA	1:B:3890:LEU:HD21	1.86	0.57
1:B:4859:PHE:HE1	1:B:4909:TYR:HD2	1.53	0.57
1:B:1793:GLU:CB	1:B:2173:GLN:CG	2.83	0.57
1:A:4859:PHE:HE1	1:A:4909:TYR:HD2	1.53	0.57
1:C:1155:LEU:HD13	1:C:1184:ILE:HD12	1.86	0.57
1:D:663:TYR:HB3	1:D:809:ALA:HB2	1.86	0.57
1:D:2291:GLN:O	1:D:2292:GLU:HG3	2.05	0.57
1:B:1619:ARG:HA	1:B:1626:TRP:CA	2.35	0.57
1:C:663:TYR:HB3	1:C:809:ALA:HB2	1.86	0.57
1:D:830:ARG:HH21	1:D:837:PRO:HB3	1.70	0.57
1:D:3806:ASN:HA	1:D:3890:LEU:HD21	1.87	0.57
1:A:1155:LEU:HD13	1:A:1184:ILE:HD12	1.86	0.56
1:A:3806:ASN:HA	1:A:3890:LEU:HD21	1.87	0.56
1:C:1072:VAL:HG12	1:C:1195:GLY:HA2	1.85	0.56
1:C:2291:GLN:O	1:C:2292:GLU:HG3	2.05	0.56
1:D:1798:LEU:N	1:D:1798:LEU:HD22	2.20	0.56
1:B:2291:GLN:O	1:B:2292:GLU:HG3	2.05	0.56
1:A:379:HIS:CD2	1:A:382:GLY:H	2.24	0.56
1:C:830:ARG:HH21	1:C:837:PRO:HB3	1.70	0.56
1:C:1933:GLU:HA	1:C:1936:LYS:HD3	1.87	0.56
1:C:4198:SER:OG	1:C:4201:ASN:ND2	2.39	0.56
1:A:379:HIS:HD2	1:A:382:GLY:H	1.53	0.56
1:A:1243:PRO:HB2	1:A:1600:LEU:HD11	1.86	0.56
1:C:2742:THR:HG23	1:C:2811:GLU:HG2	1.88	0.56
1:C:3806:ASN:HA	1:C:3890:LEU:HD21	1.87	0.56
1:D:379:HIS:CD2	1:D:382:GLY:H	2.24	0.56
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.37	0.56
1:B:578:ILE:HD12	1:B:583:ILE:HD11	1.87	0.56
1:B:830:ARG:HH21	1:B:837:PRO:HB3	1.69	0.56
1:B:2364:PHE:HB3	1:B:2368:LEU:HD23	1.87	0.56
1:A:3752:SER:N	1:A:3755:GLU:OE2	2.39	0.56
1:C:2880:GLU:HA	1:C:2883:HIS:NE2	2.21	0.56
1:B:1044:ARG:HA	1:B:1047:LEU:HD22	1.86	0.56
1:B:1793:GLU:CB	1:B:2173:GLN:HG3	2.35	0.56
1:A:56:GLN:O	1:A:309:THR:OG1	2.23	0.56
1:C:56:GLN:O	1:C:309:THR:OG1	2.23	0.56
1:C:3752:SER:N	1:C:3755:GLU:OE2	2.38	0.56
1:D:56:GLN:O	1:D:309:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1155:LEU:HD13	1:D:1184:ILE:HD12	1.87	0.56
1:B:1155:LEU:HD13	1:B:1184:ILE:HD12	1.87	0.56
1:B:4912:TYR:CD2	5:B:5106:POV:H34	2.41	0.56
1:C:379:HIS:HD2	1:C:382:GLY:H	1.53	0.56
1:C:4857:ASN:HD22	5:C:5107:POV:H34	1.70	0.56
1:C:346:CYS:SG	1:C:347:PHE:N	2.79	0.56
1:C:886:ARG:HH21	1:C:907:LEU:HD13	1.71	0.56
1:D:379:HIS:HD2	1:D:382:GLY:H	1.53	0.56
1:B:886:ARG:HH21	1:B:907:LEU:HD13	1.71	0.56
1:C:379:HIS:CD2	1:C:382:GLY:H	2.24	0.56
1:C:1078:GLU:HB2	1:C:1081:TYR:HD2	1.71	0.56
1:C:2364:PHE:HB3	1:C:2368:LEU:HD23	1.88	0.56
1:C:2916:LYS:HG3	1:C:2920:ARG:HE	1.70	0.56
1:B:5009:TYR:CZ	1:B:5013:MET:HE2	2.41	0.56
1:A:877:ASN:HD22	1:A:1045:THR:HG21	1.70	0.56
1:A:1933:GLU:HA	1:A:1936:LYS:HD3	1.87	0.56
1:C:4858:PHE:CD2	5:C:5106:POV:C33	2.88	0.56
1:D:578:ILE:HD12	1:D:583:ILE:HD11	1.87	0.56
1:D:886:ARG:HH21	1:D:907:LEU:HD13	1.71	0.56
1:B:2506:UNK:O	1:B:2511:UNK:N	2.38	0.56
1:B:2742:THR:HG23	1:B:2811:GLU:HG2	1.88	0.56
1:B:4238:CYS:O	1:B:4242:ILE:HG12	2.06	0.56
1:A:886:ARG:HH21	1:A:907:LEU:HD13	1.71	0.56
1:A:2916:LYS:HG3	1:A:2920:ARG:HE	1.70	0.56
1:D:1165:ASN:HA	1:D:1213:PHE:HE2	1.71	0.56
1:D:2916:LYS:HG3	1:D:2920:ARG:HE	1.70	0.56
1:D:2364:PHE:HB3	1:D:2368:LEU:HD23	1.88	0.55
1:D:4912:TYR:CD2	5:D:5105:POV:H34	2.41	0.55
1:B:4892:ARG:HG3	1:B:4892:ARG:NH2	2.22	0.55
1:A:2364:PHE:HB3	1:A:2368:LEU:HD23	1.88	0.55
1:C:1044:ARG:HA	1:C:1047:LEU:HD22	1.87	0.55
1:D:244:LEU:HG	1:D:246:TYR:HE1	1.71	0.55
1:D:913:LEU:HB2	1:D:918:ARG:HD2	1.88	0.55
1:B:346:CYS:SG	1:B:347:PHE:N	2.79	0.55
1:C:913:LEU:HB2	1:C:918:ARG:HD2	1.88	0.55
1:A:2742:THR:HG23	1:A:2811:GLU:HG2	1.87	0.55
1:D:877:ASN:HD22	1:D:1045:THR:HG21	1.70	0.55
1:A:244:LEU:HG	1:A:246:TYR:HE1	1.71	0.55
1:C:649:PHE:HB3	1:C:776:LEU:HD13	1.89	0.55
1:B:379:HIS:HD2	1:B:382:GLY:H	1.53	0.55
1:A:3450:UNK:O	1:A:3454:UNK:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2155:LEU:HB2	1:C:2188:ASN:ND2	2.21	0.55
1:C:4851:TYR:CD1	1:C:4916:PHE:HE1	2.24	0.55
1:D:346:CYS:SG	1:D:347:PHE:N	2.79	0.55
1:D:2880:GLU:HA	1:D:2883:HIS:NE2	2.21	0.55
1:B:1165:ASN:HA	1:B:1213:PHE:HE2	1.71	0.55
1:B:2155:LEU:HB2	1:B:2188:ASN:ND2	2.21	0.55
1:A:913:LEU:HB2	1:A:918:ARG:HD2	1.88	0.55
1:A:2770:LYS:HE3	1:A:2775:TRP:HE3	1.72	0.55
1:A:2880:GLU:HA	1:A:2883:HIS:NE2	2.21	0.55
1:D:2155:LEU:HB2	1:D:2188:ASN:ND2	2.21	0.55
1:B:649:PHE:HB3	1:B:776:LEU:HD13	1.89	0.55
1:C:3805:LEU:HD12	1:C:3890:LEU:HG	1.89	0.55
1:D:2665:UNK:C	1:D:2922:LYS:HZ1	2.20	0.55
1:D:2770:LYS:HE3	1:D:2775:TRP:HE3	1.71	0.55
1:B:877:ASN:HD22	1:B:1045:THR:HG21	1.71	0.55
1:B:3450:UNK:O	1:B:3454:UNK:N	2.40	0.55
1:A:346:CYS:SG	1:A:347:PHE:N	2.79	0.55
1:A:1078:GLU:HB2	1:A:1081:TYR:HD2	1.71	0.55
1:D:2695:UNK:H	1:D:2761:TYR:HH	1.52	0.55
1:C:3450:UNK:O	1:C:3454:UNK:N	2.40	0.55
1:D:901:LYS:HE3	1:D:903:LEU:HD12	1.89	0.55
1:D:3752:SER:N	1:D:3755:GLU:OE2	2.39	0.55
1:A:3676:ASP:HA	1:A:3679:LYS:HB2	1.89	0.54
1:C:126:SER:HB3	1:C:132:ALA:HB2	1.90	0.54
1:C:320:LYS:HA	1:C:356:TRP:HH2	1.72	0.54
1:C:877:ASN:HD22	1:C:1045:THR:HG21	1.71	0.54
1:C:4238:CYS:O	1:C:4242:ILE:HG12	2.07	0.54
1:B:379:HIS:CD2	1:B:382:GLY:H	2.24	0.54
1:B:913:LEU:HB2	1:B:918:ARG:HD2	1.88	0.54
1:C:901:LYS:HE3	1:C:903:LEU:HD12	1.90	0.54
1:B:3752:SER:N	1:B:3755:GLU:OE2	2.39	0.54
1:A:2155:LEU:HB2	1:A:2188:ASN:ND2	2.22	0.54
1:A:3722:TYR:CD2	1:A:3782:MET:CE	2.90	0.54
1:B:244:LEU:HG	1:B:246:TYR:HE1	1.71	0.54
1:A:901:LYS:HE3	1:A:903:LEU:HD12	1.89	0.54
1:C:1165:ASN:HA	1:C:1213:PHE:HE2	1.71	0.54
1:D:661:LYS:HG2	1:D:808:TYR:CD1	2.43	0.54
1:B:320:LYS:HA	1:B:356:TRP:HH2	1.73	0.54
1:B:901:LYS:HE3	1:B:903:LEU:HD12	1.89	0.54
1:B:1243:PRO:HB2	1:B:1600:LEU:HD11	1.88	0.54
1:B:1679:ASN:HB3	1:B:1797:ARG:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:PHE:HB3	1:A:776:LEU:HD13	1.89	0.54
1:A:3442:UNK:O	1:A:3446:UNK:N	2.41	0.54
1:B:2770:LYS:HE3	1:B:2775:TRP:HE3	1.71	0.54
1:A:320:LYS:HA	1:A:356:TRP:HH2	1.72	0.54
1:C:2695:UNK:H	1:C:2761:TYR:HH	1.53	0.54
1:D:144:GLU:O	1:D:175:SER:OG	2.24	0.54
1:D:649:PHE:HB3	1:D:776:LEU:HD13	1.89	0.54
1:D:3450:UNK:O	1:D:3454:UNK:N	2.40	0.54
1:B:944:GLU:HA	1:B:947:GLU:HB2	1.88	0.54
1:B:2644:UNK:C	1:B:2873:ALA:H	2.21	0.54
1:A:249:GLY:HA2	1:A:372:LEU:HD23	1.90	0.54
1:C:244:LEU:HG	1:C:246:TYR:HE1	1.72	0.54
1:C:661:LYS:HG2	1:C:808:TYR:CD1	2.43	0.54
1:B:661:LYS:HG2	1:B:808:TYR:CD1	2.43	0.54
1:B:1153:ILE:HG22	1:B:1160:ILE:HG23	1.90	0.54
1:A:2095:GLN:HA	1:A:2127:GLN:NE2	2.23	0.54
1:A:3805:LEU:HD12	1:A:3890:LEU:HG	1.89	0.54
1:D:2742:THR:HG23	1:D:2811:GLU:HG2	1.88	0.54
1:D:4238:CYS:O	1:D:4242:ILE:HG12	2.08	0.54
1:B:144:GLU:O	1:B:175:SER:OG	2.24	0.54
1:B:2921:GLU:O	1:B:2924:GLN:NE2	2.40	0.54
1:A:2099:SER:HB2	1:A:2128:TYR:HE1	1.73	0.54
1:A:2128:TYR:HB3	1:A:3669:PHE:HZ	1.73	0.54
1:C:224:HIS:NE2	1:C:385:ASP:O	2.40	0.54
1:C:2770:LYS:HE3	1:C:2775:TRP:HE3	1.72	0.54
1:C:2868:SER:N	1:C:2872:GLN:HE22	2.06	0.53
1:C:3442:UNK:O	1:C:3446:UNK:N	2.41	0.53
1:B:126:SER:HB3	1:B:132:ALA:HB2	1.90	0.53
1:A:661:LYS:HG2	1:A:808:TYR:CD1	2.43	0.53
1:A:1153:ILE:HG22	1:A:1160:ILE:HG23	1.90	0.53
1:A:2642:UNK:N	1:A:2872:GLN:HB2	2.23	0.53
1:D:350:HIS:HE1	1:D:352:ALA:HB3	1.73	0.53
1:D:2812:SER:O	1:D:2882:TYR:OH	2.26	0.53
1:D:3770:LEU:O	1:D:3770:LEU:HD23	2.09	0.53
1:A:1407:UNK:O	1:A:1409:UNK:N	2.42	0.53
1:D:126:SER:HB3	1:D:132:ALA:HB2	1.90	0.53
1:D:320:LYS:HA	1:D:356:TRP:HH2	1.72	0.53
1:D:2868:SER:N	1:D:2872:GLN:HE22	2.06	0.53
1:D:3442:UNK:O	1:D:3446:UNK:N	2.41	0.53
1:D:4892:ARG:HG3	1:D:4892:ARG:O	2.08	0.53
1:B:3442:UNK:O	1:B:3446:UNK:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ILE:HD12	1:A:583:ILE:HD11	1.90	0.53
1:A:758:ARG:HH12	1:A:764:VAL:H	1.57	0.53
1:A:1165:ASN:HA	1:A:1213:PHE:HE2	1.72	0.53
1:C:1407:UNK:O	1:C:1409:UNK:N	2.42	0.53
1:C:2095:GLN:HA	1:C:2127:GLN:NE2	2.24	0.53
1:D:2921:GLU:O	1:D:2924:GLN:NE2	2.41	0.53
1:D:3805:LEU:HD12	1:D:3890:LEU:HG	1.91	0.53
1:B:2867:LEU:HD22	1:B:2872:GLN:HG3	1.90	0.53
1:A:18:ASP:OD1	1:A:18:ASP:N	2.42	0.53
1:C:1639:LEU:N	1:C:1648:MET:O	2.41	0.53
1:D:2867:LEU:O	1:D:2868:SER:O	2.27	0.53
1:B:2644:UNK:O	1:B:2873:ALA:N	2.36	0.53
1:A:1639:LEU:N	1:A:1648:MET:O	2.42	0.53
1:A:3446:UNK:O	1:A:3451:UNK:N	2.42	0.53
1:A:4912:TYR:CD2	5:A:5106:POV:H34	2.43	0.53
1:C:144:GLU:O	1:C:175:SER:OG	2.24	0.53
1:D:2124:LEU:HD11	1:D:2128:TYR:CZ	2.44	0.53
1:B:1407:UNK:O	1:B:1409:UNK:N	2.42	0.53
1:B:3770:LEU:O	1:B:3770:LEU:HD23	2.09	0.53
1:C:350:HIS:HE1	1:C:352:ALA:HB3	1.73	0.53
1:C:1386:UNK:O	1:C:1395:UNK:N	2.42	0.53
1:D:1577:ALA:HB1	1:D:1584:ARG:HA	1.91	0.53
1:D:3722:TYR:CE1	1:D:3782:MET:HE2	2.44	0.53
1:B:1386:UNK:O	1:B:1395:UNK:N	2.42	0.53
1:A:126:SER:HB3	1:A:132:ALA:HB2	1.90	0.53
1:A:350:HIS:HE1	1:A:352:ALA:HB3	1.73	0.53
1:C:1577:ALA:HB1	1:C:1584:ARG:HA	1.91	0.53
1:B:1577:ALA:HB1	1:B:1584:ARG:HA	1.91	0.53
1:A:667:MET:SD	1:A:743:VAL:HG12	2.49	0.53
1:C:575:LEU:HD22	1:C:609:CYS:HB3	1.91	0.53
1:B:18:ASP:OD1	1:B:18:ASP:N	2.42	0.53
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.26	0.52
1:C:3676:ASP:HA	1:C:3679:LYS:HB2	1.90	0.52
1:D:1153:ILE:HG22	1:D:1160:ILE:HG23	1.90	0.52
1:D:1407:UNK:O	1:D:1409:UNK:N	2.42	0.52
1:B:2880:GLU:HA	1:B:2883:HIS:NE2	2.24	0.52
1:C:960:MET:HE3	1:C:963:ASN:HB3	1.91	0.52
1:C:3446:UNK:O	1:C:3451:UNK:N	2.42	0.52
1:A:275:ARG:H	1:A:278:GLN:HE22	1.57	0.52
1:B:758:ARG:HH12	1:B:764:VAL:H	1.57	0.52
1:B:3446:UNK:O	1:B:3451:UNK:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2356:LEU:HA	1:B:2359:ARG:HG2	1.91	0.52
1:B:2812:SER:O	1:B:2882:TYR:OH	2.27	0.52
1:B:3805:LEU:HD12	1:B:3890:LEU:HG	1.90	0.52
1:A:215:THR:OG1	1:A:271:GLY:O	2.28	0.52
1:A:3944:GLU:HG2	1:A:3947:GLY:H	1.75	0.52
1:C:2812:SER:O	1:C:2882:TYR:OH	2.27	0.52
1:C:2921:GLU:O	1:C:2924:GLN:NE2	2.41	0.52
1:D:274:LEU:HB3	1:D:339:ILE:HD12	1.92	0.52
1:D:3944:GLU:HG2	1:D:3947:GLY:H	1.75	0.52
1:B:3761:GLN:NE2	1:B:3762:ARG:HG2	2.24	0.52
1:A:3722:TYR:CD2	1:A:3782:MET:HE1	2.44	0.52
1:C:274:LEU:HB3	1:C:339:ILE:HD12	1.92	0.52
1:C:963:ASN:ND2	1:C:965:TYR:O	2.43	0.52
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.26	0.52
1:B:249:GLY:HA2	1:B:372:LEU:HD23	1.91	0.52
1:B:1122:TYR:CZ	1:B:1182:ILE:HD11	2.45	0.52
1:B:2128:TYR:HB3	1:B:3669:PHE:HZ	1.75	0.52
1:A:963:ASN:ND2	1:A:965:TYR:O	2.43	0.52
1:A:1386:UNK:O	1:A:1395:UNK:N	2.42	0.52
1:C:4856:PHE:CZ	1:D:4580:TYR:HE2	2.28	0.52
1:D:18:ASP:OD1	1:D:18:ASP:N	2.43	0.52
1:D:960:MET:HE3	1:D:963:ASN:HB3	1.90	0.52
1:D:1122:TYR:CZ	1:D:1182:ILE:HD11	2.45	0.52
1:D:1386:UNK:O	1:D:1395:UNK:N	2.42	0.52
1:D:3761:GLN:NE2	1:D:3762:ARG:HG2	2.24	0.52
1:D:3808:GLY:O	1:D:3813:GLN:NE2	2.43	0.52
1:B:1783:VAL:HG12	1:B:1783:VAL:O	2.09	0.52
1:B:2124:LEU:HD11	1:B:2128:TYR:CZ	2.45	0.52
1:B:3808:GLY:O	1:B:3813:GLN:NE2	2.43	0.52
1:B:4864:ASN:OD1	1:B:4875:LYS:NZ	2.39	0.52
1:A:1122:TYR:CZ	1:A:1182:ILE:HD11	2.45	0.52
1:A:3808:GLY:O	1:A:3813:GLN:NE2	2.43	0.52
1:C:2356:LEU:HA	1:C:2359:ARG:HG2	1.91	0.52
1:C:4984:ASN:O	1:C:4985:LEU:HG	2.10	0.52
1:D:1078:GLU:HB2	1:D:1081:TYR:HD2	1.75	0.52
1:C:3761:GLN:NE2	1:C:3762:ARG:HG2	2.24	0.52
1:C:3808:GLY:O	1:C:3813:GLN:NE2	2.43	0.52
1:B:350:HIS:HE1	1:B:352:ALA:HB3	1.73	0.52
1:A:1577:ALA:HB1	1:A:1584:ARG:HA	1.91	0.52
1:C:714:TYR:HB3	1:C:768:PHE:CE2	2.45	0.52
1:D:2356:LEU:HA	1:D:2359:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:MET:HE3	1:A:963:ASN:HB3	1.92	0.51
1:A:2124:LEU:HD11	1:A:2128:TYR:CZ	2.44	0.51
1:C:3944:GLU:HG2	1:C:3947:GLY:H	1.75	0.51
1:D:3446:UNK:O	1:D:3451:UNK:N	2.42	0.51
1:D:4567:LEU:HA	1:D:4816:ILE:HG12	1.92	0.51
1:B:1680:ARG:HB2	1:B:1796:ALA:HB3	1.87	0.51
1:B:2580:UNK:HA	1:B:2900:GLY:HA2	1.92	0.51
1:A:2695:UNK:H	1:A:2761:TYR:HH	1.53	0.51
1:D:266:ARG:O	1:D:270:SER:OG	2.27	0.51
1:D:1580:PHE:HE2	1:D:1592:PRO:HG2	1.76	0.51
1:B:275:ARG:H	1:B:278:GLN:HE22	1.58	0.51
1:B:714:TYR:HB3	1:B:768:PHE:CE2	2.45	0.51
1:C:4567:LEU:HA	1:C:4816:ILE:HG12	1.93	0.51
1:A:4251:ILE:O	1:A:4251:ILE:HG13	2.11	0.51
1:C:1122:TYR:CZ	1:C:1182:ILE:HD11	2.45	0.51
1:C:1153:ILE:HG22	1:C:1160:ILE:HG23	1.91	0.51
1:D:793:LEU:CD1	1:D:821:LEU:HD21	2.38	0.51
1:D:1933:GLU:HA	1:D:1936:LYS:HD3	1.93	0.51
1:D:4251:ILE:HG13	1:D:4251:ILE:O	2.11	0.51
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.26	0.51
1:B:4858:PHE:HE2	5:B:5106:POV:C33	2.12	0.51
1:A:3761:GLN:NE2	1:A:3762:ARG:HG2	2.24	0.51
1:A:3767:GLN:O	1:A:3772:THR:OG1	2.27	0.51
1:B:682:LEU:HD22	1:B:738:LEU:HG	1.91	0.51
1:A:224:HIS:NE2	1:A:385:ASP:O	2.43	0.51
1:A:1580:PHE:HE2	1:A:1592:PRO:HG2	1.76	0.51
1:C:667:MET:SD	1:C:743:VAL:HG12	2.51	0.51
1:C:2124:LEU:HD11	1:C:2128:TYR:CZ	2.46	0.51
1:C:4684:ASP:OD1	1:C:4684:ASP:N	2.44	0.51
1:B:963:ASN:ND2	1:B:965:TYR:O	2.43	0.51
1:B:4567:LEU:HA	1:B:4816:ILE:HG12	1.93	0.51
1:A:2921:GLU:O	1:A:2924:GLN:NE2	2.41	0.51
1:C:578:ILE:HD12	1:C:583:ILE:HD11	1.93	0.51
1:D:667:MET:SD	1:D:743:VAL:HG12	2.51	0.51
1:D:963:ASN:ND2	1:D:965:TYR:O	2.43	0.51
1:C:143:GLY:HA3	1:C:147:TRP:HE1	1.76	0.51
1:D:2580:UNK:HA	1:D:2900:GLY:HA2	1.92	0.51
1:B:4251:ILE:HG13	1:B:4251:ILE:O	2.11	0.51
1:A:143:GLY:HA3	1:A:147:TRP:HE1	1.76	0.51
1:A:274:LEU:HB3	1:A:339:ILE:HD12	1.92	0.51
1:C:758:ARG:HH12	1:C:764:VAL:H	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1617:THR:HA	1:C:1627:ALA:O	2.11	0.51
1:D:249:GLY:HA2	1:D:372:LEU:HD23	1.91	0.51
1:D:2680:UNK:O	1:D:2741:GLU:N	2.44	0.51
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.69	0.51
1:B:3944:GLU:HG2	1:B:3947:GLY:H	1.75	0.51
1:A:1087:ARG:HG3	1:A:1223:PHE:HA	1.94	0.50
1:A:2680:UNK:O	1:A:2741:GLU:N	2.45	0.50
1:A:4794:TRP:HA	1:A:4797:VAL:HG12	1.92	0.50
1:C:275:ARG:H	1:C:278:GLN:HE22	1.57	0.50
1:C:1087:ARG:HG3	1:C:1223:PHE:HA	1.94	0.50
1:D:215:THR:OG1	1:D:271:GLY:O	2.28	0.50
1:D:4851:TYR:CE1	5:D:5105:POV:H312	2.42	0.50
1:B:274:LEU:HB3	1:B:339:ILE:HD12	1.92	0.50
1:B:1786:LEU:CD1	1:B:1786:LEU:N	2.74	0.50
1:C:4251:ILE:HG13	1:C:4251:ILE:O	2.11	0.50
1:C:4864:ASN:OD1	1:C:4875:LYS:NZ	2.38	0.50
1:D:143:GLY:HA3	1:D:147:TRP:HE1	1.77	0.50
1:D:275:ARG:H	1:D:278:GLN:HE22	1.57	0.50
1:D:714:TYR:HB3	1:D:768:PHE:CE2	2.45	0.50
1:A:661:LYS:HE2	1:A:808:TYR:CE2	2.47	0.50
1:A:4567:LEU:HA	1:A:4816:ILE:HG12	1.92	0.50
1:C:2680:UNK:O	1:C:2741:GLU:N	2.44	0.50
1:D:1087:ARG:HG3	1:D:1223:PHE:HA	1.93	0.50
1:D:2099:SER:HB2	1:D:2128:TYR:HE1	1.75	0.50
1:A:27:THR:OG1	1:A:29:LEU:O	2.30	0.50
1:A:921:ASN:O	1:A:924:MET:HG3	2.12	0.50
1:D:921:ASN:O	1:D:924:MET:HG3	2.12	0.50
1:D:2102:VAL:HG11	1:D:2124:LEU:HB2	1.94	0.50
1:B:2102:VAL:HG11	1:B:2124:LEU:HB2	1.94	0.50
1:A:221:ARG:NH1	1:A:253:CYS:O	2.45	0.50
1:D:626:LEU:HD23	1:D:628:GLY:H	1.76	0.50
1:D:2626:UNK:H	1:D:2892:GLN:NE2	2.10	0.50
1:B:667:MET:SD	1:B:743:VAL:HG12	2.51	0.50
1:B:921:ASN:O	1:B:924:MET:HG3	2.12	0.50
1:B:1078:GLU:HB2	1:B:1081:TYR:HD2	1.75	0.50
1:D:2128:TYR:HB3	1:D:3669:PHE:HZ	1.76	0.50
1:B:2680:UNK:O	1:B:2741:GLU:N	2.45	0.50
1:B:3890:LEU:HD12	1:B:3893:GLU:HB2	1.94	0.50
1:B:4583:SER:HG	1:B:4630:TYR:HE1	1.58	0.50
1:A:2626:UNK:H	1:A:2892:GLN:NE2	2.10	0.50
1:C:3561:UNK:O	1:C:3563:UNK:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:LEU:HD23	1:D:525:LEU:HD13	1.94	0.50
1:D:3561:UNK:O	1:D:3563:UNK:N	2.45	0.50
1:B:27:THR:OG1	1:B:29:LEU:O	2.29	0.50
1:B:661:LYS:HE2	1:B:808:TYR:CE2	2.47	0.50
1:B:2291:GLN:NE2	1:B:2292:GLU:H	2.09	0.50
1:A:210:GLU:OE2	1:A:273:HIS:NE2	2.45	0.50
1:C:921:ASN:O	1:C:924:MET:HG3	2.11	0.50
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.69	0.50
1:D:758:ARG:HH12	1:D:764:VAL:H	1.57	0.50
1:D:2877:GLN:O	1:D:2877:GLN:NE2	2.45	0.50
1:B:867:LEU:HD22	1:B:933:LEU:HD21	1.94	0.50
1:B:1933:GLU:HA	1:B:1936:LYS:HD3	1.93	0.50
1:A:2665:UNK:C	1:A:2922:LYS:HZ1	2.24	0.50
1:C:2102:VAL:HG11	1:C:2124:LEU:HB2	1.94	0.50
1:C:2626:UNK:H	1:C:2892:GLN:NE2	2.10	0.50
1:C:4861:LYS:HG2	1:C:4862:PHE:N	2.27	0.50
1:D:867:LEU:HD22	1:D:933:LEU:HD21	1.94	0.50
1:B:215:THR:OG1	1:B:271:GLY:O	2.29	0.50
1:B:1087:ARG:HG3	1:B:1223:PHE:HA	1.94	0.50
1:A:2291:GLN:NE2	1:A:2292:GLU:H	2.09	0.49
1:C:2291:GLN:NE2	1:C:2292:GLU:H	2.09	0.49
1:C:3117:UNK:O	1:C:3121:UNK:N	2.45	0.49
1:C:3670:GLU:OE2	1:C:3731:LYS:HG3	2.12	0.49
1:C:3890:LEU:HD12	1:C:3893:GLU:HB2	1.94	0.49
1:C:4915:VAL:O	1:C:4919:THR:HG22	2.12	0.49
1:D:210:GLU:OE2	1:D:273:HIS:NE2	2.45	0.49
1:B:1580:PHE:HE2	1:B:1592:PRO:HG2	1.77	0.49
1:B:2868:SER:N	1:B:2872:GLN:HE22	2.10	0.49
1:B:3561:UNK:O	1:B:3563:UNK:N	2.45	0.49
1:B:4858:PHE:CD2	5:B:5106:POV:H33	2.46	0.49
1:A:266:ARG:O	1:A:270:SER:OG	2.26	0.49
1:A:2679:UNK:HA	1:A:2741:GLU:HA	1.94	0.49
1:C:215:THR:OG1	1:C:271:GLY:O	2.28	0.49
1:C:661:LYS:HE2	1:C:808:TYR:CE2	2.47	0.49
1:B:143:GLY:HA3	1:B:147:TRP:HE1	1.77	0.49
1:B:626:LEU:HD23	1:B:628:GLY:H	1.76	0.49
1:A:144:GLU:O	1:A:175:SER:OG	2.24	0.49
1:A:2812:SER:O	1:A:2882:TYR:OH	2.28	0.49
1:A:3117:UNK:O	1:A:3121:UNK:N	2.46	0.49
1:A:3561:UNK:O	1:A:3563:UNK:N	2.45	0.49
1:A:4059:LEU:HD13	1:A:4167:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4579:PHE:HD2	1:A:4639:MET:SD	2.34	0.49
1:A:4849:TYR:HD2	1:A:4850:LEU:HD23	1.78	0.49
1:C:867:LEU:HD22	1:C:933:LEU:HD21	1.95	0.49
1:C:1580:PHE:HE2	1:C:1592:PRO:HG2	1.78	0.49
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.94	0.49
1:B:207:SER:HB3	1:B:334:MET:HE2	1.94	0.49
1:A:1742:THR:OG1	1:A:1769:THR:OG1	2.24	0.49
1:C:703:GLY:N	1:C:1647:CYS:SG	2.86	0.49
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.94	0.49
1:D:3890:LEU:HD12	1:D:3893:GLU:HB2	1.94	0.49
1:B:3117:UNK:O	1:B:3121:UNK:N	2.45	0.49
1:A:2102:VAL:HG11	1:A:2124:LEU:HB2	1.94	0.49
1:C:27:THR:OG1	1:C:29:LEU:O	2.29	0.49
1:C:1991:THR:O	1:C:1995:THR:HG23	2.13	0.49
1:C:2679:UNK:HA	1:C:2741:GLU:HA	1.94	0.49
1:C:4121:GLU:HG3	1:C:4122:MET:H	1.78	0.49
1:D:647:ASN:OD1	1:D:821:LEU:HD12	2.13	0.49
1:B:1127:HIS:ND1	1:B:1128:ARG:HG3	2.27	0.49
1:B:4684:ASP:OD1	1:B:4684:ASP:N	2.44	0.49
1:B:4871:GLU:N	1:B:4872:PRO:HD3	2.28	0.49
1:A:626:LEU:HD23	1:A:628:GLY:H	1.77	0.49
1:A:2580:UNK:HA	1:A:2900:GLY:HA2	1.94	0.49
1:C:18:ASP:OD1	1:C:18:ASP:N	2.41	0.49
1:C:3767:GLN:O	1:C:3772:THR:OG1	2.26	0.49
1:D:4121:GLU:HG3	1:D:4122:MET:H	1.78	0.49
1:D:4871:GLU:N	1:D:4872:PRO:HD3	2.28	0.49
1:B:266:ARG:O	1:B:270:SER:OG	2.26	0.49
1:A:233:ILE:HG22	1:A:242:ARG:HG2	1.94	0.49
1:A:238:SER:OG	1:A:240:ASP:OD1	2.30	0.49
1:A:2642:UNK:N	1:A:2876:GLU:OE1	2.45	0.49
1:A:3890:LEU:HD12	1:A:3893:GLU:HB2	1.94	0.49
1:A:4068:LEU:HA	1:A:4071:ILE:HG22	1.95	0.49
1:A:4871:GLU:N	1:A:4872:PRO:HD3	2.28	0.49
1:C:4871:GLU:N	1:C:4872:PRO:HD3	2.28	0.49
1:D:1991:THR:O	1:D:1995:THR:HG23	2.13	0.49
1:D:4198:SER:OG	1:D:4201:ASN:ND2	2.46	0.49
1:B:960:MET:HE3	1:B:963:ASN:HB3	1.93	0.49
1:B:2626:UNK:H	1:B:2892:GLN:NE2	2.10	0.49
1:A:2359:ARG:NH2	1:D:179:TYR:OH	2.42	0.49
1:A:4858:PHE:HE2	5:A:5106:POV:C33	2.11	0.49
1:D:233:ILE:HG22	1:D:242:ARG:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3500:UNK:O	1:D:3504:UNK:N	2.46	0.49
1:D:3767:GLN:O	1:D:3772:THR:OG1	2.28	0.49
1:B:233:ILE:HG22	1:B:242:ARG:HG2	1.94	0.49
1:B:1616:GLU:O	1:B:1628:VAL:HA	2.12	0.49
1:B:3676:ASP:HA	1:B:3679:LYS:HB2	1.95	0.49
1:A:867:LEU:HD22	1:A:933:LEU:HD21	1.95	0.49
1:A:4851:TYR:CE1	5:A:5106:POV:H312	2.45	0.49
1:C:1742:THR:OG1	1:C:1769:THR:OG1	2.24	0.49
1:C:2642:UNK:C	1:C:2875:ALA:HB3	2.43	0.49
1:D:661:LYS:HE2	1:D:808:TYR:CE2	2.47	0.49
1:D:3117:UNK:O	1:D:3121:UNK:N	2.45	0.49
1:B:445:LEU:HD23	1:B:525:LEU:HD13	1.95	0.49
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.94	0.49
1:A:1679:ASN:O	1:A:1797:ARG:NH2	2.46	0.49
1:D:1742:THR:O	1:D:1745:ILE:HG22	2.13	0.49
1:D:2291:GLN:NE2	1:D:2292:GLU:H	2.10	0.49
1:B:4953:ASP:HA	1:B:4956:THR:HG22	1.95	0.49
1:A:445:LEU:HD23	1:A:525:LEU:HD13	1.94	0.48
1:C:233:ILE:HG22	1:C:242:ARG:HG2	1.94	0.48
1:C:2128:TYR:HB3	1:C:3669:PHE:HZ	1.77	0.48
1:D:221:ARG:NH1	1:D:253:CYS:O	2.46	0.48
1:D:2642:UNK:C	1:D:2875:ALA:HB3	2.43	0.48
1:D:2667:UNK:HA	1:D:2809:ILE:HD11	1.95	0.48
1:B:134:ASP:OD1	1:B:134:ASP:N	2.45	0.48
1:B:1786:LEU:HD13	1:B:1786:LEU:N	2.28	0.48
1:B:1991:THR:O	1:B:1995:THR:HG23	2.13	0.48
1:A:1742:THR:O	1:A:1745:ILE:HG22	2.13	0.48
1:A:2128:TYR:HB3	1:A:3669:PHE:CZ	2.48	0.48
1:A:3500:UNK:O	1:A:3504:UNK:N	2.46	0.48
1:A:4177:TYR:CE1	1:A:4199:GLU:HB3	2.48	0.48
1:C:134:ASP:N	1:C:134:ASP:OD1	2.45	0.48
1:B:1742:THR:OG1	1:B:1769:THR:OG1	2.24	0.48
1:B:2667:UNK:HA	1:B:2809:ILE:HD11	1.95	0.48
1:A:703:GLY:N	1:A:1647:CYS:SG	2.86	0.48
1:C:221:ARG:NH1	1:C:253:CYS:O	2.46	0.48
1:C:1618:ARG:O	1:C:1619:ARG:C	2.51	0.48
1:B:4152:GLU:OE2	1:B:4180:ARG:NH1	2.47	0.48
1:A:134:ASP:N	1:A:134:ASP:OD1	2.45	0.48
1:A:1991:THR:O	1:A:1995:THR:HG23	2.13	0.48
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.26	0.48
1:D:505:GLU:HG2	1:D:512:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4865:LYS:HG2	1:D:4875:LYS:CE	2.44	0.48
1:B:4851:TYR:CE1	5:B:5106:POV:H312	2.40	0.48
1:A:293:LEU:HD11	1:A:297:GLN:N	2.24	0.48
1:A:2667:UNK:HA	1:A:2809:ILE:HD11	1.95	0.48
1:C:682:LEU:HD22	1:C:738:LEU:HG	1.95	0.48
1:C:2667:UNK:HA	1:C:2809:ILE:HD11	1.96	0.48
1:D:682:LEU:HD22	1:D:738:LEU:HG	1.95	0.48
1:B:1742:THR:O	1:B:1745:ILE:HG22	2.13	0.48
1:A:1618:ARG:O	1:A:1626:TRP:CA	2.62	0.48
1:C:1932:PRO:HD2	1:C:1935:VAL:HG12	1.95	0.48
1:D:134:ASP:OD1	1:D:134:ASP:N	2.45	0.48
1:D:1130:GLN:OE1	1:D:1136:SER:OG	2.32	0.48
1:D:4858:PHE:CD2	5:D:5105:POV:H33	2.46	0.48
1:B:1618:ARG:O	1:B:1627:ALA:N	2.47	0.48
1:B:2679:UNK:HA	1:B:2741:GLU:HA	1.95	0.48
1:A:4198:SER:OG	1:A:4198:SER:O	2.31	0.48
1:A:4684:ASP:OD1	1:A:4684:ASP:N	2.44	0.48
1:C:1742:THR:O	1:C:1745:ILE:HG22	2.13	0.48
1:C:3500:UNK:O	1:C:3504:UNK:N	2.46	0.48
1:D:27:THR:OG1	1:D:29:LEU:O	2.32	0.48
1:A:61:ASP:OD1	1:A:61:ASP:N	2.47	0.48
1:A:505:GLU:HG2	1:A:512:ALA:HB2	1.96	0.48
1:C:626:LEU:HD23	1:C:628:GLY:H	1.78	0.48
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.32	0.48
1:C:2665:UNK:C	1:C:2922:LYS:HZ1	2.26	0.48
1:D:4900:GLU:OE2	1:D:4900:GLU:N	2.47	0.48
1:B:210:GLU:OE2	1:B:273:HIS:NE2	2.47	0.48
1:B:3986:TRP:HD1	1:B:4047:MET:HG3	1.78	0.48
1:C:61:ASP:OD1	1:C:61:ASP:N	2.47	0.48
1:C:249:GLY:HA2	1:C:372:LEU:HD23	1.94	0.48
1:C:675:LEU:HG	1:C:676:THR:H	1.79	0.48
1:D:2867:LEU:C	1:D:2872:GLN:HE22	2.17	0.48
1:A:1932:PRO:HD2	1:A:1935:VAL:HG12	1.95	0.48
1:A:4242:ILE:HD12	1:A:4993:MET:HG3	1.95	0.48
1:A:4863:TYR:HA	1:A:4901:ILE:HG23	1.96	0.48
1:A:4912:TYR:HD2	5:A:5106:POV:H34	1.79	0.48
1:C:1154:ASP:OD2	1:C:1156:THR:OG1	2.32	0.48
1:C:2580:UNK:HA	1:C:2900:GLY:HA2	1.94	0.48
1:D:2162:ILE:HG23	1:D:2178:MET:HE3	1.95	0.48
1:D:4175:ARG:HG2	1:D:4175:ARG:HH11	1.79	0.48
1:D:4580:TYR:HH	1:D:4629:TYR:HD1	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3451:UNK:O	1:B:3455:UNK:N	2.47	0.48
1:B:3500:UNK:O	1:B:3504:UNK:N	2.46	0.48
1:B:3767:GLN:O	1:B:3772:THR:OG1	2.28	0.48
1:A:2877:GLN:O	1:A:2877:GLN:NE2	2.47	0.47
1:A:3451:UNK:O	1:A:3455:UNK:N	2.47	0.47
1:C:505:GLU:HG2	1:C:512:ALA:HB2	1.95	0.47
1:C:2642:UNK:N	1:C:2872:GLN:HB2	2.28	0.47
1:D:4580:TYR:OH	1:D:4629:TYR:HB3	2.14	0.47
1:B:675:LEU:HG	1:B:676:THR:H	1.79	0.47
1:B:3699:HIS:HD2	1:B:3771:HIS:HD2	1.61	0.47
1:A:758:ARG:NH2	1:A:763:PRO:HD2	2.29	0.47
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.94	0.47
1:A:3986:TRP:HD1	1:A:4047:MET:HG3	1.79	0.47
1:A:4567:LEU:HG	1:A:4816:ILE:HG13	1.96	0.47
1:C:238:SER:OG	1:C:240:ASP:OD1	2.30	0.47
1:C:1749:PRO:HG3	1:C:1760:HIS:CE1	2.49	0.47
1:C:3980:LEU:HD21	1:C:3985:LEU:HD22	1.96	0.47
1:C:4152:GLU:OE2	1:C:4180:ARG:NH1	2.47	0.47
1:D:675:LEU:HG	1:D:676:THR:H	1.79	0.47
1:D:758:ARG:NH2	1:D:763:PRO:HD2	2.29	0.47
1:B:2606:UNK:O	1:B:2650:UNK:HA	2.14	0.47
1:B:2641:UNK:HA	1:B:2872:GLN:HG3	1.97	0.47
1:C:262:LEU:HB2	1:C:280:LEU:HD13	1.96	0.47
1:C:2644:UNK:O	1:C:2873:ALA:N	2.41	0.47
1:D:3451:UNK:O	1:D:3455:UNK:N	2.47	0.47
1:D:4579:PHE:HD2	1:D:4639:MET:SD	2.36	0.47
1:B:505:GLU:HG2	1:B:512:ALA:HB2	1.96	0.47
1:B:3980:LEU:HD21	1:B:3985:LEU:HD22	1.97	0.47
1:B:4121:GLU:HG3	1:B:4122:MET:H	1.78	0.47
1:B:4579:PHE:HD2	1:B:4639:MET:SD	2.37	0.47
1:A:2644:UNK:CB	1:A:2874:MET:H	2.27	0.47
1:A:3661:TRP:HE3	1:A:3663:LEU:HD22	1.80	0.47
1:C:210:GLU:OE2	1:C:273:HIS:NE2	2.47	0.47
1:C:4924:VAL:O	1:C:4928:LEU:HB2	2.14	0.47
1:D:2679:UNK:HA	1:D:2741:GLU:HA	1.94	0.47
1:D:3772:THR:HG22	1:D:3815:LYS:HD2	1.96	0.47
1:D:3980:LEU:HD21	1:D:3985:LEU:HD22	1.97	0.47
1:D:3986:TRP:HD1	1:D:4047:MET:HG3	1.79	0.47
1:D:4152:GLU:OE2	1:D:4180:ARG:NH1	2.47	0.47
1:B:1130:GLN:OE1	1:B:1136:SER:OG	2.31	0.47
1:B:1749:PRO:HG3	1:B:1760:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4579:PHE:HB2	1:B:4639:MET:SD	2.55	0.47
1:A:3980:LEU:HD21	1:A:3985:LEU:HD22	1.96	0.47
1:C:2128:TYR:HB3	1:C:3669:PHE:CZ	2.49	0.47
1:C:2877:GLN:O	1:C:2877:GLN:NE2	2.45	0.47
1:D:4684:ASP:N	1:D:4684:ASP:OD1	2.45	0.47
1:A:3497:UNK:O	1:A:3502:UNK:N	2.48	0.47
1:A:4152:GLU:OE2	1:A:4180:ARG:NH1	2.47	0.47
1:C:266:ARG:O	1:C:270:SER:OG	2.27	0.47
1:D:2641:UNK:HA	1:D:2872:GLN:HG3	1.96	0.47
1:B:262:LEU:HB2	1:B:280:LEU:HD13	1.97	0.47
1:B:3497:UNK:O	1:B:3502:UNK:N	2.48	0.47
1:A:262:LEU:HB2	1:A:280:LEU:HD13	1.97	0.47
1:A:375:LYS:HD3	1:A:377:ILE:HD11	1.96	0.47
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.32	0.47
1:A:3699:HIS:HD2	1:A:3771:HIS:HD2	1.61	0.47
1:A:4858:PHE:CD2	5:A:5106:POV:H33	2.46	0.47
1:C:2099:SER:HB2	1:C:2128:TYR:HE1	1.79	0.47
1:C:2644:UNK:CB	1:C:2874:MET:H	2.28	0.47
1:C:4059:LEU:HD13	1:C:4167:ALA:HB2	1.96	0.47
1:B:221:ARG:NH1	1:B:253:CYS:O	2.48	0.47
1:B:1237:TRP:CH2	1:B:1652:GLU:HG2	2.49	0.47
1:A:714:TYR:HB3	1:A:768:PHE:CE2	2.49	0.47
1:A:1618:ARG:O	1:A:1626:TRP:HA	2.15	0.47
1:A:1749:PRO:HG3	1:A:1760:HIS:CE1	2.49	0.47
1:C:3451:UNK:O	1:C:3455:UNK:N	2.47	0.47
1:C:3986:TRP:HD1	1:C:4047:MET:HG3	1.79	0.47
1:C:4865:LYS:HG2	1:C:4875:LYS:CE	2.44	0.47
1:D:2644:UNK:CB	1:D:2874:MET:H	2.28	0.47
1:B:1154:ASP:OD2	1:B:1156:THR:OG1	2.32	0.47
1:B:4175:ARG:HG2	1:B:4175:ARG:HH11	1.79	0.47
1:A:310:LYS:HE3	1:A:352:ALA:HB2	1.97	0.47
1:A:4175:ARG:HG2	1:A:4175:ARG:HH11	1.79	0.47
1:C:758:ARG:NH2	1:C:763:PRO:HD2	2.30	0.47
1:C:955:LEU:O	1:C:966:LYS:NZ	2.48	0.47
1:C:3661:TRP:HE3	1:C:3663:LEU:HD22	1.80	0.47
1:D:1237:TRP:CH2	1:D:1652:GLU:HG2	2.49	0.47
1:D:1683:HIS:CE1	1:D:1780:PRO:HA	2.49	0.47
1:D:2642:UNK:N	1:D:2872:GLN:HB2	2.28	0.47
1:D:3497:UNK:O	1:D:3502:UNK:N	2.48	0.47
1:D:4156:HIS:NE2	1:D:5036:LEU:HD11	2.30	0.47
1:B:2099:SER:HB2	1:B:2128:TYR:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4177:TYR:CE1	1:B:4199:GLU:HB3	2.50	0.47
1:D:238:SER:OG	1:D:240:ASP:OD1	2.29	0.47
1:D:375:LYS:HD3	1:D:377:ILE:HD11	1.97	0.47
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.32	0.47
1:D:3670:GLU:OE1	1:D:3731:LYS:HE3	2.14	0.47
1:B:4156:HIS:NE2	1:B:5036:LEU:HD11	2.30	0.47
1:A:1969:LEU:HD13	1:A:2009:LEU:HD11	1.97	0.46
1:A:4764:LEU:O	1:A:4765:LEU:HG	2.15	0.46
1:C:4156:HIS:NE2	1:C:5036:LEU:HD11	2.30	0.46
1:C:4175:ARG:HH11	1:C:4175:ARG:HG2	1.79	0.46
1:B:2648:UNK:HA	1:B:2869:ARG:CZ	2.45	0.46
1:B:3818:ASP:OD1	1:B:3819:TYR:N	2.49	0.46
1:B:5004:THR:HG22	1:B:5005:GLY:N	2.30	0.46
1:A:877:ASN:O	1:A:880:GLU:HG3	2.16	0.46
1:A:1130:GLN:OE1	1:A:1136:SER:OG	2.33	0.46
1:A:2802:LYS:HA	1:A:2806:ARG:HB2	1.97	0.46
1:C:445:LEU:HD23	1:C:525:LEU:HD13	1.96	0.46
1:D:61:ASP:OD1	1:D:61:ASP:N	2.47	0.46
1:D:262:LEU:HB2	1:D:280:LEU:HD13	1.97	0.46
1:D:1749:PRO:HG3	1:D:1760:HIS:CE1	2.49	0.46
1:D:3722:TYR:CE2	1:D:3782:MET:HE3	2.50	0.46
1:B:4567:LEU:HG	1:B:4816:ILE:HG13	1.98	0.46
1:A:2867:LEU:O	1:A:2868:SER:C	2.53	0.46
1:A:3535:UNK:O	1:A:3537:UNK:N	2.49	0.46
1:C:375:LYS:HD3	1:C:377:ILE:HD11	1.97	0.46
1:C:2641:UNK:HA	1:C:2872:GLN:HG3	1.96	0.46
1:C:3497:UNK:O	1:C:3502:UNK:N	2.48	0.46
1:D:293:LEU:HD11	1:D:297:GLN:N	2.24	0.46
1:D:3489:UNK:O	1:D:3491:UNK:N	2.49	0.46
1:D:4219:PHE:HD1	1:D:4950:VAL:HG11	1.80	0.46
1:B:758:ARG:NH2	1:B:763:PRO:HD2	2.29	0.46
1:B:3772:THR:HG22	1:B:3815:LYS:HD2	1.97	0.46
1:B:3773:ARG:H	1:B:3773:ARG:HD3	1.79	0.46
1:A:294:THR:HG23	1:A:295:GLU:N	2.31	0.46
1:A:675:LEU:HG	1:A:676:THR:H	1.80	0.46
1:A:2882:TYR:O	1:A:2886:TRP:HD1	1.99	0.46
1:C:310:LYS:HE3	1:C:352:ALA:HB2	1.97	0.46
1:C:3489:UNK:O	1:C:3491:UNK:N	2.48	0.46
1:B:747:CYS:SG	1:B:756:SER:HB3	2.56	0.46
1:B:1969:LEU:HD13	1:B:2009:LEU:HD11	1.97	0.46
1:B:4059:LEU:HD13	1:B:4167:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5004:THR:HG22	1:A:5005:GLY:N	2.31	0.46
1:C:2875:ALA:HB1	1:C:2939:ARG:HD3	1.98	0.46
1:D:877:ASN:O	1:D:880:GLU:HG3	2.16	0.46
1:D:955:LEU:O	1:D:966:LYS:NZ	2.48	0.46
1:D:1969:LEU:HD13	1:D:2009:LEU:HD11	1.97	0.46
1:D:2802:LYS:HA	1:D:2806:ARG:HB2	1.97	0.46
1:D:3749:VAL:O	1:D:3751:VAL:HG23	2.16	0.46
1:D:4059:LEU:HD13	1:D:4167:ALA:HB2	1.95	0.46
1:B:3670:GLU:OE1	1:B:3731:LYS:HE3	2.15	0.46
