



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:23 PM UTC

PDB ID : 7WTD / pdb_00007wtd
EMDB ID : EMD-32779
Title : Cryo-EM structure of human pyruvate carboxylase with acetyl-CoA in the intermediate state 1
Authors : Chai, P.; Lan, P.; Wu, J.; Lei, M.
Deposited on : 2022-02-04
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

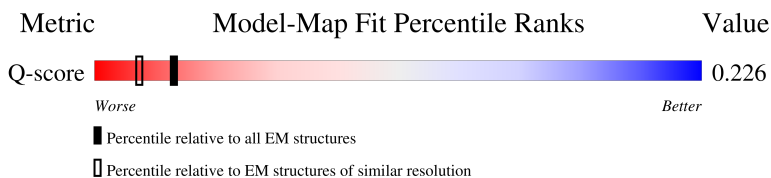
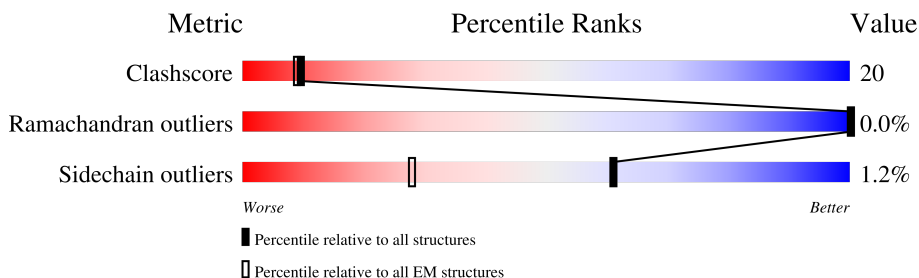
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	A	1178	
1	B	1178	
1	C	1178	
1	D	1178	

2 Entry composition [i](#)

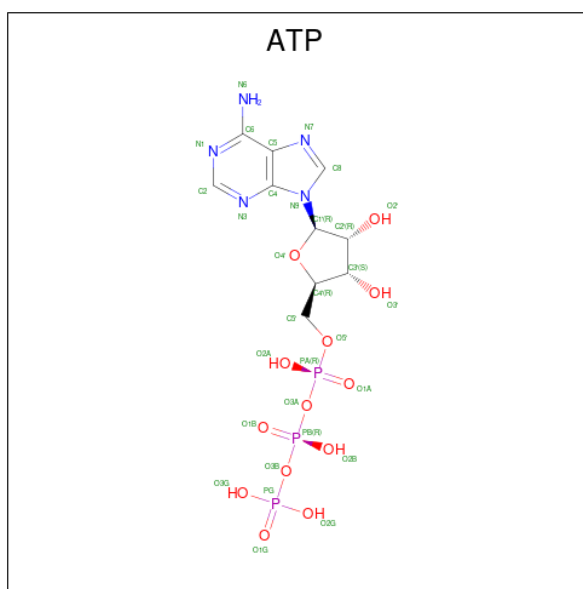
There are 3 unique types of molecules in this entry. The entry contains 27137 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate carboxylase, mitochondrial.

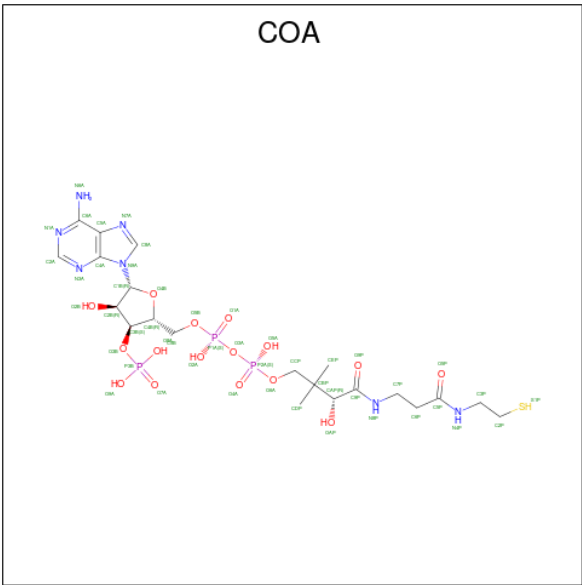
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4625	2938	796	863	28		
1	B	600	Total	C	N	O	S	0	0
			4625	2938	796	863	28		
1	C	1146	Total	C	N	O	S	0	0
			8869	5612	1559	1651	47		
1	D	1145	Total	C	N	O	S	0	0
			8860	5607	1558	1648	47		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