1:A:2644:UNK:O	1:A:2873:ALA:N	2.43	0.46
1:A:3749:VAL:O	1:A:3751:VAL:HG23	2.16	0.46
1:C:877:ASN:O	1:C:880:GLU:HG3	2.16	0.46
1:C:1087:ARG:HB2	1:C:1223:PHE:CE2	2.51	0.46
1:C:3773:ARG:H	1:C:3773:ARG:HD3	1.79	0.46
1:D:2867:LEU:N	1:D:2872:GLN:NE2	2.64	0.46
1:B:375:LYS:HD3	1:B:377:ILE:HD11	1.96	0.46
1:B:3535:UNK:O	1:B:3537:UNK:N	2.49	0.46
1:A:1078:GLU:HB2	1:A:1081:TYR:CD2	2.50	0.46
1:A:1087:ARG:HB2	1:A:1223:PHE:CE2	2.51	0.46
1:A:2924:GLN:NE2	1:A:2925:GLU:HG3	2.31	0.46
1:A:3454:UNK:O	1:A:3458:UNK:N	2.49	0.46
1:A:4156:HIS:NE2	1:A:5036:LEU:HD11	2.30	0.46
1:C:747:CYS:SG	1:C:756:SER:HB3	2.56	0.46
1:C:2880:GLU:HA	1:C:2883:HIS:CE1	2.51	0.46
1:D:310:LYS:HE3	1:D:352:ALA:HB2	1.97	0.46
1:D:747:CYS:SG	1:D:756:SER:HB3	2.56	0.46
1:D:1618:ARG:O	1:D:1626:TRP:N	2.48	0.46
1:D:2644:UNK:H	1:D:2872:GLN:HA	1.81	0.46
1:D:3454:UNK:O	1:D:3458:UNK:N	2.49	0.46
1:B:3454:UNK:O	1:B:3458:UNK:N	2.49	0.46
1:B:3722:TYR:CD2	1:B:3782:MET:CE	2.99	0.46
1:A:3818:ASP:OD1	1:A:3819:TYR:N	2.49	0.46
1:C:1969:LEU:HD13	1:C:2009:LEU:HD11	1.97	0.46
1:C:4764:LEU:O	1:C:4765:LEU:HG	2.16	0.46
1:D:219:VAL:HG12	1:D:261:ARG:HB2	1.98	0.46
1:B:3749:VAL:O	1:B:3751:VAL:HG23	2.16	0.46
1:B:3983:SER:OG	1:B:3984:ARG:N	2.49	0.46
1:A:3773:ARG:H	1:A:3773:ARG:HD3	1.79	0.46
1:A:4802:GLY:O	1:A:4805:ASN:HB3	2.16	0.46
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.38	0.46
1:D:1742:THR:OG1	1:D:1769:THR:OG1	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3818:ASP:OD1	1:D:3819:TYR:N	2.49	0.46
1:D:4567:LEU:HG	1:D:4816:ILE:HG13	1.98	0.46
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.32	0.46
1:A:955:LEU:O	1:A:966:LYS:NZ	2.49	0.46
1:D:320:LYS:HA	1:D:356:TRP:CH2	2.51	0.46
1:D:2880:GLU:HA	1:D:2883:HIS:CE1	2.51	0.46
1:D:4764:LEU:O	1:D:4765:LEU:HG	2.15	0.46
1:B:294:THR:HG23	1:B:295:GLU:N	2.31	0.46
1:B:955:LEU:O	1:B:966:LYS:NZ	2.48	0.46
1:A:445:LEU:HB3	1:A:521:LEU:CD2	2.46	0.45
1:A:2880:GLU:HA	1:A:2883:HIS:CE1	2.51	0.45
1:C:294:THR:HG23	1:C:295:GLU:N	2.31	0.45
1:C:1130:GLN:OE1	1:C:1136:SER:OG	2.33	0.45
1:C:2924:GLN:NE2	1:C:2925:GLU:HG3	2.31	0.45
1:D:2875:ALA:HB1	1:D:2939:ARG:HD3	1.98	0.45
1:B:1087:ARG:HB2	1:B:1223:PHE:CE2	2.51	0.45
1:B:4764:LEU:O	1:B:4765:LEU:HG	2.15	0.45
1:A:773:LEU:HD23	1:A:773:LEU:H	1.82	0.45
1:A:998:ARG:HA	1:A:1002:ALA:HB3	1.98	0.45
1:A:3489:UNK:O	1:A:3491:UNK:N	2.48	0.45
1:A:3749:VAL:O	1:A:3750:GLU:HG2	2.16	0.45
1:A:3772:THR:HG22	1:A:3815:LYS:HD2	1.97	0.45
1:A:5027:CYS:O	1:A:5028:PHE:HB3	2.16	0.45
1:C:3749:VAL:O	1:C:3751:VAL:HG23	2.16	0.45
1:D:3856:LEU:HD23	1:D:3856:LEU:H	1.82	0.45
1:D:5004:THR:HG22	1:D:5005:GLY:N	2.30	0.45
1:D:5027:CYS:O	1:D:5028:PHE:HB3	2.16	0.45
1:B:3794:VAL:HG11	1:B:3835:LEU:HD11	1.98	0.45
1:B:4112:LEU:O	1:B:4115:SER:OG	2.33	0.45
1:A:597:HIS:HB2	1:A:1665:HIS:ND1	2.32	0.45
1:A:4865:LYS:NZ	1:A:4875:LYS:HE3	2.31	0.45
1:C:3454:UNK:O	1:C:3458:UNK:N	2.49	0.45
1:C:3749:VAL:O	1:C:3750:GLU:HG2	2.17	0.45
1:C:3818:ASP:OD1	1:C:3819:TYR:N	2.48	0.45
1:C:5027:CYS:O	1:C:5028:PHE:HB3	2.16	0.45
1:D:2606:UNK:O	1:D:2650:UNK:HA	2.17	0.45
1:D:3535:UNK:O	1:D:3537:UNK:N	2.49	0.45
1:D:3773:ARG:H	1:D:3773:ARG:HD3	1.79	0.45
1:D:4198:SER:OG	1:D:4198:SER:O	2.30	0.45
1:D:4579:PHE:HB2	1:D:4639:MET:SD	2.57	0.45
1:B:5027:CYS:O	1:B:5028:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4219:PHE:HD1	1:A:4950:VAL:HG11	1.80	0.45
1:C:320:LYS:HA	1:C:356:TRP:CH2	2.51	0.45
1:C:773:LEU:HD23	1:C:773:LEU:H	1.81	0.45
1:C:2644:UNK:H	1:C:2872:GLN:HA	1.81	0.45
1:C:2882:TYR:O	1:C:2886:TRP:HD1	2.00	0.45
1:C:3535:UNK:O	1:C:3537:UNK:N	2.49	0.45
1:D:3749:VAL:O	1:D:3750:GLU:HG2	2.17	0.45
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.50	0.45
1:B:2882:TYR:O	1:B:2886:TRP:HD1	2.00	0.45
1:B:3489:UNK:O	1:B:3491:UNK:N	2.48	0.45
1:B:3749:VAL:O	1:B:3750:GLU:HG2	2.17	0.45
1:A:747:CYS:SG	1:A:756:SER:HB3	2.56	0.45
1:A:3856:LEU:HD23	1:A:3856:LEU:H	1.82	0.45
1:C:1155:LEU:HD13	1:C:1184:ILE:HG23	1.98	0.45
1:D:1155:LEU:HD13	1:D:1184:ILE:HG23	1.98	0.45
1:D:2882:TYR:O	1:D:2886:TRP:HD1	2.00	0.45
1:D:2932:MET:SD	1:D:2932:MET:N	2.90	0.45
1:D:4849:TYR:HD2	1:D:4850:LEU:HD23	1.82	0.45
1:B:2924:GLN:NE2	1:B:2925:GLU:HG3	2.31	0.45
1:A:1207:ASP:OD1	1:A:1207:ASP:N	2.48	0.45
1:C:534:ARG:HG2	1:C:534:ARG:HH11	1.82	0.45
1:C:809:ALA:N	1:C:810:PRO:HD3	2.32	0.45
1:C:4219:PHE:HD1	1:C:4950:VAL:HG11	1.81	0.45
1:C:5004:THR:HG22	1:C:5005:GLY:N	2.30	0.45
1:D:1087:ARG:HB2	1:D:1223:PHE:CE2	2.51	0.45
1:D:1651:LEU:HD13	1:D:1702:HIS:NE2	2.32	0.45
1:D:1783:VAL:HG12	1:D:1783:VAL:O	2.17	0.45
1:D:2924:GLN:NE2	1:D:2925:GLU:HG3	2.31	0.45
1:B:310:LYS:HE3	1:B:352:ALA:HB2	1.97	0.45
1:B:1680:ARG:CB	1:B:1796:ALA:HB1	2.44	0.45
1:B:1797:ARG:O	1:B:1798:LEU:C	2.51	0.45
1:B:2802:LYS:HA	1:B:2806:ARG:HB2	1.97	0.45
1:B:2932:MET:SD	1:B:2932:MET:N	2.90	0.45
1:B:4039:MET:HB3	1:B:4042:ARG:HH21	1.82	0.45
1:C:2802:LYS:HA	1:C:2806:ARG:HB2	1.97	0.45
1:C:3856:LEU:HD23	1:C:3856:LEU:H	1.82	0.45
1:C:4857:ASN:ND2	5:C:5107:POV:H34	2.32	0.45
1:D:445:LEU:HB3	1:D:521:LEU:CD2	2.47	0.45
1:D:652:ARG:HH21	1:D:773:LEU:HD13	1.82	0.45
1:D:998:ARG:HA	1:D:1002:ALA:HB3	1.98	0.45
1:B:773:LEU:H	1:B:773:LEU:HD23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:PRO:HD3	1:A:1605:TRP:NE1	2.32	0.45
1:C:219:VAL:HG12	1:C:261:ARG:HB2	1.98	0.45
1:C:1111:PRO:HD3	1:C:1605:TRP:NE1	2.32	0.45
1:C:4733:GLY:HA3	1:C:4736:ARG:HG3	1.99	0.45
1:D:761:GLY:C	1:D:763:PRO:HD3	2.37	0.45
1:D:809:ALA:N	1:D:810:PRO:HD3	2.32	0.45
1:D:1111:PRO:HD3	1:D:1605:TRP:NE1	2.32	0.45
1:B:877:ASN:O	1:B:880:GLU:HG3	2.16	0.45
1:B:3856:LEU:H	1:B:3856:LEU:HD23	1.82	0.45
1:B:3946:GLN:OE1	1:B:3949:ARG:NH2	2.50	0.45
1:A:1580:PHE:CE2	1:A:1592:PRO:HG2	2.52	0.45
1:A:2336:ARG:HG3	1:A:2435:ARG:HD2	1.99	0.45
1:A:2867:LEU:N	1:A:2872:GLN:NE2	2.65	0.45
1:A:3699:HIS:HD2	1:A:3771:HIS:CD2	2.35	0.45
1:C:293:LEU:HD11	1:C:297:GLN:N	2.24	0.45
1:C:3772:THR:HG22	1:C:3815:LYS:HD2	1.98	0.45
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.50	0.45
1:B:703:GLY:N	1:B:1647:CYS:SG	2.90	0.45
1:B:1683:HIS:CE1	1:B:1780:PRO:HA	2.52	0.45
1:B:2162:ILE:HG23	1:B:2178:MET:HE3	1.98	0.45
1:B:2336:ARG:HG3	1:B:2435:ARG:HD2	1.99	0.45
1:B:2930:LEU:HD23	1:B:2930:LEU:HA	1.88	0.45
1:A:3722:TYR:CG	1:A:3782:MET:HE1	2.52	0.45
1:A:4851:TYR:OH	1:A:4919:THR:HG23	2.16	0.45
1:C:761:GLY:C	1:C:763:PRO:HD3	2.38	0.45
1:C:4567:LEU:HG	1:C:4816:ILE:HG13	1.98	0.45
1:B:219:VAL:HG12	1:B:261:ARG:HB2	1.97	0.45
1:B:1680:ARG:HB2	1:B:1796:ALA:HB1	1.91	0.45
1:B:2880:GLU:HA	1:B:2883:HIS:CE1	2.52	0.45
1:B:3297:UNK:HA	1:B:3302:UNK:HA	1.99	0.45
1:A:875:ALA:HA	1:A:878:ILE:HG12	1.99	0.44
1:C:998:ARG:HA	1:C:1002:ALA:HB3	1.98	0.44
1:C:2932:MET:SD	1:C:2932:MET:N	2.90	0.44
1:D:2895:GLU:OE2	1:D:2902:HIS:NE2	2.50	0.44
1:D:4733:GLY:HA3	1:D:4736:ARG:HG3	1.99	0.44
1:B:809:ALA:N	1:B:810:PRO:HD3	2.32	0.44
1:B:2128:TYR:HB3	1:B:3669:PHE:CZ	2.51	0.44
1:A:219:VAL:HG12	1:A:261:ARG:HB2	1.99	0.44
1:C:2606:UNK:O	1:C:2650:UNK:HA	2.17	0.44
1:D:703:GLY:N	1:D:1647:CYS:SG	2.90	0.44
1:D:821:LEU:HG	1:D:821:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1932:PRO:HD2	1:D:1935:VAL:HG12	1.99	0.44
1:B:626:LEU:HD23	1:B:628:GLY:N	2.32	0.44
1:B:875:ALA:HA	1:B:878:ILE:HG12	1.99	0.44
1:B:1651:LEU:HD13	1:B:1702:HIS:NE2	2.32	0.44
1:B:1932:PRO:HD2	1:B:1935:VAL:HG12	1.99	0.44
1:B:2665:UNK:O	1:B:2922:LYS:NZ	2.50	0.44
1:D:1580:PHE:CE2	1:D:1592:PRO:HG2	2.52	0.44
1:D:2128:TYR:HB3	1:D:3669:PHE:CZ	2.52	0.44
1:D:2336:ARG:HG3	1:D:2435:ARG:HD2	2.00	0.44
1:D:3794:VAL:HG11	1:D:3835:LEU:HD11	1.98	0.44
1:D:4912:TYR:HD2	5:D:5105:POV:H34	1.80	0.44
1:A:320:LYS:HA	1:A:356:TRP:CH2	2.51	0.44
1:A:2142:TYR:CG	1:A:2197:LEU:HD13	2.53	0.44
1:C:1966:VAL:HG21	1:C:3649:ALA:HB1	1.99	0.44
1:C:2142:TYR:CG	1:C:2197:LEU:HD13	2.53	0.44
1:C:2336:ARG:HG3	1:C:2435:ARG:HD2	1.99	0.44
1:C:2911:LEU:HD11	1:C:2914:LYS:HG3	1.99	0.44
1:C:2930:LEU:HD23	1:C:2930:LEU:HA	1.88	0.44
1:C:4039:MET:HB3	1:C:4042:ARG:HH21	1.82	0.44
1:C:4958:CYS:O	4:C:5104:ACP:C2	2.66	0.44
1:D:2142:TYR:CG	1:D:2197:LEU:HD13	2.53	0.44
1:D:2911:LEU:HD11	1:D:2914:LYS:HG3	1.99	0.44
1:D:3297:UNK:HA	1:D:3302:UNK:HA	1.99	0.44
1:B:2911:LEU:HD11	1:B:2914:LYS:HG3	1.99	0.44
1:B:4793:GLY:O	1:B:4797:VAL:HG23	2.17	0.44
1:A:761:GLY:C	1:A:763:PRO:HD3	2.37	0.44
1:A:3946:GLN:OE1	1:A:3949:ARG:NH2	2.50	0.44
1:A:4039:MET:HB3	1:A:4042:ARG:HH21	1.82	0.44
1:A:4583:SER:HG	1:A:4630:TYR:HE1	1.62	0.44
1:C:875:ALA:HA	1:C:878:ILE:HG12	1.99	0.44
1:C:3790:THR:HG22	1:C:3835:LEU:HG	1.99	0.44
1:D:1805:GLU:HA	1:D:1808:ARG:NE	2.33	0.44
1:D:2239:PHE:O	1:D:2242:ILE:HG22	2.18	0.44
1:B:445:LEU:HB3	1:B:521:LEU:CD2	2.47	0.44
1:B:1111:PRO:HD3	1:B:1605:TRP:NE1	2.32	0.44
1:A:2911:LEU:HD11	1:A:2914:LYS:HG3	2.00	0.44
1:A:2932:MET:SD	1:A:2932:MET:N	2.90	0.44
1:C:805:PRO:HB2	1:C:808:TYR:CD2	2.53	0.44
1:C:1969:LEU:HD23	1:C:1969:LEU:HA	1.87	0.44
1:C:3946:GLN:OE1	1:C:3949:ARG:NH2	2.51	0.44
1:D:294:THR:HG23	1:D:295:GLU:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:ARG:HH21	1:B:773:LEU:HD13	1.83	0.44
1:B:761:GLY:C	1:B:763:PRO:HD3	2.37	0.44
1:B:4733:GLY:HA3	1:B:4736:ARG:HG3	1.99	0.44
1:B:4912:TYR:HD2	5:B:5106:POV:H34	1.80	0.44
1:A:1966:VAL:HG21	1:A:3649:ALA:HB1	1.99	0.44
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.50	0.44
1:A:3794:VAL:HG11	1:A:3835:LEU:HD11	1.99	0.44
1:A:4733:GLY:HA3	1:A:4736:ARG:HG3	1.99	0.44
1:C:1237:TRP:CH2	1:C:1652:GLU:HG2	2.53	0.44
1:C:3297:UNK:HA	1:C:3302:UNK:HA	1.99	0.44
1:C:4849:TYR:HD2	1:C:4850:LEU:HD23	1.83	0.44
1:D:27:THR:OG1	1:D:31:GLU:O	2.29	0.44
1:D:597:HIS:HB2	1:D:1665:HIS:ND1	2.32	0.44
1:D:879:HIS:CG	1:D:921:ASN:HD22	2.36	0.44
1:D:3661:TRP:CE2	1:D:3662:ILE:HG22	2.53	0.44
1:D:4793:GLY:O	1:D:4797:VAL:HG23	2.18	0.44
1:B:998:ARG:HA	1:B:1002:ALA:HB3	1.98	0.44
1:B:1735:ILE:HD11	1:B:2201:LEU:HD11	1.99	0.44
1:B:2095:GLN:HA	1:B:2127:GLN:OE1	2.18	0.44
1:B:4198:SER:OG	1:B:4198:SER:O	2.31	0.44
1:A:796:ARG:HH21	1:A:820:ARG:HH22	1.66	0.44
1:A:831:ARG:HE	1:A:840:VAL:HG11	1.83	0.44
1:A:1155:LEU:HD13	1:A:1184:ILE:HG23	1.98	0.44
1:A:2606:UNK:O	1:A:2650:UNK:HA	2.18	0.44
1:A:3835:LEU:HD21	1:A:3880:PHE:CZ	2.52	0.44
1:C:445:LEU:HB3	1:C:521:LEU:CD2	2.47	0.44
1:C:2288:LEU:O	1:C:3849:ARG:NH1	2.50	0.44
1:C:3338:UNK:O	1:C:3342:UNK:N	2.51	0.44
1:C:3794:VAL:HG11	1:C:3835:LEU:HD11	1.99	0.44
1:D:3946:GLN:OE1	1:D:3949:ARG:NH2	2.51	0.44
1:D:4844:LEU:O	1:D:4848:VAL:HG23	2.18	0.44
1:B:805:PRO:HB2	1:B:808:TYR:CD2	2.53	0.44
1:B:3661:TRP:CE2	1:B:3662:ILE:HG22	2.53	0.44
1:B:4913:ARG:HH11	1:B:4913:ARG:HG2	1.82	0.44
1:A:661:LYS:HD2	1:A:748:LEU:O	2.18	0.44
1:C:2239:PHE:O	1:C:2242:ILE:HG22	2.18	0.44
1:C:4580:TYR:OH	1:C:4629:TYR:HB3	2.18	0.44
1:D:350:HIS:CE1	1:D:352:ALA:HB3	2.53	0.44
1:D:773:LEU:HD23	1:D:773:LEU:H	1.81	0.44
1:D:1639:LEU:HD23	1:D:1640:HIS:N	2.33	0.44
1:D:4177:TYR:CE1	1:D:4199:GLU:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2877:GLN:O	1:B:2877:GLN:NE2	2.44	0.44
1:B:3790:THR:HG22	1:B:3835:LEU:HG	1.99	0.44
1:A:809:ALA:N	1:A:810:PRO:HD3	2.32	0.43
1:A:3297:UNK:HA	1:A:3302:UNK:HA	1.99	0.43
1:C:661:LYS:HD2	1:C:748:LEU:O	2.18	0.43
1:C:879:HIS:CG	1:C:921:ASN:HD22	2.36	0.43
1:B:2895:GLU:OE2	1:B:2902:HIS:NE2	2.50	0.43
1:B:3937:TYR:OH	1:B:3944:GLU:OE2	2.31	0.43
1:C:1078:GLU:HB2	1:C:1081:TYR:CD2	2.50	0.43
1:C:2891:LYS:O	1:C:2894:LEU:HD23	2.19	0.43
1:C:4071:ILE:HD11	1:C:4102:GLN:HE21	1.83	0.43
1:C:4981:GLU:HB2	1:C:4982:GLU:OE2	2.19	0.43
1:D:928:THR:HA	1:D:931:THR:HG22	2.01	0.43
1:B:758:ARG:NH1	1:B:762:CYS:HA	2.33	0.43
1:B:1155:LEU:HD13	1:B:1184:ILE:HG23	1.99	0.43
1:B:2643:UNK:HA	1:B:2871:LEU:O	2.18	0.43
1:C:597:HIS:HB2	1:C:1665:HIS:ND1	2.32	0.43
1:C:652:ARG:HH21	1:C:773:LEU:HD13	1.83	0.43
1:C:758:ARG:NH1	1:C:762:CYS:HA	2.34	0.43
1:C:4921:PHE:CE2	1:D:4892:ARG:HB2	2.52	0.43
1:D:805:PRO:HB2	1:D:808:TYR:CD2	2.53	0.43
1:D:1735:ILE:HD11	1:D:2201:LEU:HD11	2.00	0.43
1:B:320:LYS:HA	1:B:356:TRP:CH2	2.52	0.43
1:B:4981:GLU:HB2	1:B:4982:GLU:OE2	2.18	0.43
1:A:350:HIS:CE1	1:A:352:ALA:HB3	2.53	0.43
1:A:652:ARG:HH21	1:A:773:LEU:HD13	1.83	0.43
1:A:758:ARG:NH1	1:A:762:CYS:HA	2.33	0.43
1:A:2239:PHE:O	1:A:2242:ILE:HG22	2.18	0.43
1:A:2930:LEU:HD23	1:A:2930:LEU:HA	1.88	0.43
1:A:3338:UNK:O	1:A:3342:UNK:N	2.51	0.43
1:C:928:THR:HA	1:C:931:THR:HG22	2.01	0.43
1:C:2895:GLU:OE2	1:C:2902:HIS:NE2	2.51	0.43
1:C:3835:LEU:HD21	1:C:3880:PHE:CZ	2.53	0.43
1:D:875:ALA:HA	1:D:878:ILE:HG12	1.99	0.43
1:D:2912:THR:OG1	1:D:2914:LYS:NZ	2.39	0.43
1:D:3338:UNK:O	1:D:3342:UNK:N	2.51	0.43
1:D:3713:LYS:HE2	1:D:3713:LYS:HB3	1.86	0.43
1:D:4039:MET:HB3	1:D:4042:ARG:HH21	1.82	0.43
1:B:2239:PHE:O	1:B:2242:ILE:HG22	2.18	0.43
1:A:1313:UNK:O	1:A:1315:UNK:N	2.51	0.43
1:A:2895:GLU:OE2	1:A:2902:HIS:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ARG:HA	1:C:402:ARG:HD2	1.87	0.43
1:C:1683:HIS:CE1	1:C:1780:PRO:HA	2.52	0.43
1:D:157:ARG:CZ	1:D:164:ARG:HH22	2.32	0.43
1:D:831:ARG:HE	1:D:840:VAL:HG11	1.84	0.43
1:D:1087:ARG:HB2	1:D:1223:PHE:CD2	2.54	0.43
1:D:2433:LEU:HD22	1:D:2457:LEU:HD21	2.00	0.43
1:D:3835:LEU:HD21	1:D:3880:PHE:CZ	2.53	0.43
1:D:5004:THR:HG22	1:D:5005:GLY:H	1.83	0.43
1:B:597:HIS:HB2	1:B:1665:HIS:ND1	2.32	0.43
1:B:2142:TYR:CG	1:B:2197:LEU:HD13	2.53	0.43
1:B:3338:UNK:O	1:B:3342:UNK:N	2.51	0.43
1:B:4580:TYR:OH	1:B:4629:TYR:HB3	2.18	0.43
1:A:805:PRO:HB2	1:A:808:TYR:CD2	2.53	0.43
1:A:1307:UNK:O	1:A:1309:UNK:N	2.51	0.43
1:C:1204:LEU:HD12	1:C:1226:PHE:HB3	2.01	0.43
1:C:1307:UNK:O	1:C:1309:UNK:N	2.51	0.43
1:C:1313:UNK:O	1:C:1315:UNK:N	2.51	0.43
1:D:626:LEU:HD23	1:D:628:GLY:N	2.32	0.43
1:B:27:THR:OG1	1:B:31:GLU:O	2.28	0.43
1:B:61:ASP:OD1	1:B:61:ASP:N	2.47	0.43
1:B:157:ARG:CZ	1:B:164:ARG:HH22	2.31	0.43
1:B:293:LEU:HD11	1:B:297:GLN:N	2.24	0.43
1:B:831:ARG:HE	1:B:840:VAL:HG11	1.83	0.43
1:B:1969:LEU:HD23	1:B:1969:LEU:HA	1.87	0.43
1:B:4242:ILE:HD12	1:B:4993:MET:HG2	1.99	0.43
1:A:660:GLY:HA3	1:A:750:LEU:HD21	2.00	0.43
1:A:928:THR:HA	1:A:931:THR:HG22	2.01	0.43
1:A:3790:THR:HG22	1:A:3835:LEU:HG	1.99	0.43
1:D:2891:LYS:O	1:D:2894:LEU:HD23	2.19	0.43
1:D:3790:THR:HG22	1:D:3835:LEU:HG	1.99	0.43
1:D:4011:GLU:O	1:D:4015:GLU:HG3	2.18	0.43
1:B:2666:UNK:HA	1:B:2922:LYS:HZ3	1.83	0.43
1:B:4071:ILE:HD11	1:B:4102:GLN:HE21	1.84	0.43
1:B:4851:TYR:CE1	5:B:5106:POV:H31E	2.54	0.43
1:B:4995:LEU:HD23	1:B:4995:LEU:HA	1.90	0.43
1:A:1237:TRP:CH2	1:A:1652:GLU:HG2	2.53	0.43
1:A:1680:ARG:HH12	1:A:1786:LEU:HD12	1.84	0.43
1:D:661:LYS:HD2	1:D:748:LEU:O	2.19	0.43
1:D:758:ARG:NH1	1:D:762:CYS:HA	2.34	0.43
1:D:1154:ASP:OD2	1:D:1156:THR:OG1	2.32	0.43
1:D:1307:UNK:O	1:D:1309:UNK:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1580:PHE:CE2	1:B:1592:PRO:HG2	2.54	0.43
1:B:3835:LEU:HD21	1:B:3880:PHE:CZ	2.53	0.43
1:B:4865:LYS:HG2	1:B:4875:LYS:CE	2.49	0.43
1:A:879:HIS:CG	1:A:921:ASN:HD22	2.36	0.43
1:A:1735:ILE:HD11	1:A:2201:LEU:HD11	1.99	0.43
1:C:626:LEU:HD23	1:C:628:GLY:N	2.34	0.43
1:C:660:GLY:HA3	1:C:750:LEU:HD21	2.01	0.43
1:C:831:ARG:HE	1:C:840:VAL:HG11	1.84	0.43
1:C:1087:ARG:HB2	1:C:1223:PHE:CD2	2.54	0.43
1:C:1651:LEU:HD13	1:C:1702:HIS:NE2	2.34	0.43
1:D:2095:GLN:HA	1:D:2127:GLN:OE1	2.18	0.43
1:D:4583:SER:HG	1:D:4630:TYR:HE1	1.64	0.43
1:B:661:LYS:HD2	1:B:748:LEU:O	2.19	0.43
1:B:1307:UNK:O	1:B:1309:UNK:N	2.51	0.43
1:A:1087:ARG:HB2	1:A:1223:PHE:CD2	2.54	0.43
1:A:2648:UNK:HA	1:A:2869:ARG:CZ	2.49	0.43
1:A:2912:THR:OG1	1:A:2914:LYS:NZ	2.38	0.43
1:A:3891:LEU:HD23	1:A:3891:LEU:HA	1.91	0.43
1:A:5004:THR:HG22	1:A:5005:GLY:H	1.84	0.43
1:C:1580:PHE:CE2	1:C:1592:PRO:HG2	2.54	0.43
1:C:3798:LEU:HD23	1:C:3798:LEU:HA	1.85	0.43
1:D:2930:LEU:HD23	1:D:2930:LEU:HA	1.88	0.43
1:B:1207:ASP:OD1	1:B:1207:ASP:N	2.48	0.43
1:A:2356:LEU:HA	1:A:2359:ARG:HG2	2.00	0.42
1:A:2891:LYS:O	1:A:2894:LEU:HD23	2.18	0.42
1:C:707:VAL:HG13	1:C:713:SER:HB3	2.01	0.42
1:C:1735:ILE:HD11	1:C:2201:LEU:HD11	2.01	0.42
1:A:758:ARG:CZ	1:A:762:CYS:H	2.33	0.42
1:A:765:GLN:HG3	1:A:1387:UNK:C	2.50	0.42
1:A:2880:GLU:OE1	1:A:2883:HIS:NE2	2.42	0.42
1:C:5004:THR:HG22	1:C:5005:GLY:H	1.84	0.42
1:D:4851:TYR:OH	1:D:4919:THR:HG23	2.19	0.42
1:B:1313:UNK:O	1:B:1315:UNK:N	2.51	0.42
1:B:1966:VAL:HG21	1:B:3649:ALA:HB1	2.00	0.42
1:A:157:ARG:CZ	1:A:164:ARG:HH22	2.32	0.42
1:A:1204:LEU:HD12	1:A:1226:PHE:HB3	2.01	0.42
1:A:1651:LEU:HD13	1:A:1702:HIS:NE2	2.34	0.42
1:A:2182:ILE:O	1:A:2185:ILE:HG22	2.19	0.42
1:A:4981:GLU:HB2	1:A:4982:GLU:OE2	2.19	0.42
1:D:707:VAL:HG13	1:D:713:SER:HB3	2.01	0.42
1:D:3969:ILE:HG23	1:D:3977:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:ARG:CZ	1:B:762:CYS:H	2.33	0.42
1:B:2891:LYS:O	1:B:2894:LEU:HD23	2.19	0.42
1:B:2912:THR:OG1	1:B:2914:LYS:NZ	2.39	0.42
1:B:4849:TYR:HD2	1:B:4850:LEU:HD23	1.84	0.42
1:A:1639:LEU:HD23	1:A:1640:HIS:N	2.34	0.42
1:C:955:LEU:HB3	1:C:966:LYS:HZ1	1.84	0.42
1:C:4583:SER:HG	1:C:4630:TYR:HE1	1.65	0.42
1:C:4913:ARG:HG3	1:C:4913:ARG:HH11	1.84	0.42
1:D:1798:LEU:N	1:D:1798:LEU:CD2	2.81	0.42
1:D:4112:LEU:O	1:D:4115:SER:OG	2.34	0.42
1:B:660:GLY:HA3	1:B:750:LEU:HD21	2.01	0.42
1:A:626:LEU:HD23	1:A:628:GLY:N	2.33	0.42
1:C:1176:GLU:CD	1:C:1176:GLU:H	2.23	0.42
1:C:1639:LEU:HD23	1:C:1640:HIS:N	2.34	0.42
1:D:4071:ILE:HD11	1:D:4102:GLN:HE21	1.84	0.42
1:B:238:SER:OG	1:B:240:ASP:OD1	2.34	0.42
1:B:4851:TYR:CD1	1:B:4916:PHE:HE1	2.37	0.42
1:A:801:LYS:HE2	1:A:801:LYS:HB3	1.93	0.42
1:A:2643:UNK:HA	1:A:2871:LEU:O	2.19	0.42
1:A:4745:LEU:HD23	1:A:4745:LEU:HA	1.92	0.42
1:B:695:TYR:HA	1:B:696:PRO:HD3	1.95	0.42
1:B:879:HIS:CG	1:B:921:ASN:HD22	2.37	0.42
1:C:796:ARG:HH21	1:C:820:ARG:HH22	1.66	0.42
1:C:2463:LEU:HD23	1:C:2464:ASP:N	2.35	0.42
1:C:4197:ILE:O	1:C:4198:SER:OG	2.32	0.42
1:C:4921:PHE:CD2	1:D:4892:ARG:HD2	2.54	0.42
1:D:659:TYR:CG	1:D:810:PRO:HG2	2.55	0.42
1:D:1176:GLU:CD	1:D:1176:GLU:H	2.23	0.42
1:B:5004:THR:HG22	1:B:5005:GLY:H	1.84	0.42
1:A:2463:LEU:HD23	1:A:2464:ASP:N	2.35	0.42
1:A:4864:ASN:HA	1:A:4875:LYS:HE2	2.00	0.42
1:C:659:TYR:CG	1:C:810:PRO:HG2	2.55	0.42
1:C:2626:UNK:H	1:C:2892:GLN:HE21	1.68	0.42
1:D:54:ASN:HB2	1:D:57:ASN:HB2	2.01	0.42
1:D:758:ARG:CZ	1:D:762:CYS:H	2.32	0.42
1:D:1204:LEU:HD12	1:D:1226:PHE:HB3	2.02	0.42
1:B:932:LEU:HD12	1:B:933:LEU:HD22	2.02	0.42
1:B:1078:GLU:HB2	1:B:1081:TYR:CD2	2.53	0.42
1:B:4892:ARG:C	1:B:4894:GLY:H	2.23	0.42
1:A:2433:LEU:HD23	1:A:2433:LEU:HA	1.87	0.42
1:A:3969:ILE:HG23	1:A:3977:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASN:HB2	1:C:57:ASN:HB2	2.01	0.42
1:C:350:HIS:CE1	1:C:352:ALA:HB3	2.53	0.42
1:C:722:TRP:CD1	1:C:727:ALA:HA	2.55	0.42
1:D:660:GLY:HA3	1:D:750:LEU:HD21	2.01	0.42
1:D:765:GLN:OE1	1:D:765:GLN:N	2.53	0.42
1:D:1313:UNK:O	1:D:1315:UNK:N	2.51	0.42
1:B:350:HIS:CE1	1:B:352:ALA:HB3	2.53	0.42
1:B:765:GLN:OE1	1:B:765:GLN:N	2.53	0.42
1:B:3751:VAL:HG12	1:B:3756:LYS:HB2	2.02	0.42
1:A:659:TYR:CG	1:A:810:PRO:HG2	2.55	0.42
1:A:1974:ARG:HH21	1:A:3642:TYR:HB2	1.85	0.42
1:A:2368:LEU:HD13	1:A:2376:LEU:HD11	2.02	0.42
1:A:2579:UNK:N	1:A:2902:HIS:O	2.53	0.42
1:C:2182:ILE:O	1:C:2185:ILE:HG22	2.20	0.42
1:D:181:HIS:ND1	1:D:198:THR:OG1	2.53	0.42
1:D:214:VAL:HG22	1:D:341:TYR:CE1	2.55	0.42
1:D:765:GLN:HG3	1:D:1387:UNK:C	2.50	0.42
1:D:2626:UNK:H	1:D:2892:GLN:HE21	1.68	0.42
1:D:4851:TYR:CD1	1:D:4916:PHE:HE1	2.38	0.42
1:B:214:VAL:HG22	1:B:341:TYR:CE1	2.55	0.42
1:B:796:ARG:HH21	1:B:820:ARG:HH22	1.67	0.42
1:B:1618:ARG:O	1:B:1626:TRP:C	2.57	0.42
1:C:1077:ALA:HB2	1:C:1190:PRO:HG2	2.02	0.41
1:C:1974:ARG:HH21	1:C:3642:TYR:HB2	1.85	0.41
1:C:4793:GLY:O	1:C:4797:VAL:HG23	2.19	0.41
1:D:3751:VAL:HG12	1:D:3756:LYS:HB2	2.02	0.41
1:D:3798:LEU:HD23	1:D:3798:LEU:HA	1.85	0.41
1:D:4239:GLU:CD	1:D:4679:ARG:HH22	2.22	0.41
1:D:4745:LEU:HD23	1:D:4745:LEU:HA	1.92	0.41
1:C:526:LEU:O	1:C:530:ILE:HD12	2.20	0.41
1:C:758:ARG:CZ	1:C:762:CYS:H	2.33	0.41
1:C:765:GLN:N	1:C:765:GLN:OE1	2.53	0.41
1:C:4851:TYR:O	1:C:4855:ALA:N	2.48	0.41
1:D:526:LEU:O	1:D:530:ILE:HD12	2.20	0.41
1:D:722:TRP:CD1	1:D:727:ALA:HA	2.55	0.41
1:D:1966:VAL:HG21	1:D:3649:ALA:HB1	2.01	0.41
5:D:5105:POV:O12	5:D:5105:POV:C15	2.68	0.41
1:B:526:LEU:O	1:B:530:ILE:HD12	2.20	0.41
1:B:765:GLN:HG3	1:B:1387:UNK:C	2.50	0.41
1:B:1087:ARG:HB2	1:B:1223:PHE:CD2	2.54	0.41
1:B:1176:GLU:H	1:B:1176:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2463:LEU:HD23	1:B:2464:ASP:N	2.35	0.41
1:A:222:LEU:HD23	1:A:222:LEU:H	1.85	0.41
1:A:1154:ASP:OD2	1:A:1156:THR:OG1	2.32	0.41
1:C:4861:LYS:O	1:C:4863:TYR:N	2.54	0.41
1:D:1974:ARG:HH21	1:D:3642:TYR:HB2	1.85	0.41
1:D:2182:ILE:O	1:D:2185:ILE:HG22	2.21	0.41
1:D:2299:VAL:HG11	1:D:2356:LEU:CD2	2.51	0.41
1:D:3778:MET:O	1:D:3782:MET:HG2	2.20	0.41
1:B:54:ASN:HB2	1:B:57:ASN:HB2	2.01	0.41
1:B:479:GLN:HG3	1:B:536:ASN:OD1	2.20	0.41
1:B:659:TYR:CG	1:B:810:PRO:HG2	2.55	0.41
1:B:3713:LYS:HE2	1:B:3713:LYS:HB3	1.86	0.41
1:A:683:ARG:HE	1:A:717:ASP:HB2	1.85	0.41
1:C:445:LEU:HB3	1:C:521:LEU:HD21	2.03	0.41
1:C:4027:LEU:HD23	1:C:4027:LEU:HA	1.92	0.41
1:D:2297:LYS:O	1:D:2300:SER:OG	2.34	0.41
1:D:2463:LEU:HD23	1:D:2464:ASP:N	2.35	0.41
1:B:1639:LEU:HD23	1:B:1640:HIS:N	2.34	0.41
1:A:526:LEU:O	1:A:530:ILE:HD12	2.20	0.41
1:A:3661:TRP:CE2	1:A:3662:ILE:HG22	2.56	0.41
1:A:3798:LEU:HD23	1:A:3798:LEU:HA	1.85	0.41
1:C:479:GLN:HG3	1:C:536:ASN:OD1	2.21	0.41
1:C:3661:TRP:CE2	1:C:3662:ILE:HG22	2.56	0.41
1:B:222:LEU:HD23	1:B:222:LEU:H	1.85	0.41
1:B:1204:LEU:HD12	1:B:1226:PHE:HB3	2.02	0.41
1:B:4892:ARG:C	1:B:4894:GLY:N	2.74	0.41
1:A:687:ALA:HB3	1:A:778:PHE:CZ	2.55	0.41
1:A:4580:TYR:OH	1:A:4629:TYR:HB3	2.21	0.41
1:C:1617:THR:CB	1:C:1628:VAL:HG22	2.49	0.41
1:C:4865:LYS:H	1:C:4875:LYS:CE	2.29	0.41
5:C:5106:POV:C13	1:D:4629:TYR:CE2	3.02	0.41
1:D:4030:LEU:HD23	1:D:4030:LEU:HA	1.88	0.41
1:D:5013:MET:HE1	1:D:5021:PHE:HB3	2.03	0.41
1:B:246:TYR:HB3	1:B:373:LYS:HZ1	1.86	0.41
1:A:765:GLN:OE1	1:A:765:GLN:N	2.53	0.41
1:A:1176:GLU:H	1:A:1176:GLU:CD	2.23	0.41
1:A:4865:LYS:HG2	1:A:4875:LYS:CE	2.50	0.41
1:C:765:GLN:HG3	1:C:1387:UNK:C	2.50	0.41
1:D:978:THR:HA	1:D:979:PRO:HD3	1.95	0.41
1:D:3906:GLN:N	1:D:3906:GLN:OE1	2.54	0.41
1:D:4079:ASP:OD1	1:D:4080:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:VAL:HG11	1:B:1048:GLY:HA2	2.03	0.41
1:B:2665:UNK:C	1:B:2922:LYS:HZ1	2.32	0.41
1:B:3780:LEU:HD23	1:B:3780:LEU:HA	1.86	0.41
1:B:3962:PHE:O	1:B:3966:THR:HG23	2.20	0.41
1:B:4999:ASP:HB3	1:B:5002:GLU:HG2	2.03	0.41
5:B:5106:POV:O12	5:B:5106:POV:C15	2.69	0.41
1:A:224:HIS:O	1:A:229:GLU:HB2	2.20	0.41
1:A:4876:CYS:HB2	1:A:4882:CYS:HB2	1.51	0.41
1:A:4892:ARG:O	1:A:4894:GLY:N	2.53	0.41
1:C:2368:LEU:HD13	1:C:2376:LEU:HD11	2.03	0.41
1:B:1974:ARG:HH21	1:B:3642:TYR:HB2	1.85	0.41
1:B:4907:ASP:OD1	1:B:4907:ASP:N	2.53	0.41
1:A:54:ASN:HB2	1:A:57:ASN:HB2	2.01	0.41
1:A:975:VAL:HG11	1:A:1048:GLY:HA2	2.03	0.41
1:A:4079:ASP:OD1	1:A:4080:TYR:N	2.54	0.41
5:A:5106:POV:O12	5:A:5106:POV:C15	2.69	0.41
1:C:631:LEU:HD12	1:C:631:LEU:HA	1.96	0.41
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	2.03	0.41
1:C:3751:VAL:HG12	1:C:3756:LYS:HB2	2.02	0.41
1:C:3962:PHE:O	1:C:3966:THR:HG23	2.21	0.41
1:C:3969:ILE:HG23	1:C:3977:GLN:HG2	2.02	0.41
1:C:4205:TRP:HH2	1:C:4214:LYS:HD3	1.86	0.41
1:C:4921:PHE:HD2	1:D:4892:ARG:HD2	1.86	0.41
1:D:13:PHE:HE1	1:D:164:ARG:HD2	1.86	0.41
1:D:222:LEU:HD23	1:D:222:LEU:H	1.85	0.41
1:D:975:VAL:HG11	1:D:1048:GLY:HA2	2.03	0.41
1:D:4792:LEU:HD23	1:D:4792:LEU:HA	1.86	0.41
1:B:722:TRP:CD1	1:B:727:ALA:HA	2.55	0.41
1:B:1639:LEU:N	1:B:1648:MET:O	2.54	0.41
1:B:1815:LEU:HD13	1:B:1845:VAL:HG21	2.03	0.41
1:B:2875:ALA:HB1	1:B:2939:ARG:HD3	2.03	0.41
1:B:3969:ILE:HG23	1:B:3977:GLN:HG2	2.02	0.41
1:A:3906:GLN:N	1:A:3906:GLN:OE1	2.54	0.41
1:A:3937:TYR:OH	1:A:3944:GLU:OE2	2.31	0.41
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.21	0.41
1:C:224:HIS:O	1:C:229:GLU:HB2	2.21	0.41
1:C:4177:TYR:CE1	1:C:4199:GLU:HB3	2.56	0.41
1:C:4907:ASP:N	1:C:4907:ASP:OD1	2.54	0.41
1:D:1078:GLU:HB2	1:D:1081:TYR:CD2	2.53	0.41
1:D:2579:UNK:N	1:D:2902:HIS:O	2.54	0.41
1:D:3962:PHE:O	1:D:3966:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4154:VAL:O	1:D:4154:VAL:HG13	2.21	0.41
1:D:4907:ASP:OD1	1:D:4907:ASP:N	2.53	0.41
1:D:4999:ASP:HB3	1:D:5002:GLU:HG2	2.03	0.41
1:B:445:LEU:HB3	1:B:521:LEU:HD21	2.03	0.41
1:B:928:THR:HA	1:B:931:THR:HG22	2.02	0.41
1:B:2299:VAL:HG11	1:B:2356:LEU:CD2	2.51	0.41
1:B:4736:ARG:O	1:B:4739:GLU:HG3	2.21	0.41
1:A:220:LEU:HD23	1:A:260:TRP:O	2.21	0.40
1:A:629:ARG:HB3	1:A:634:GLN:CD	2.41	0.40
1:A:1077:ALA:HB2	1:A:1190:PRO:HG2	2.02	0.40
1:A:4156:HIS:N	1:A:4161:ARG:HH12	2.19	0.40
1:A:4907:ASP:N	1:A:4907:ASP:OD1	2.53	0.40
1:C:2579:UNK:N	1:C:2902:HIS:O	2.53	0.40
1:C:3827:GLY:HA2	1:C:3830:GLN:HG2	2.03	0.40
1:C:3906:GLN:OE1	1:C:3906:GLN:N	2.54	0.40
1:C:4154:VAL:HG13	1:C:4154:VAL:O	2.21	0.40
1:B:661:LYS:HE3	1:B:747:CYS:HB2	2.03	0.40
1:B:1617:THR:HA	1:B:1628:VAL:HG22	2.01	0.40
1:B:2182:ILE:O	1:B:2185:ILE:HG22	2.21	0.40
1:B:2626:UNK:H	1:B:2892:GLN:HE21	1.68	0.40
1:A:412:ASN:HA	1:A:415:ILE:HG22	2.03	0.40
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.40	0.40
1:A:3751:VAL:HG12	1:A:3756:LYS:HB2	2.02	0.40
1:A:4060:LYS:O	1:A:4064:MET:HG3	2.22	0.40
1:A:4094:GLN:HG3	1:A:4108:ILE:HG21	2.03	0.40
1:C:157:ARG:CZ	1:C:164:ARG:HH22	2.34	0.40
1:C:214:VAL:HG22	1:C:341:TYR:CE1	2.55	0.40
1:C:220:LEU:HD23	1:C:260:TRP:O	2.22	0.40
1:C:222:LEU:HD23	1:C:222:LEU:H	1.85	0.40
1:C:975:VAL:HG11	1:C:1048:GLY:HA2	2.03	0.40
1:C:2380:ILE:O	1:C:2384:ILE:HG12	2.22	0.40
5:C:5106:POV:O12	5:C:5106:POV:C15	2.69	0.40
1:D:224:HIS:O	1:D:229:GLU:HB2	2.20	0.40
1:D:553:ARG:CZ	1:D:1593:PRO:HG3	2.51	0.40
1:D:1639:LEU:N	1:D:1648:MET:O	2.55	0.40
1:D:1819:VAL:HG12	1:D:1926:LEU:HD13	2.03	0.40
1:D:3827:GLY:HA2	1:D:3830:GLN:HG2	2.03	0.40
1:D:3937:TYR:OH	1:D:3944:GLU:OE2	2.31	0.40
1:D:4027:LEU:HD23	1:D:4027:LEU:HA	1.92	0.40
1:B:139:GLU:OE2	1:B:139:GLU:N	2.52	0.40
1:B:412:ASN:HA	1:B:415:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ARG:HB3	1:B:634:GLN:CD	2.42	0.40
1:A:214:VAL:HG22	1:A:341:TYR:CE1	2.55	0.40
1:A:553:ARG:CZ	1:A:1593:PRO:HG3	2.51	0.40
1:A:2114:PRO:HA	1:A:2117:VAL:HG12	2.03	0.40
1:C:4867:GLU:OE1	1:C:4875:LYS:NZ	2.39	0.40
1:D:1618:ARG:O	1:D:1626:TRP:C	2.55	0.40
1:D:2285:GLU:OE1	1:D:2285:GLU:N	2.55	0.40
1:D:4876:CYS:HB2	1:D:4882:CYS:HB2	1.51	0.40
1:B:2380:ILE:O	1:B:2384:ILE:HG12	2.22	0.40
1:B:4156:HIS:N	1:B:4161:ARG:HH12	2.20	0.40
1:B:4983:HIS:O	1:B:4983:HIS:ND1	2.53	0.40
1:B:4984:ASN:O	1:B:4985:LEU:HG	2.22	0.40
1:A:2626:UNK:H	1:A:2892:GLN:HE21	1.68	0.40
1:A:4242:ILE:HD12	1:A:4993:MET:SD	2.61	0.40
1:D:103:TYR:CE2	1:D:163:VAL:HG12	2.56	0.40
1:D:479:GLN:HG3	1:D:536:ASN:OD1	2.21	0.40
1:D:805:PRO:HB2	1:D:808:TYR:CE2	2.56	0.40
1:D:2644:UNK:O	1:D:2873:ALA:N	2.41	0.40
1:B:213:TYR:CD1	1:B:337:PRO:HB2	2.56	0.40
1:B:220:LEU:HD23	1:B:260:TRP:O	2.22	0.40
1:B:4154:VAL:HG13	1:B:4154:VAL:O	2.22	0.40
1:B:4745:LEU:HD23	1:B:4745:LEU:HA	1.92	0.40
1:A:213:TYR:CD1	1:A:337:PRO:HB2	2.57	0.40
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	2.04	0.40
1:A:2868:SER:OG	1:A:2869:ARG:N	2.55	0.40
1:A:4154:VAL:O	1:A:4154:VAL:HG13	2.22	0.40
1:A:4239:GLU:CD	1:A:4679:ARG:HH22	2.22	0.40
1:C:687:ALA:HB3	1:C:778:PHE:CZ	2.57	0.40
1:C:920:TYR:O	1:C:923:GLN:HG2	2.22	0.40
1:C:4030:LEU:HD23	1:C:4030:LEU:HA	1.88	0.40
1:C:4999:ASP:HB3	1:C:5002:GLU:HG2	2.03	0.40
1:D:629:ARG:HB3	1:D:634:GLN:CD	2.41	0.40
1:D:758:ARG:NE	1:D:762:CYS:H	2.20	0.40
1:B:103:TYR:CE2	1:B:163:VAL:HG12	2.57	0.40
1:B:805:PRO:HB2	1:B:808:TYR:CE2	2.56	0.40
1:B:2579:UNK:N	1:B:2902:HIS:O	2.54	0.40
1:B:3906:GLN:N	1:B:3906:GLN:OE1	2.54	0.40
1:B:4876:CYS:HB2	1:B:4882:CYS:HB2	1.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	3203/5037 (64%)	2993 (93%)	207 (6%)	3 (0%)	51 83
1	B	3203/5037 (64%)	2988 (93%)	215 (7%)	0	100 100
1	C	3203/5037 (64%)	2989 (93%)	212 (7%)	2 (0%)	51 83
1	D	3203/5037 (64%)	2994 (94%)	207 (6%)	2 (0%)	51 83
All	All	12812/20148 (64%)	11964 (93%)	841 (7%)	7 (0%)	54 83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1797	ARG
1	A	2868	SER
1	C	1796	ALA
1	D	2868	SER
1	C	1797	ARG
1	A	1781	CYS
1	D	1795	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2512/3264 (77%)	2502 (100%)	10 (0%)	91 95
1	B	2512/3264 (77%)	2500 (100%)	12 (0%)	88 94
1	C	2512/3264 (77%)	2499 (100%)	13 (0%)	88 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	2508/3264 (77%)	2500 (100%)	8 (0%)	92 96
All	All	10044/13056 (77%)	10001 (100%)	43 (0%)	91 95

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ARG
1	A	553	ARG
1	A	1087	ARG
1	A	1141	ARG
1	A	2441	HIS
1	A	2920	ARG
1	A	3773	ARG
1	A	4631	PHE
1	A	4891	VAL
1	A	4892	ARG
1	C	178	ARG
1	C	553	ARG
1	C	1087	ARG
1	C	1141	ARG
1	C	1786	LEU
1	C	2441	HIS
1	C	2920	ARG
1	C	3773	ARG
1	C	4631	PHE
1	C	4632	LEU
1	C	4857	ASN
1	C	4859	PHE
1	C	4861	LYS
1	D	178	ARG
1	D	553	ARG
1	D	1141	ARG
1	D	2441	HIS
1	D	2920	ARG
1	D	3773	ARG
1	D	4631	PHE
1	D	4632	LEU
1	B	178	ARG
1	B	553	ARG
1	B	1087	ARG
1	B	1141	ARG
1	B	1786	LEU

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Mol	Chain	Res	Type
1	B	2441	HIS
1	B	2920	ARG
1	B	3773	ARG
1	B	3781	GLN
1	B	4631	PHE
1	B	4632	LEU
1	B	4891	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	379	HIS
1	A	921	ASN
1	A	2127	GLN
1	A	2188	ASN
1	A	3699	HIS
1	A	4201	ASN
1	C	278	GLN
1	C	379	HIS
1	C	634	GLN
1	C	921	ASN
1	C	1693	GLN
1	C	2127	GLN
1	C	2188	ASN
1	C	2291	GLN
1	C	2872	GLN
1	C	4201	ASN
1	C	4857	ASN
1	D	278	GLN
1	D	379	HIS
1	D	921	ASN
1	D	1693	GLN
1	D	2188	ASN
1	D	2872	GLN
1	D	3699	HIS
1	D	4201	ASN
1	B	278	GLN
1	B	379	HIS
1	B	634	GLN
1	B	921	ASN
1	B	2188	ASN

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Mol	Chain	Res	Type
1	B	2291	GLN
1	B	2872	GLN
1	B	3699	HIS
1	B	4201	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 12 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	POV	C	5107	-	14,14,51	48.40	2 (14%)	12,12,59	3.56	1 (8%)
5	POV	A	5105	-	14,14,51	48.40	2 (14%)	12,12,59	3.56	1 (8%)
4	ACP	D	5104	-	27,33,33	1.37	5 (18%)	32,52,52	1.59	6 (18%)
5	POV	C	5106	-	44,44,51	0.89	0	50,52,59	0.76	2 (4%)
5	POV	B	5106	-	44,44,51	0.89	0	50,52,59	0.76	2 (4%)
5	POV	D	5105	-	44,44,51	0.89	0	50,52,59	0.76	2 (4%)
4	ACP	C	5104	-	27,33,33	1.41	5 (18%)	32,52,52	1.62	6 (18%)
5	POV	A	5106	-	44,44,51	0.89	0	50,52,59	0.76	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	POV	B	5105	-	14,14,51	48.40	2 (14%)	12,12,59	3.56	1 (8%)
4	ACP	A	5104	-	27,33,33	1.41	5 (18%)	32,52,52	1.62	6 (18%)
4	ACP	B	5104	-	27,33,33	1.41	5 (18%)	32,52,52	1.63	6 (18%)
5	POV	C	5105	-	14,14,51	48.40	2 (14%)	12,12,59	3.56	1 (8%)

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	POV	C	5107	-	-	2/11/11/55	-
5	POV	A	5105	-	-	2/11/11/55	-
4	ACP	D	5104	-	-	6/15/38/38	0/3/3/3
5	POV	C	5106	-	-	21/48/48/55	-
5	POV	B	5106	-	-	21/48/48/55	-
5	POV	D	5105	-	-	21/48/48/55	-
4	ACP	C	5104	-	-	6/15/38/38	0/3/3/3
5	POV	A	5106	-	-	21/48/48/55	-
5	POV	B	5105	-	-	2/11/11/55	-
4	ACP	A	5104	-	-	6/15/38/38	0/3/3/3
4	ACP	B	5104	-	-	6/15/38/38	0/3/3/3
5	POV	C	5105	-	-	2/11/11/55	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5105	POV	C314-C313	181.01	16.36	1.49
5	C	5107	POV	C314-C313	181.01	16.36	1.49
5	C	5105	POV	C314-C313	181.00	16.36	1.49
5	B	5105	POV	C314-C313	181.00	16.36	1.49
5	A	5105	POV	C32-C33	-3.57	1.26	1.51
5	B	5105	POV	C32-C33	-3.56	1.26	1.51
5	C	5105	POV	C32-C33	-3.56	1.26	1.51
5	C	5107	POV	C32-C33	-3.55	1.26	1.51
4	A	5104	ACP	O4'-C4'	-3.05	1.38	1.45
4	C	5104	ACP	O4'-C4'	-3.03	1.38	1.45
4	B	5104	ACP	O4'-C4'	-3.03	1.38	1.45
4	A	5104	ACP	PG-O2G	2.82	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5104	ACP	PG-O2G	2.82	1.61	1.54
4	C	5104	ACP	PG-O2G	2.79	1.61	1.54
4	B	5104	ACP	PG-O2G	2.79	1.61	1.54
4	C	5104	ACP	PG-O3G	2.75	1.61	1.54
4	A	5104	ACP	PG-O3G	2.75	1.61	1.54
4	D	5104	ACP	PG-O3G	2.75	1.61	1.54
4	B	5104	ACP	PG-O3G	2.73	1.61	1.54
4	D	5104	ACP	O4'-C4'	-2.43	1.39	1.45
4	A	5104	ACP	PB-O3A	2.43	1.61	1.58
4	D	5104	ACP	PB-O3A	2.40	1.61	1.58
4	C	5104	ACP	PB-O3A	2.39	1.61	1.58
4	B	5104	ACP	PB-O3A	2.38	1.61	1.58
4	B	5104	ACP	PB-O2B	2.17	1.61	1.56
4	C	5104	ACP	PB-O2B	2.16	1.61	1.56
4	D	5104	ACP	PB-O2B	2.15	1.61	1.56
4	A	5104	ACP	PB-O2B	2.14	1.61	1.56

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	5105	POV	C314-C313-C312	-11.94	22.80	113.42
5	B	5105	POV	C314-C313-C312	-11.94	22.82	113.42
5	C	5107	POV	C314-C313-C312	-11.93	22.84	113.42
5	A	5105	POV	C314-C313-C312	-11.93	22.85	113.42
4	C	5104	ACP	PB-O3A-PA	-4.77	117.42	132.56
4	A	5104	ACP	PB-O3A-PA	-4.77	117.43	132.56
4	B	5104	ACP	PB-O3A-PA	-4.77	117.45	132.56
4	D	5104	ACP	PB-O3A-PA	-4.76	117.45	132.56
4	B	5104	ACP	N3-C2-N1	-3.84	122.67	128.68
4	C	5104	ACP	N3-C2-N1	-3.83	122.69	128.68
4	D	5104	ACP	N3-C2-N1	-3.83	122.70	128.68
4	A	5104	ACP	N3-C2-N1	-3.81	122.73	128.68
4	D	5104	ACP	C3'-C2'-C1'	2.99	105.47	100.98
4	B	5104	ACP	C3'-C2'-C1'	2.99	105.47	100.98
4	C	5104	ACP	C3'-C2'-C1'	2.96	105.44	100.98
4	A	5104	ACP	C3'-C2'-C1'	2.96	105.43	100.98
5	D	5105	POV	O13-P-O12	-2.56	95.85	107.75
5	B	5106	POV	O13-P-O12	-2.56	95.86	107.75
5	A	5106	POV	O13-P-O12	-2.55	95.88	107.75
5	C	5106	POV	O13-P-O12	-2.55	95.90	107.75
4	B	5104	ACP	C1'-N9-C4	-2.33	122.55	126.64
4	C	5104	ACP	C1'-N9-C4	-2.31	122.58	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5104	ACP	C1'-N9-C4	-2.30	122.60	126.64
4	A	5104	ACP	C4-C5-N7	-2.29	107.01	109.40
4	C	5104	ACP	C4-C5-N7	-2.28	107.02	109.40
4	D	5104	ACP	C1'-N9-C4	-2.28	122.64	126.64
4	D	5104	ACP	C4-C5-N7	-2.28	107.03	109.40
4	B	5104	ACP	C4-C5-N7	-2.28	107.03	109.40
4	B	5104	ACP	C2-N1-C6	2.11	122.37	118.75
4	C	5104	ACP	C2-N1-C6	2.08	122.31	118.75
4	A	5104	ACP	C2-N1-C6	2.08	122.31	118.75
4	D	5104	ACP	C2-N1-C6	2.05	122.26	118.75
5	D	5105	POV	O11-P-O14	2.02	116.96	109.07
5	A	5106	POV	O11-P-O14	2.01	116.93	109.07
5	C	5106	POV	O11-P-O14	2.01	116.93	109.07
5	B	5106	POV	O11-P-O14	2.01	116.92	109.07

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5104	ACP	PB-C3B-PG-O1G
4	A	5104	ACP	PB-C3B-PG-O2G
4	A	5104	ACP	PB-C3B-PG-O3G
4	A	5104	ACP	PG-C3B-PB-O1B
4	A	5104	ACP	PG-C3B-PB-O3A
4	C	5104	ACP	PB-C3B-PG-O1G
4	C	5104	ACP	PB-C3B-PG-O2G
4	C	5104	ACP	PB-C3B-PG-O3G
4	C	5104	ACP	PG-C3B-PB-O1B
4	C	5104	ACP	PG-C3B-PB-O3A
4	D	5104	ACP	PB-C3B-PG-O1G
4	D	5104	ACP	PB-C3B-PG-O2G
4	D	5104	ACP	PB-C3B-PG-O3G
4	D	5104	ACP	PG-C3B-PB-O1B
4	D	5104	ACP	PG-C3B-PB-O3A
4	B	5104	ACP	PB-C3B-PG-O1G
4	B	5104	ACP	PB-C3B-PG-O2G
4	B	5104	ACP	PB-C3B-PG-O3G
4	B	5104	ACP	PG-C3B-PB-O1B
4	B	5104	ACP	PG-C3B-PB-O3A
5	A	5106	POV	C1-O11-P-O12
5	A	5106	POV	C11-O12-P-O11
5	A	5106	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
5	C	5106	POV	C1-O11-P-O12
5	C	5106	POV	C11-O12-P-O11
5	C	5106	POV	C11-O12-P-O14
5	D	5105	POV	C1-O11-P-O12
5	D	5105	POV	C11-O12-P-O11
5	D	5105	POV	C11-O12-P-O14
5	B	5106	POV	C1-O11-P-O12
5	B	5106	POV	C11-O12-P-O11
5	B	5106	POV	C11-O12-P-O14
5	A	5106	POV	O21-C2-C3-O31
5	C	5106	POV	O21-C2-C3-O31
5	D	5105	POV	O21-C2-C3-O31
5	B	5106	POV	O21-C2-C3-O31
5	C	5106	POV	C31-C32-C33-C34
5	D	5105	POV	C31-C32-C33-C34
5	B	5106	POV	C31-C32-C33-C34
5	A	5106	POV	C31-C32-C33-C34
5	A	5106	POV	C311-C312-C313-C314
5	C	5106	POV	C311-C312-C313-C314
5	D	5105	POV	C311-C312-C313-C314
5	B	5106	POV	C311-C312-C313-C314
5	A	5106	POV	C26-C27-C28-C29
5	C	5106	POV	C26-C27-C28-C29
5	D	5105	POV	C26-C27-C28-C29
5	B	5106	POV	C26-C27-C28-C29
5	A	5105	POV	C311-C310-C39-C38
5	C	5107	POV	C311-C310-C39-C38
5	B	5105	POV	C311-C310-C39-C38
5	C	5105	POV	C311-C310-C39-C38
5	A	5106	POV	C37-C38-C39-C310
5	C	5106	POV	C37-C38-C39-C310
5	D	5105	POV	C37-C38-C39-C310
5	B	5106	POV	C37-C38-C39-C310
5	A	5106	POV	O11-C1-C2-O21
5	C	5106	POV	O11-C1-C2-O21
5	D	5105	POV	O11-C1-C2-O21
5	B	5106	POV	O11-C1-C2-O21
5	C	5106	POV	C22-C23-C24-C25
5	D	5105	POV	C22-C23-C24-C25
5	A	5106	POV	C22-C23-C24-C25
5	B	5106	POV	C22-C23-C24-C25
5	A	5106	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
5	C	5106	POV	C1-C2-C3-O31
5	D	5105	POV	C1-C2-C3-O31
5	B	5106	POV	C1-C2-C3-O31
5	B	5106	POV	C34-C35-C36-C37
5	A	5106	POV	C34-C35-C36-C37
5	C	5106	POV	C34-C35-C36-C37
5	D	5105	POV	C34-C35-C36-C37
5	A	5106	POV	C311-C310-C39-C38
5	D	5105	POV	C311-C310-C39-C38
5	B	5106	POV	C311-C310-C39-C38
5	C	5106	POV	C311-C310-C39-C38
5	C	5105	POV	C311-C312-C313-C314
5	C	5107	POV	C311-C312-C313-C314
5	B	5105	POV	C311-C312-C313-C314
5	A	5105	POV	C311-C312-C313-C314
5	A	5106	POV	C33-C34-C35-C36
5	C	5106	POV	C33-C34-C35-C36
5	D	5105	POV	C33-C34-C35-C36
5	B	5106	POV	C33-C34-C35-C36
5	A	5106	POV	C1-O11-P-O14
5	C	5106	POV	C1-O11-P-O14
5	D	5105	POV	C1-O11-P-O14
5	B	5106	POV	C1-O11-P-O14
5	A	5106	POV	O11-C1-C2-C3
5	C	5106	POV	O11-C1-C2-C3
5	D	5105	POV	O11-C1-C2-C3
5	B	5106	POV	O11-C1-C2-C3
4	A	5104	ACP	PG-C3B-PB-O2B
4	C	5104	ACP	PG-C3B-PB-O2B
4	D	5104	ACP	PG-C3B-PB-O2B
4	B	5104	ACP	PG-C3B-PB-O2B
5	A	5106	POV	C3-C2-O21-C21
5	C	5106	POV	C3-C2-O21-C21
5	D	5105	POV	C3-C2-O21-C21
5	B	5106	POV	C3-C2-O21-C21
5	A	5106	POV	C27-C28-C29-C210
5	C	5106	POV	C27-C28-C29-C210
5	D	5105	POV	C27-C28-C29-C210
5	B	5106	POV	C27-C28-C29-C210
5	C	5106	POV	C32-C33-C34-C35
5	B	5106	POV	C32-C33-C34-C35
5	D	5105	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
5	A	5106	POV	C32-C33-C34-C35
5	A	5106	POV	O31-C31-C32-C33
5	C	5106	POV	O31-C31-C32-C33
5	D	5105	POV	O31-C31-C32-C33
5	B	5106	POV	O31-C31-C32-C33
5	A	5106	POV	O32-C31-C32-C33
5	B	5106	POV	O32-C31-C32-C33
5	C	5106	POV	O32-C31-C32-C33
5	D	5105	POV	O32-C31-C32-C33

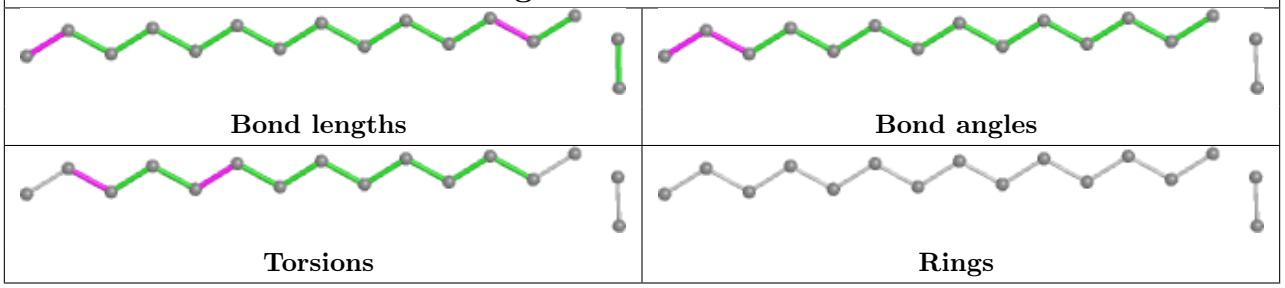
There are no ring outliers.

12 monomers are involved in 75 short contacts:

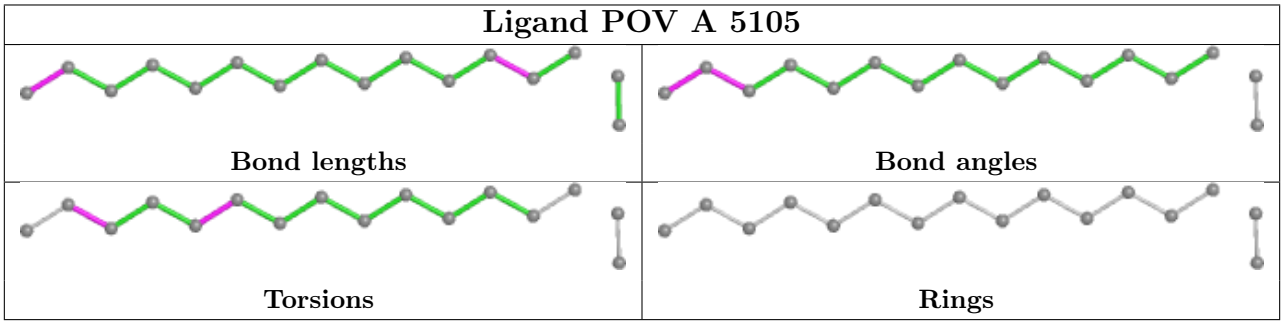
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5107	POV	4	0
5	A	5105	POV	2	0
4	D	5104	ACP	1	0
5	C	5106	POV	11	0
5	B	5106	POV	17	0
5	D	5105	POV	16	0
4	C	5104	ACP	2	0
5	A	5106	POV	16	0
5	B	5105	POV	2	0
4	A	5104	ACP	1	0
4	B	5104	ACP	1	0
5	C	5105	POV	2	0

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.

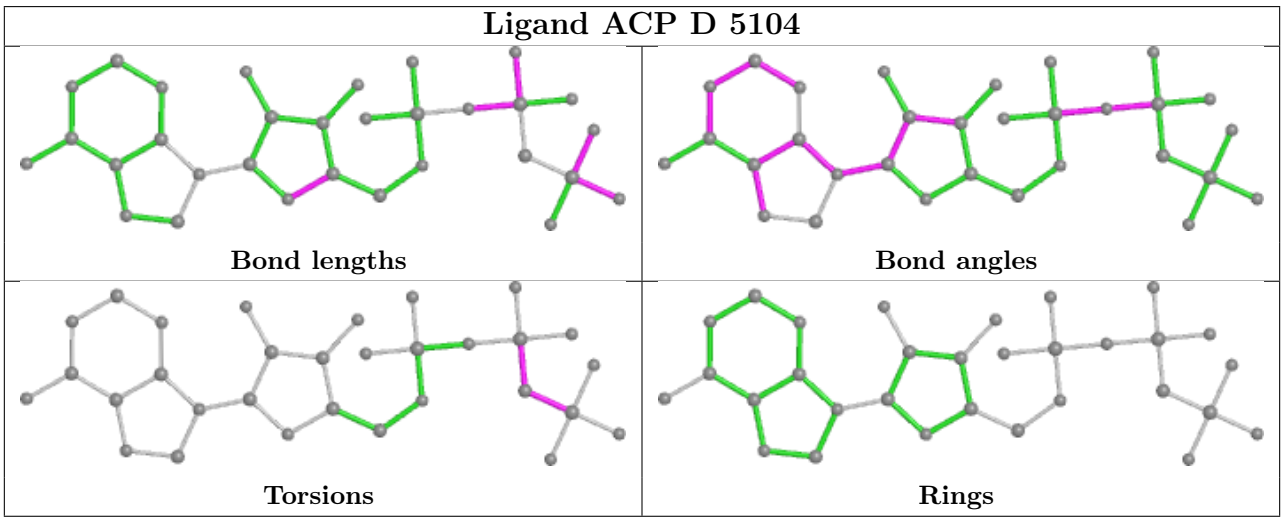
Ligand POV C 5107



Ligand POV A 5105



Ligand ACP D 5104



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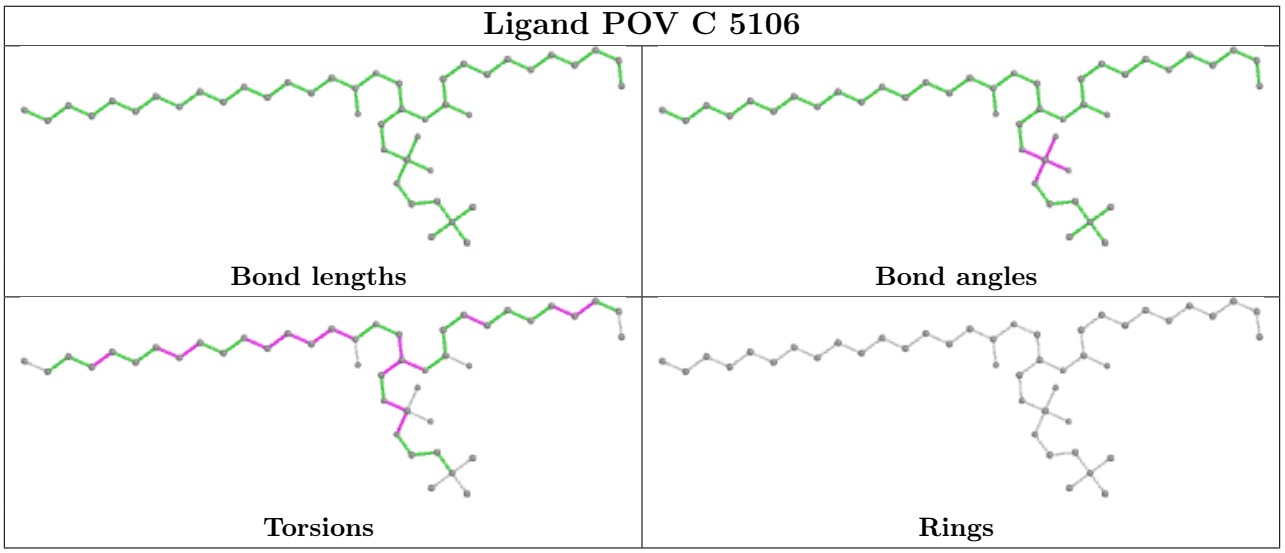
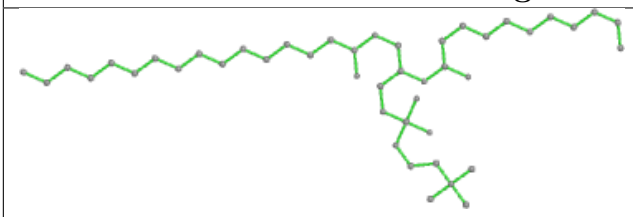
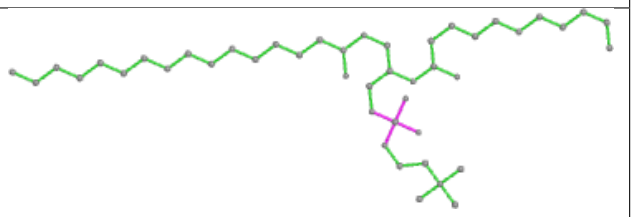


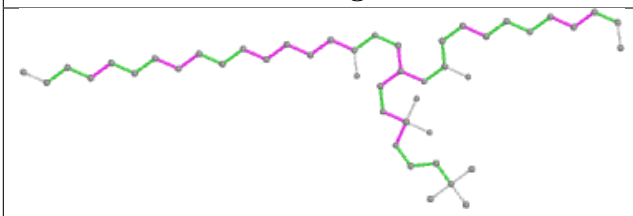
Ligand POV B 5106



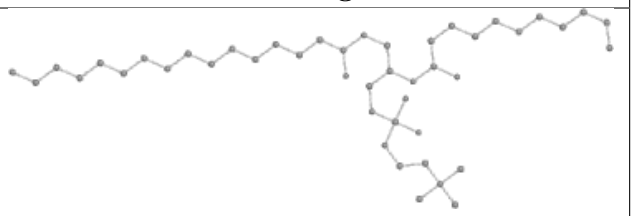
Bond lengths



Bond angles

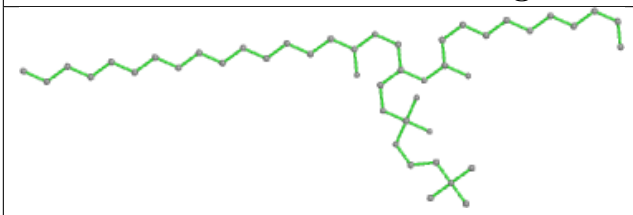


Torsions

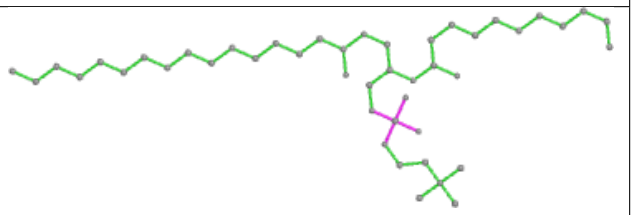


Rings

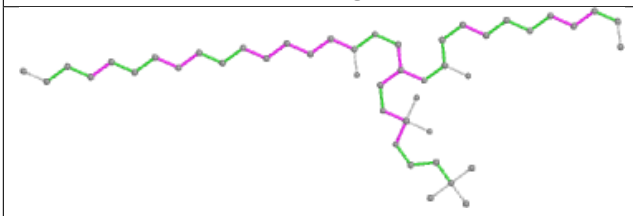
Ligand POV D 5105



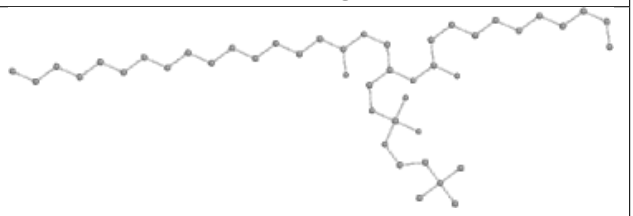
Bond lengths



Bond angles

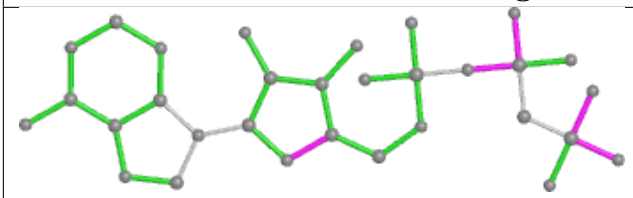


Torsions

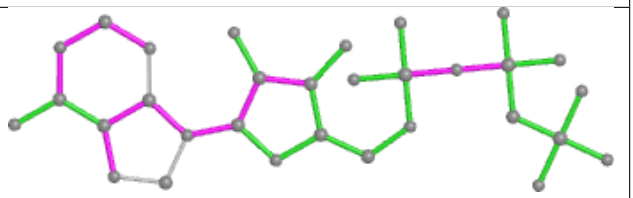


Rings

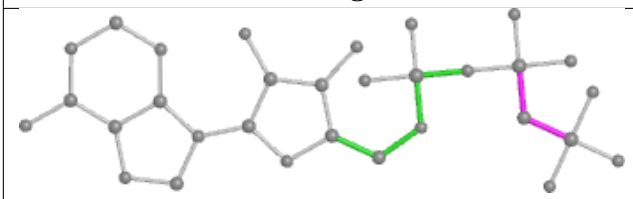
Ligand ACP C 5104



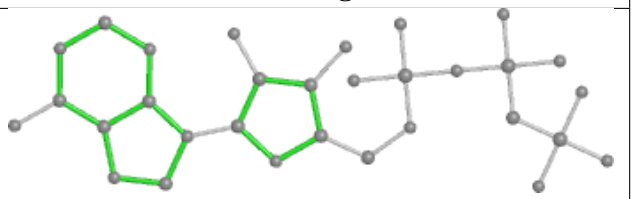
Bond lengths



Bond angles

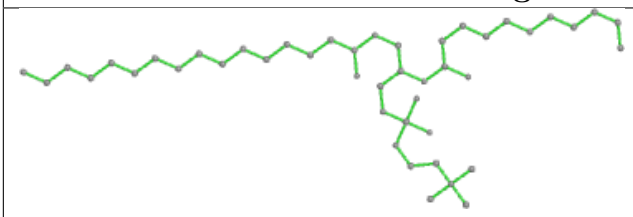


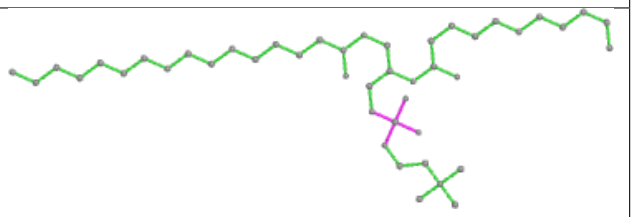
Torsions

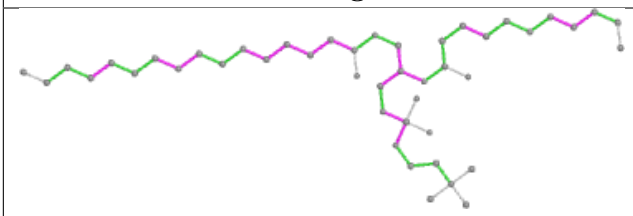


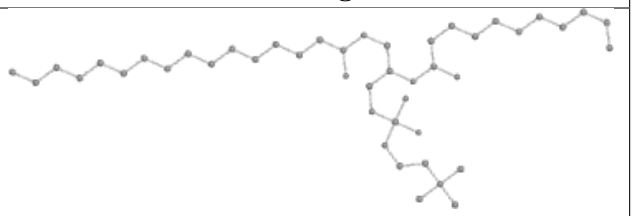
Rings

Ligand POV A 5106

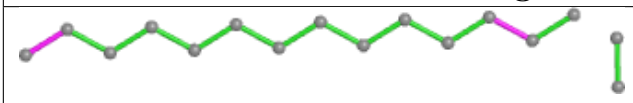

Bond lengths

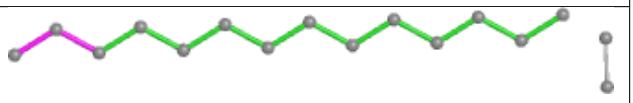

Bond angles

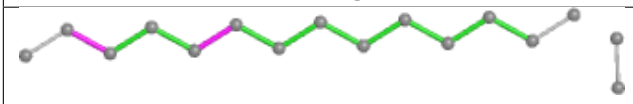

Torsions

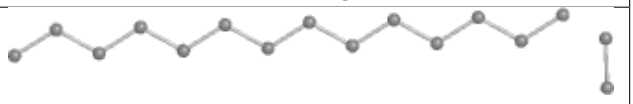

Rings

Ligand POV B 5105

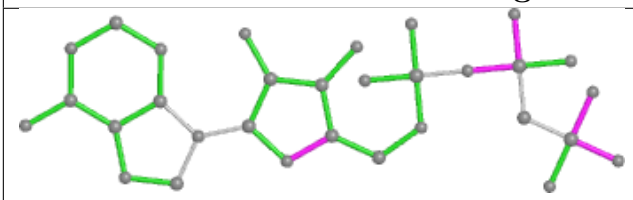

Bond lengths

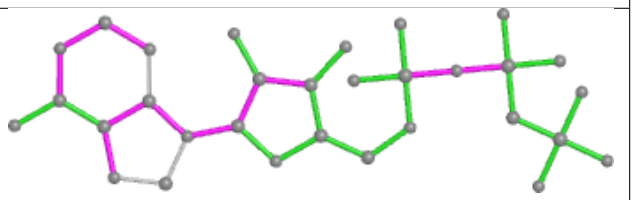

Bond angles

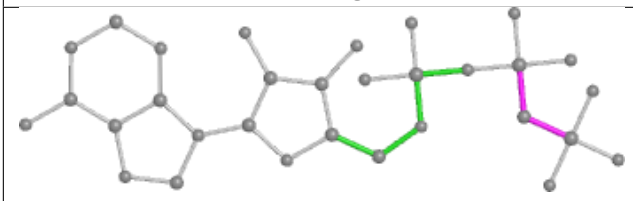

Torsions

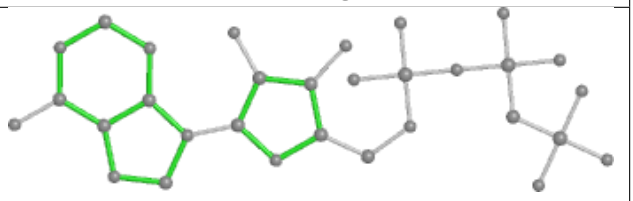

Rings

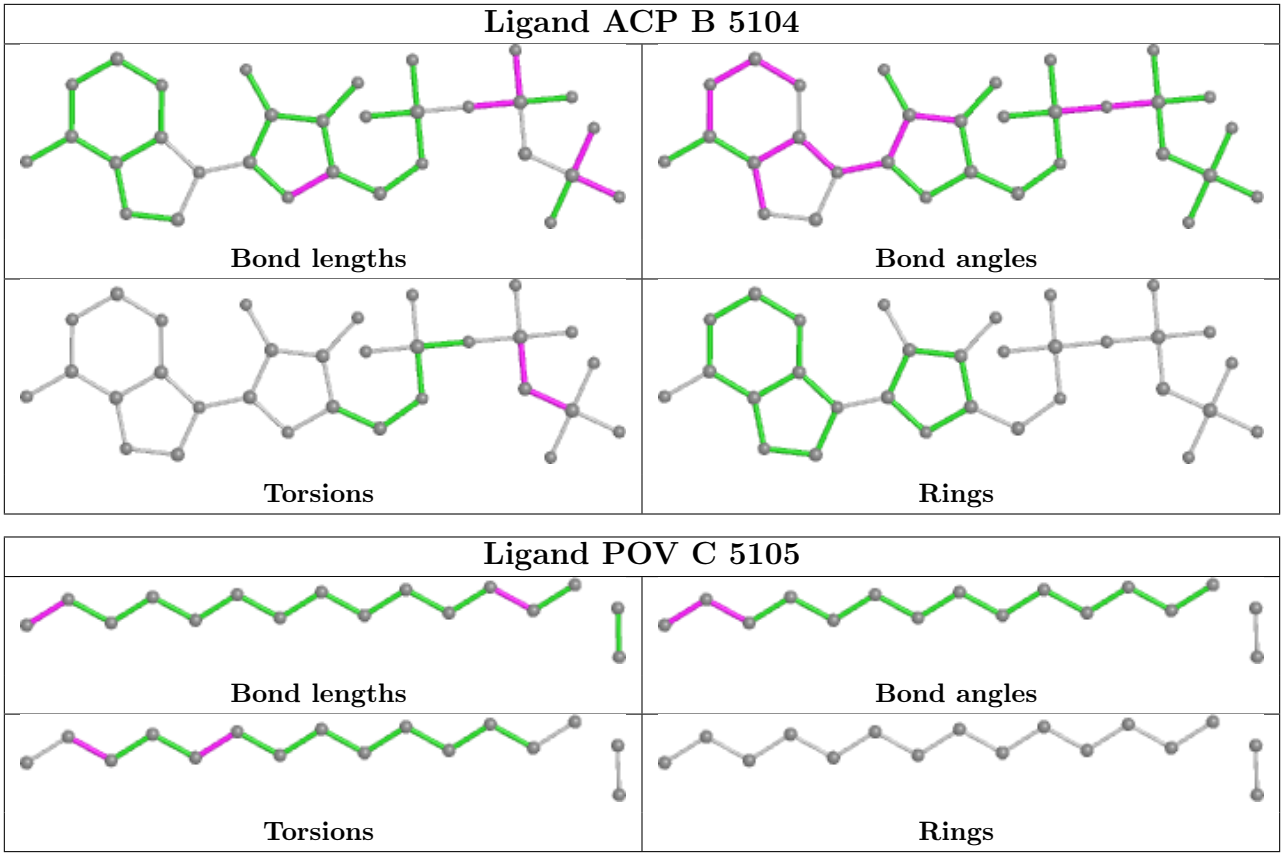
Ligand ACP A 5104


Bond lengths


Bond angles


Torsions


Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	7
1	D	7
1	B	7
1	A	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3122:UNK	C	3123:UNK	N	14.33
1	D	3122:UNK	C	3123:UNK	N	14.33
1	B	3122:UNK	C	3123:UNK	N	14.33
1	A	3122:UNK	C	3123:UNK	N	14.32

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3221:UNK	C	3222:UNK	N	13.70
1	C	3221:UNK	C	3222:UNK	N	13.70
1	D	3221:UNK	C	3222:UNK	N	13.70
1	B	3221:UNK	C	3222:UNK	N	13.70
1	C	3510:UNK	C	3511:UNK	N	13.52
1	D	3510:UNK	C	3511:UNK	N	13.52
1	B	3510:UNK	C	3511:UNK	N	13.52
1	A	3510:UNK	C	3511:UNK	N	13.51
1	B	3288:UNK	C	3289:UNK	N	13.29
1	A	3288:UNK	C	3289:UNK	N	13.28
1	C	3288:UNK	C	3289:UNK	N	13.28
1	D	3288:UNK	C	3289:UNK	N	13.28
1	A	3191:UNK	C	3192:UNK	N	8.26
1	C	3191:UNK	C	3192:UNK	N	8.26
1	B	3191:UNK	C	3192:UNK	N	8.26
1	D	3191:UNK	C	3192:UNK	N	8.25
1	C	3302:UNK	C	3303:UNK	N	8.15
1	D	3302:UNK	C	3303:UNK	N	8.15
1	A	3302:UNK	C	3303:UNK	N	8.14
1	B	3302:UNK	C	3303:UNK	N	8.14
1	A	1297:UNK	C	1298:UNK	N	7.59
1	C	1297:UNK	C	1298:UNK	N	7.59
1	D	1297:UNK	C	1298:UNK	N	7.59
1	B	1297:UNK	C	1298:UNK	N	7.59

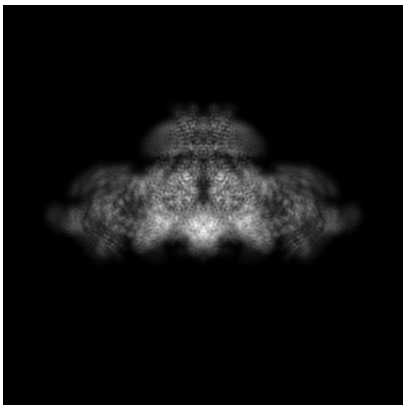
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25828. These allow visual inspection of the internal detail of the map and identification of artifacts.

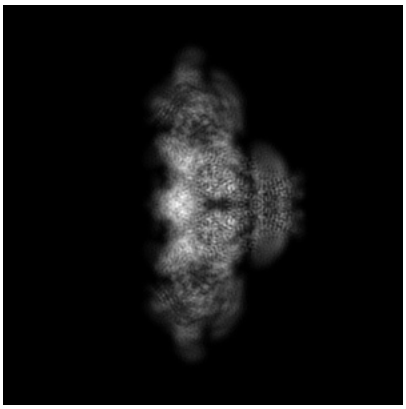
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

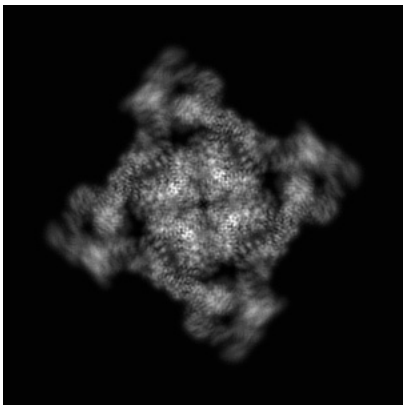
6.1.1 Primary map



X

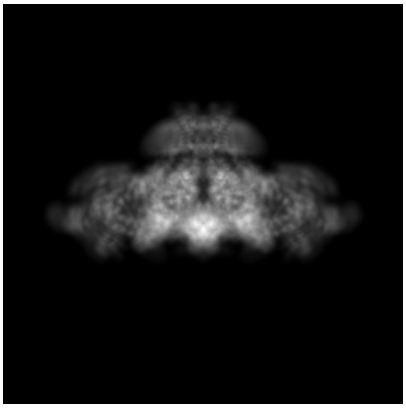


Y

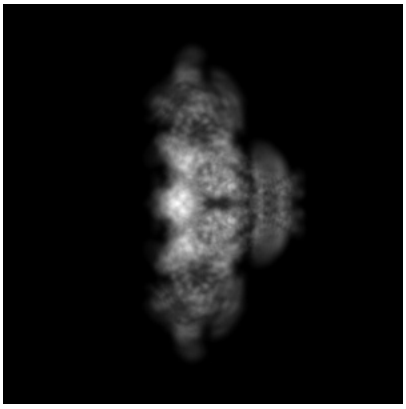


Z

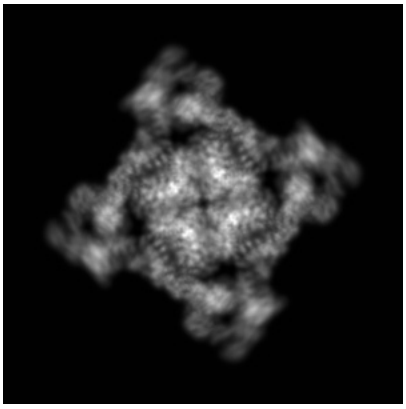
6.1.2 Raw map



X



Y

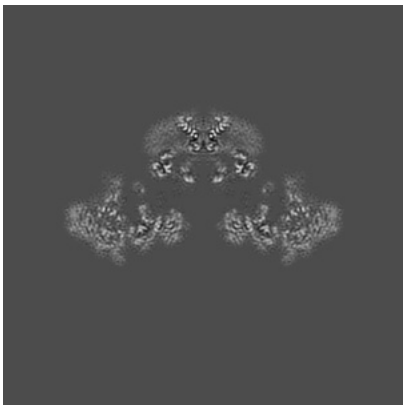


Z

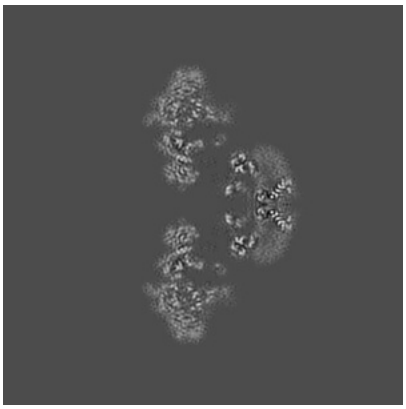
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

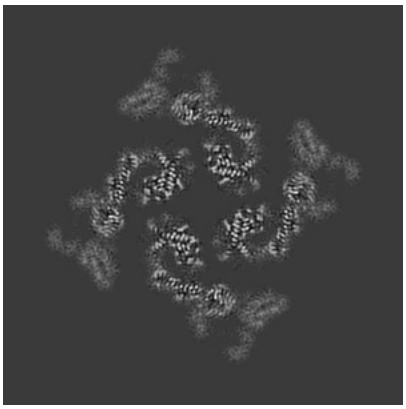
6.2.1 Primary map



X Index: 216

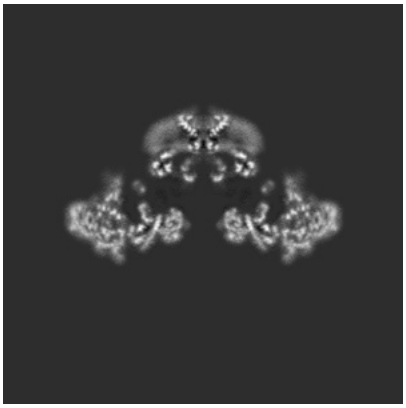


Y Index: 216

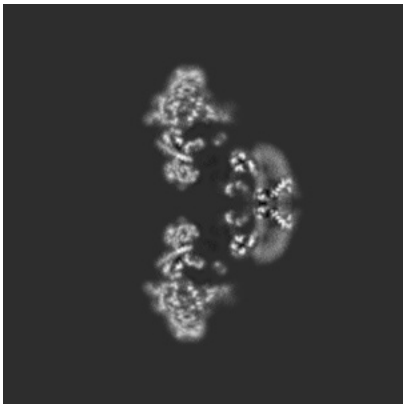


Z Index: 216

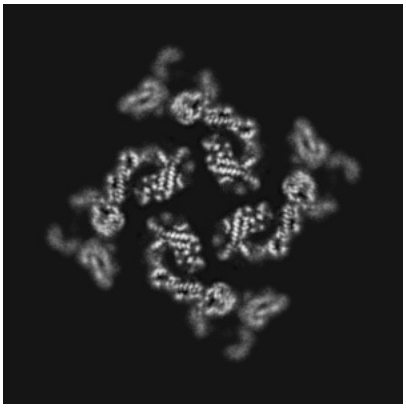
6.2.2 Raw map



X Index: 216



Y Index: 216

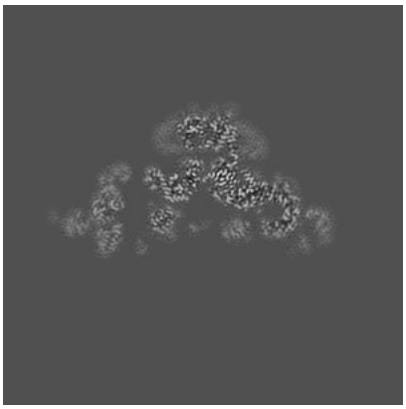


Z Index: 216

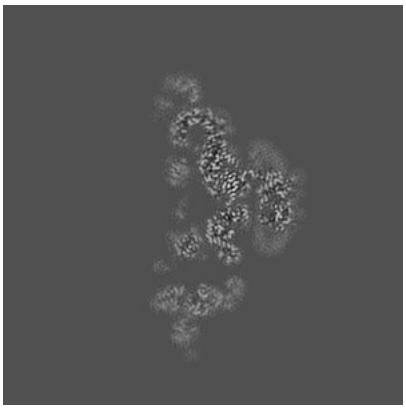
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

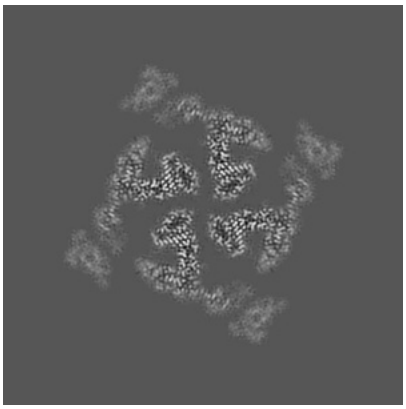
6.3.1 Primary map



X Index: 233

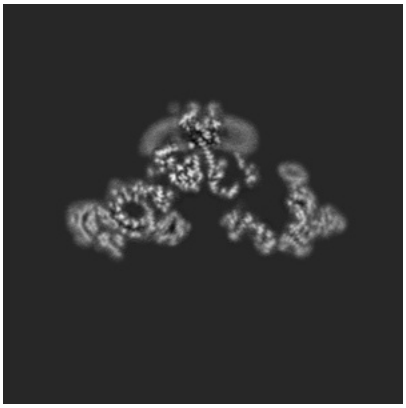


Y Index: 199

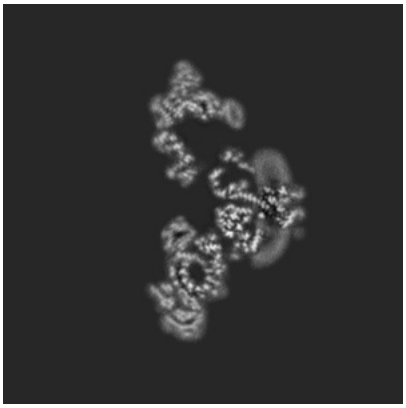


Z Index: 228

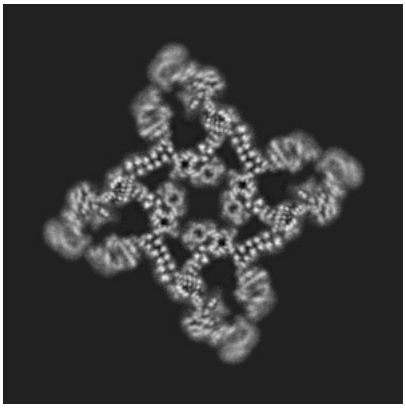
6.3.2 Raw map



X Index: 207



Y Index: 225

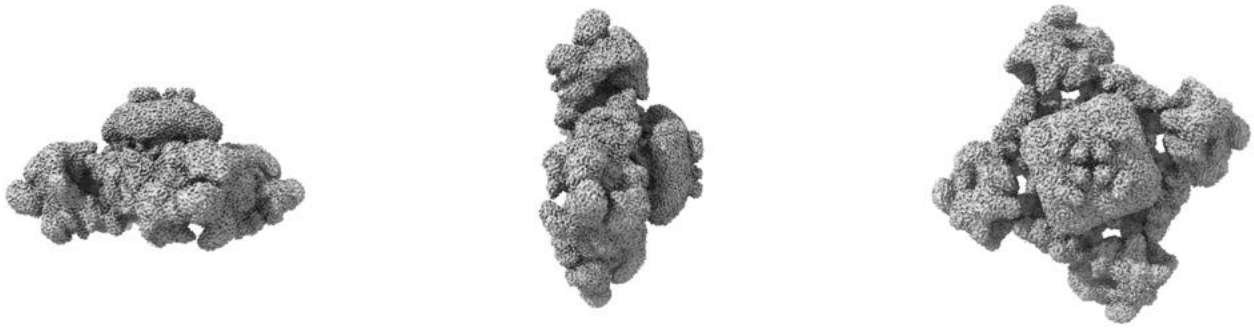


Z Index: 198

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

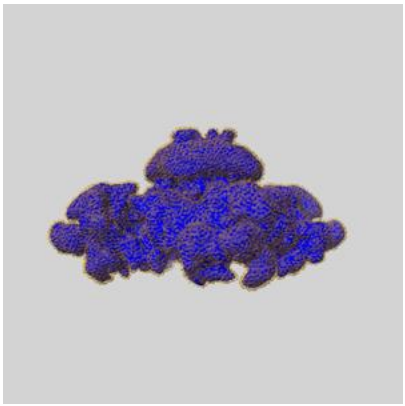
6.5 Mask visualisation

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

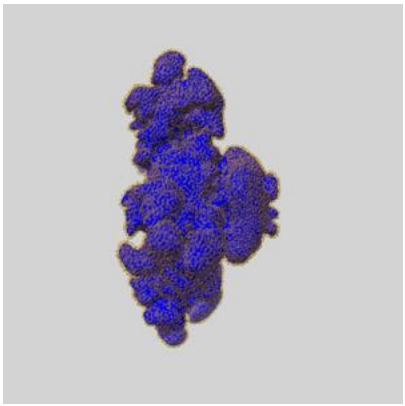
A mask typically either:

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

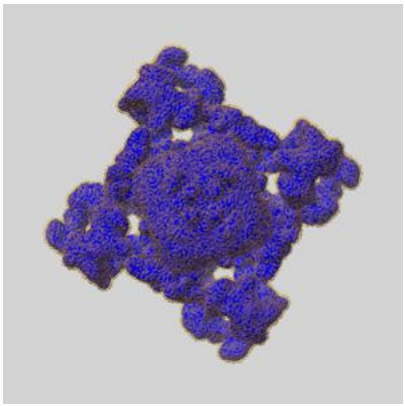
6.5.1 emd_25828_msk_1.map



X



Y

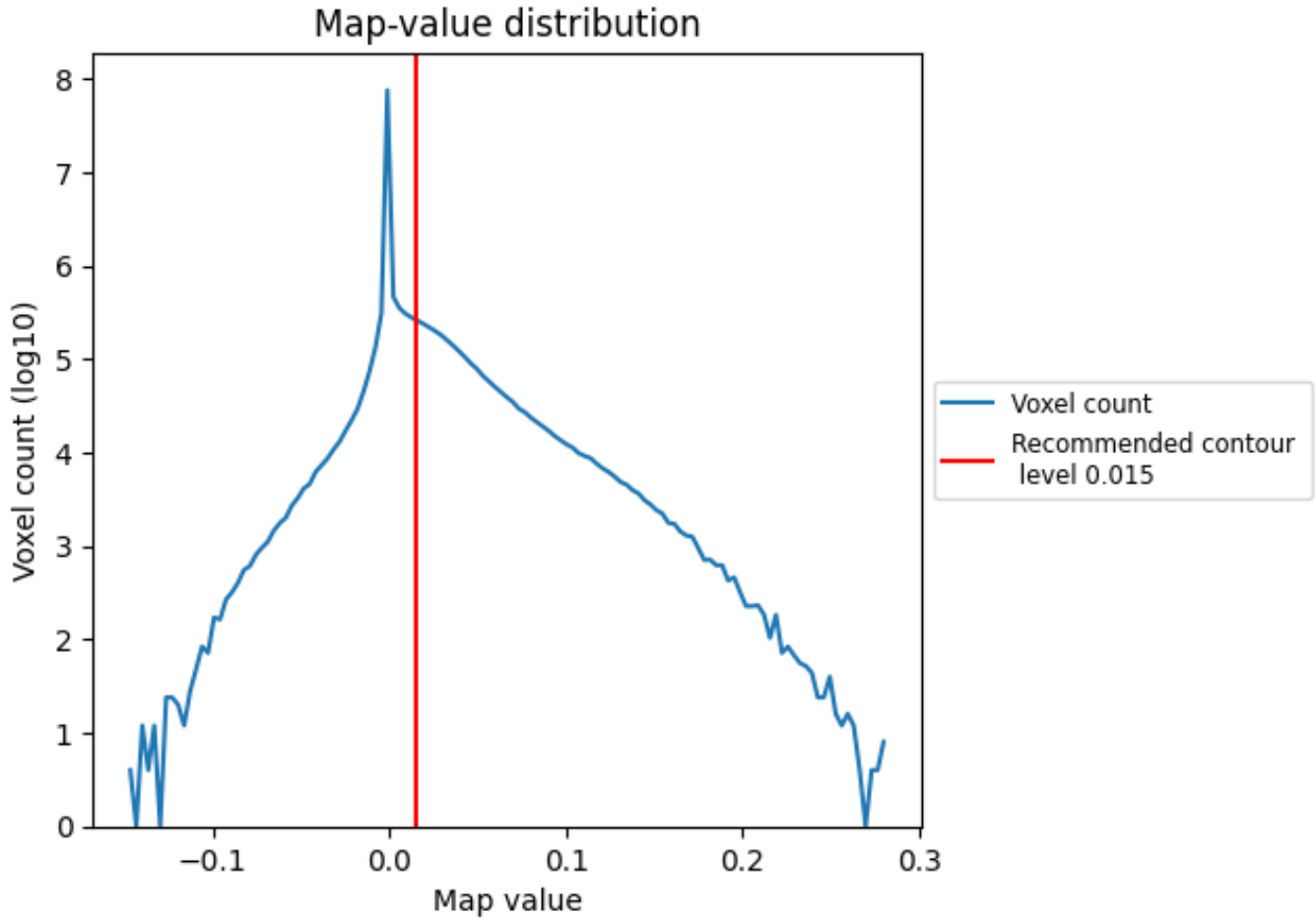


Z

7 Map analysis

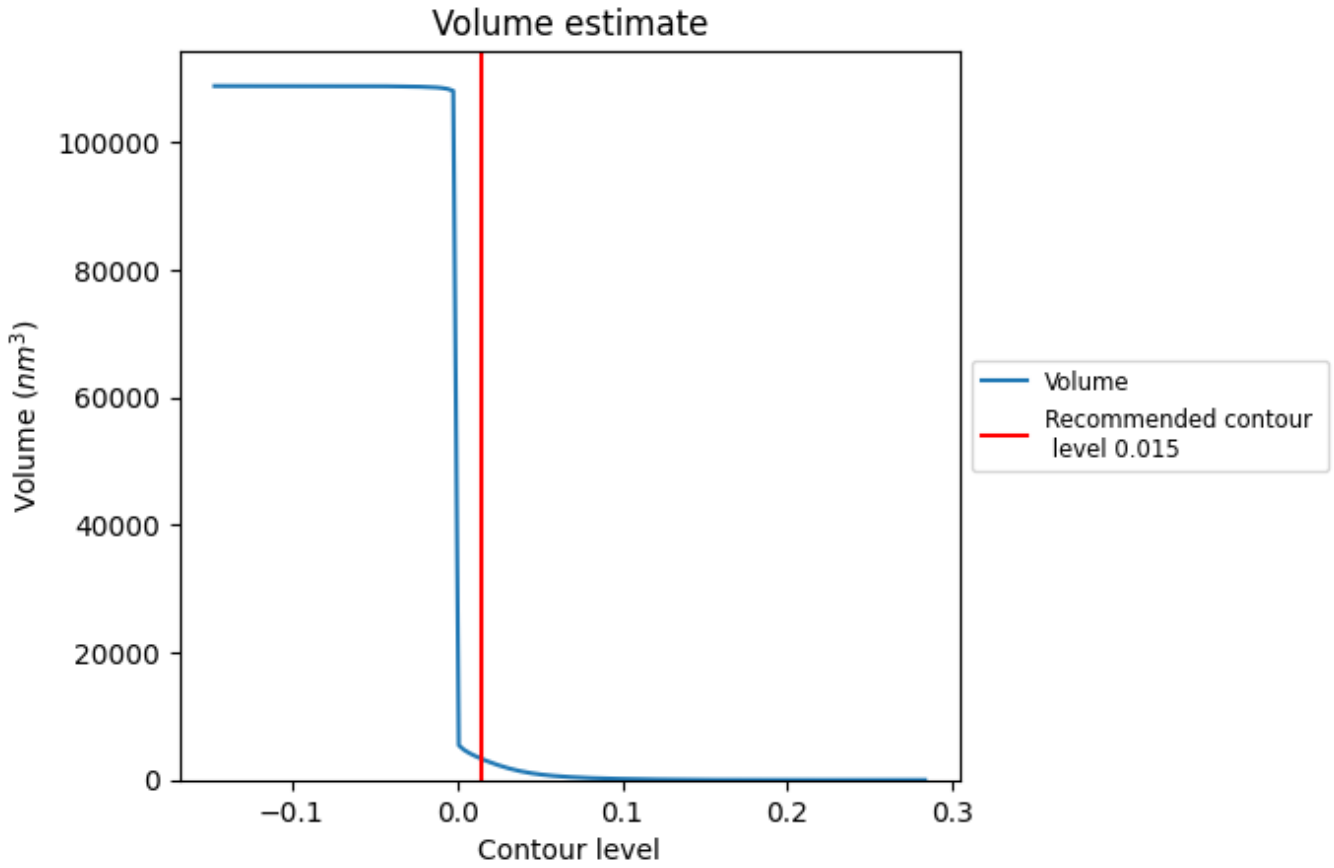
This section contains the results of statistical analysis of the map.

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.

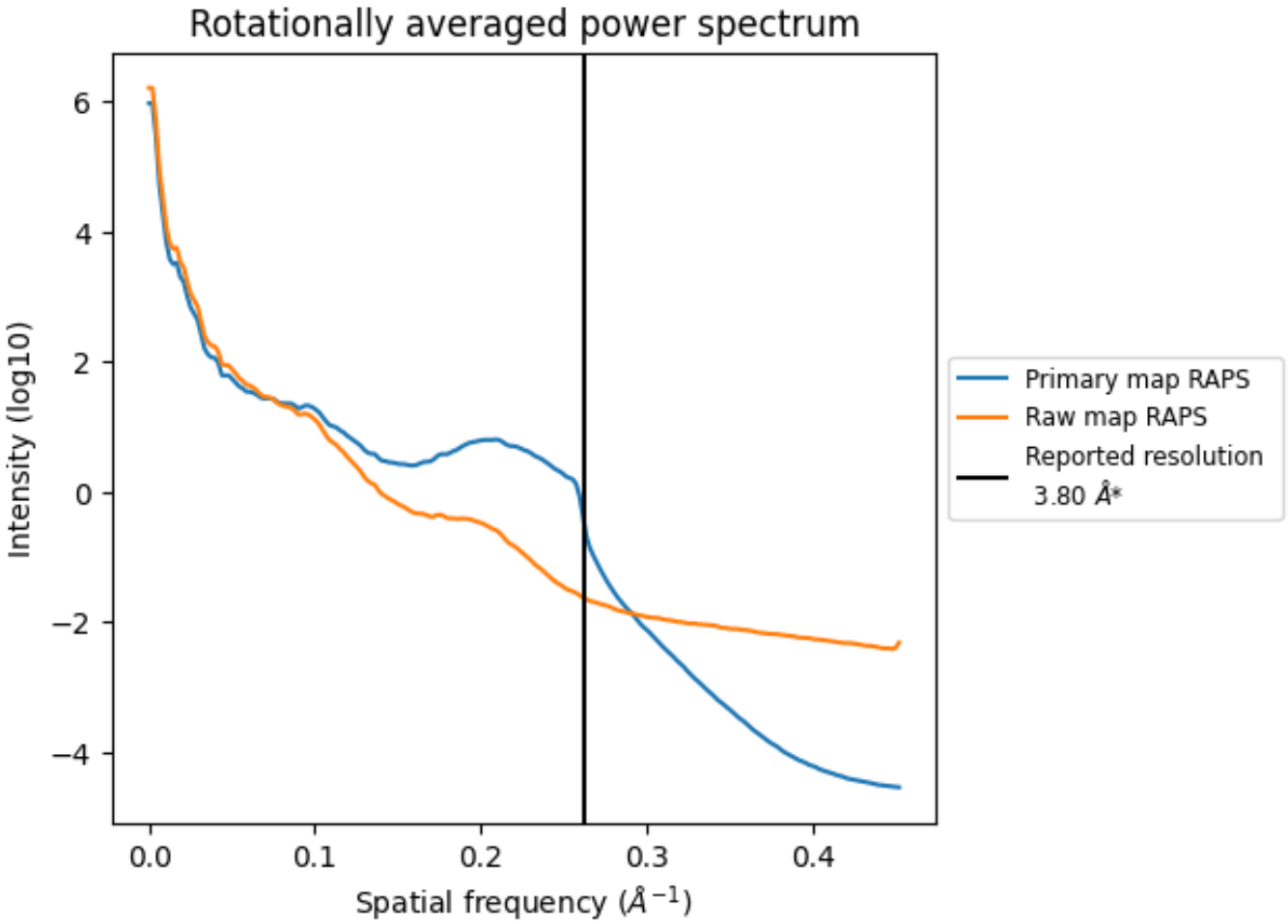
7.2 Volume estimate



The volume at the recommended contour level is 3290 nm^3; this corresponds to an approximate mass of 2972 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)

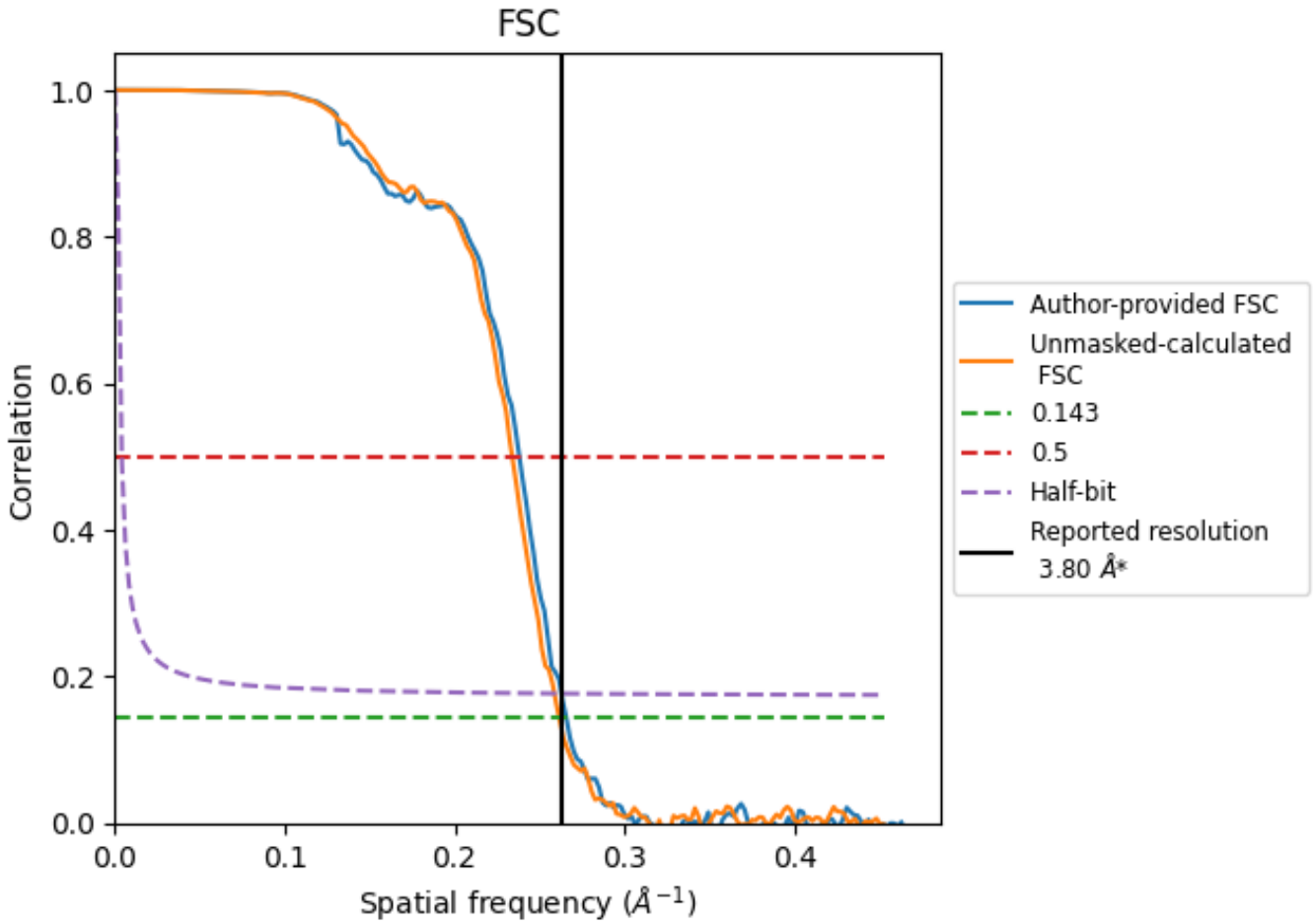


*Reported resolution corresponds to spatial frequency of 0.263 $Å^{-1}$

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

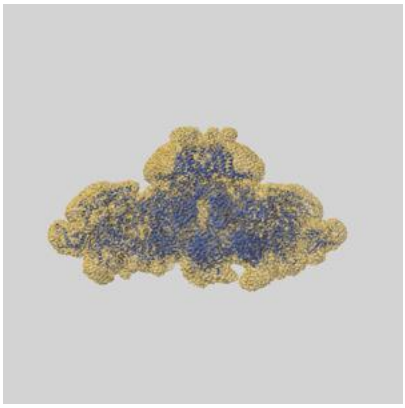
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.20	3.80
Unmasked-calculated*	3.82	4.28	3.87

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

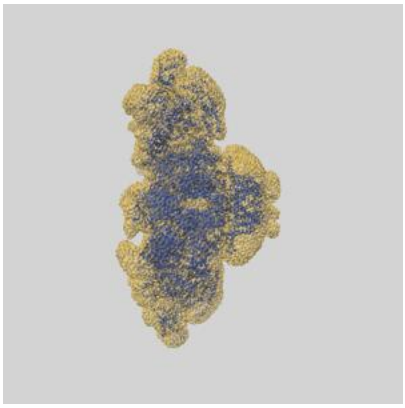
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25828 and PDB model 7TDG. Per-residue inclusion information can be found in section 3 on page 6.

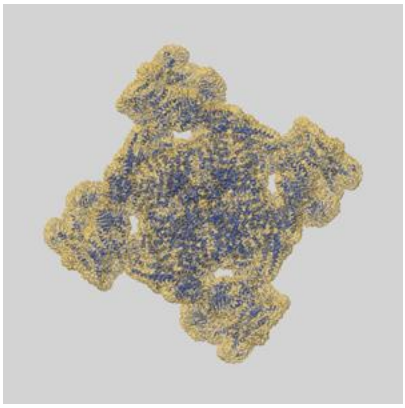
9.1 Map-model overlay



X



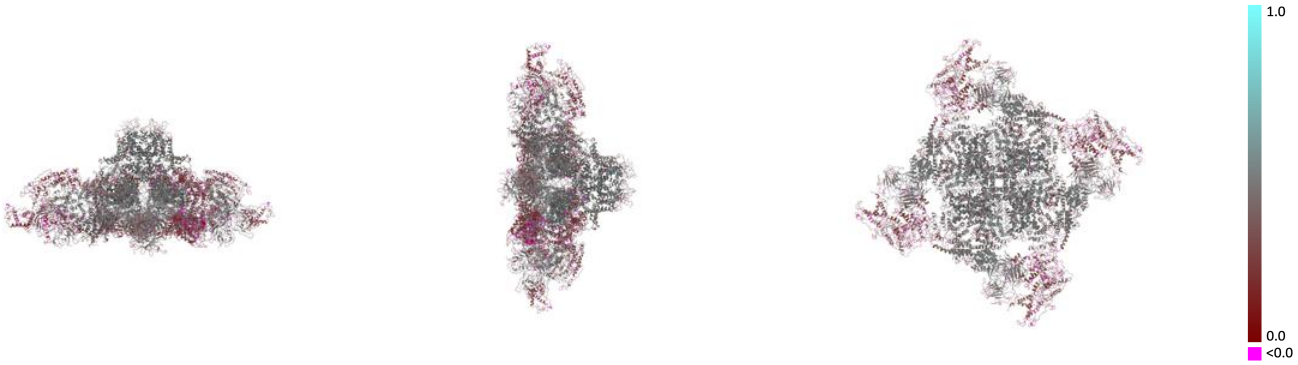
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

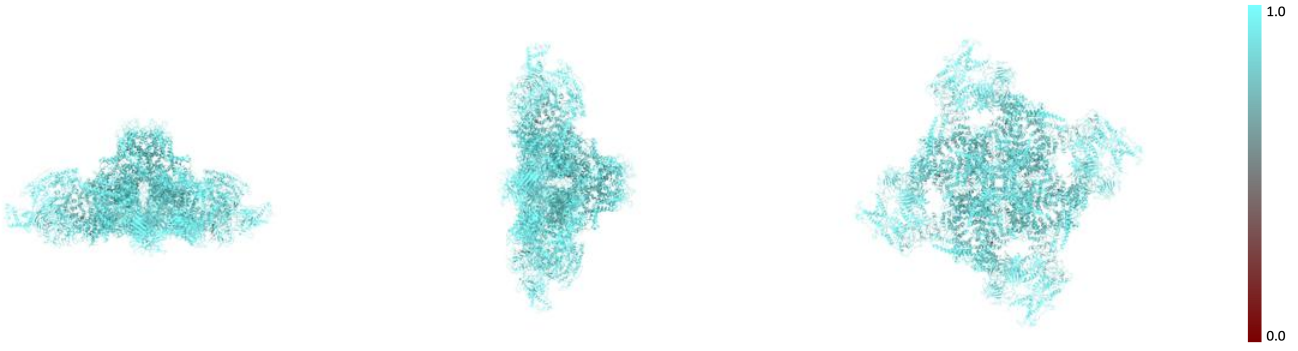
9.2 Q-score mapped to coordinate model



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.

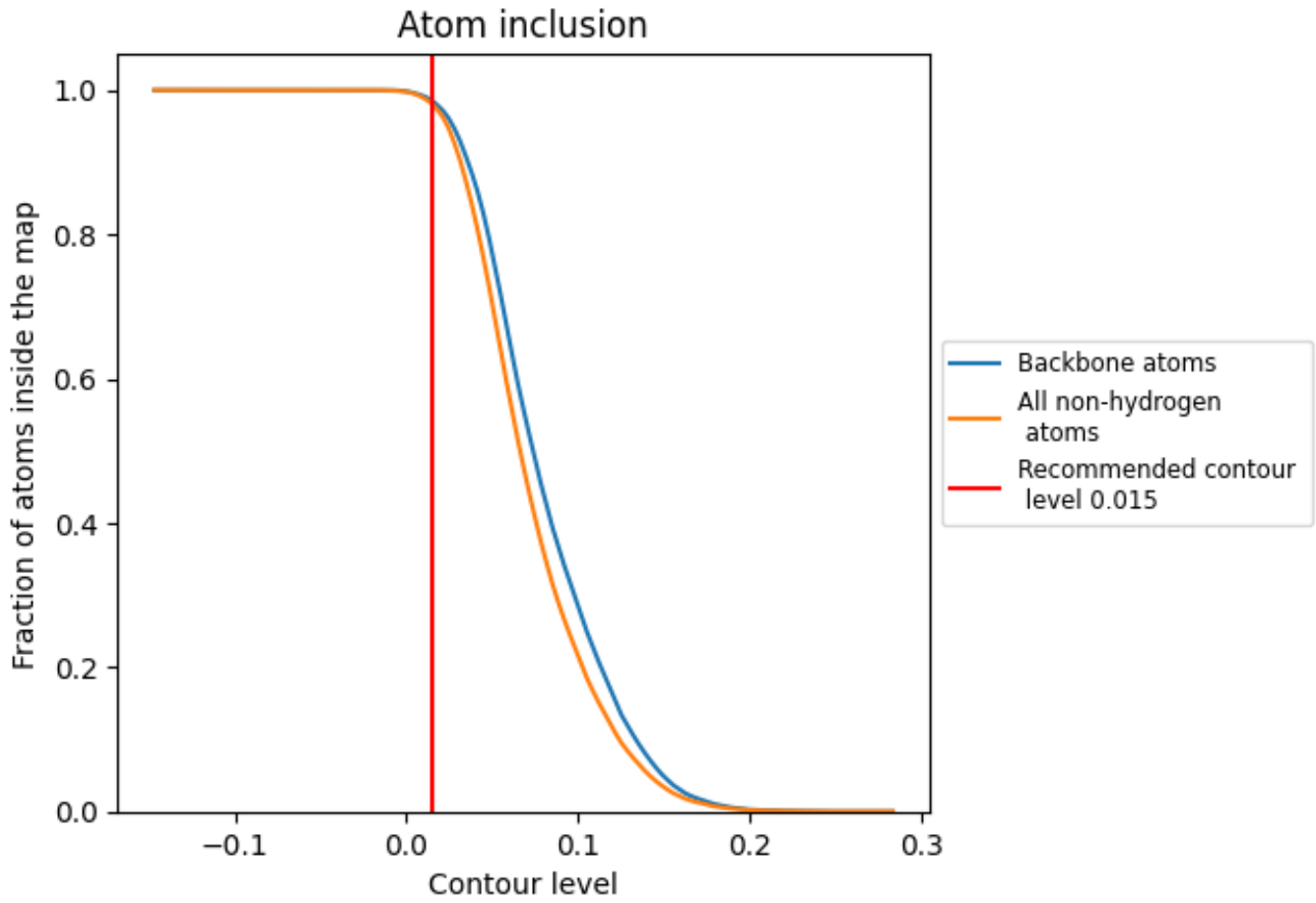
9.3 Atom inclusion mapped to coordinate model



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9808	0.3860
A	0.9812	0.3860
B	0.9807	0.3860
C	0.9806	0.3860
D	0.9807	0.3850