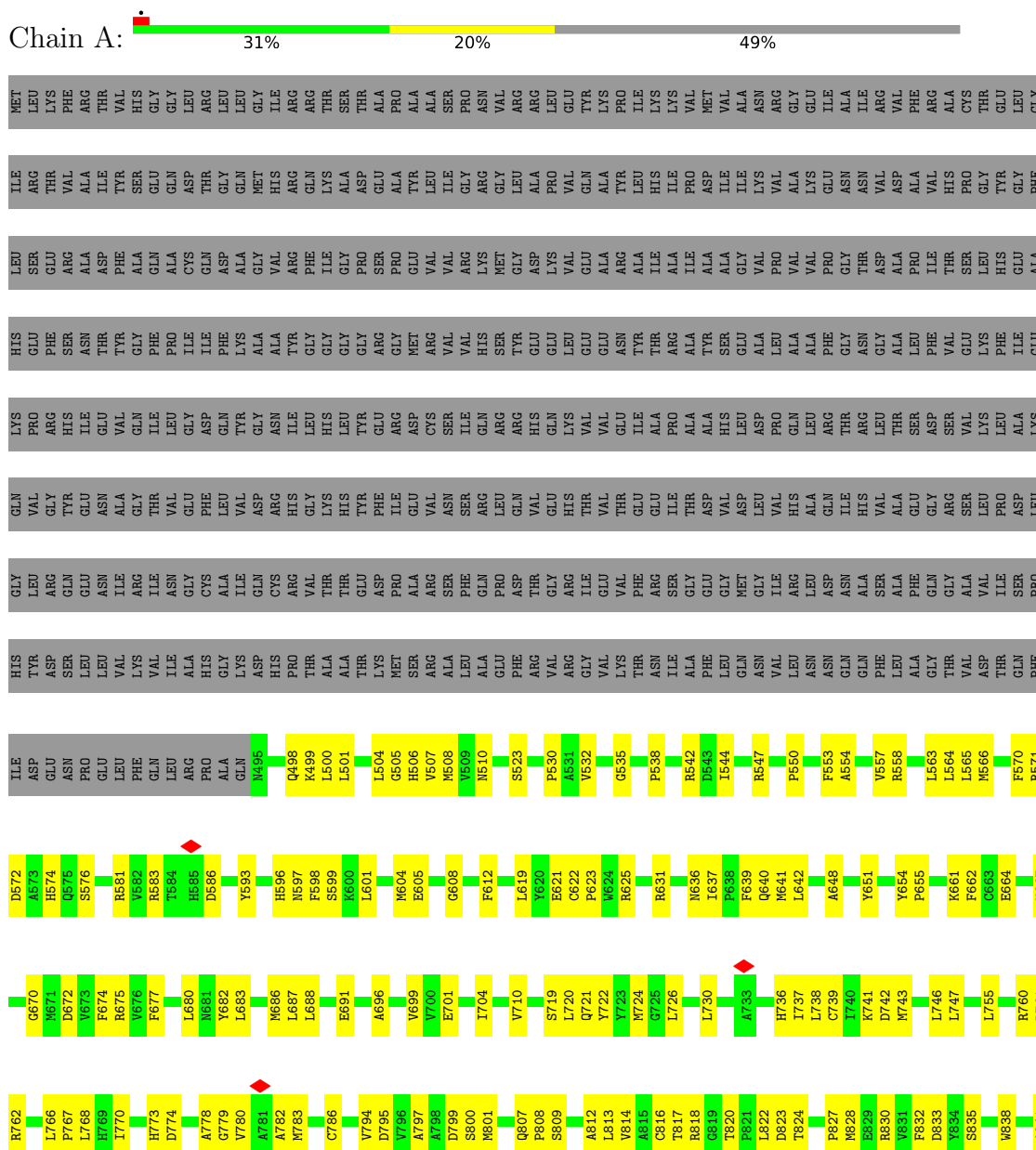


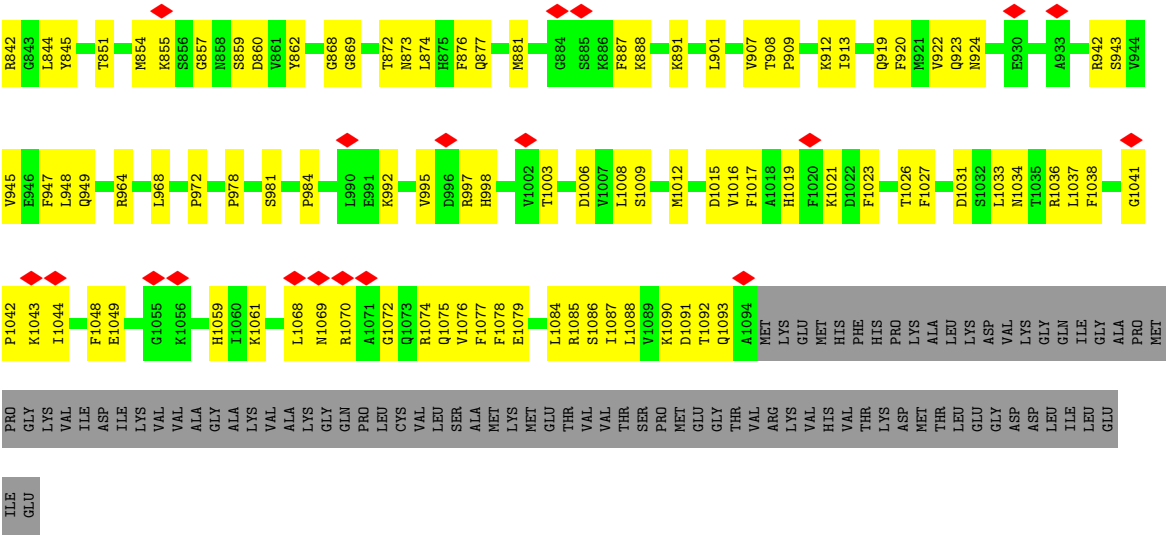
Mol	Chain	Residues	Atoms						AltConf
3	C	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
3	D	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

3 Residue-property plots

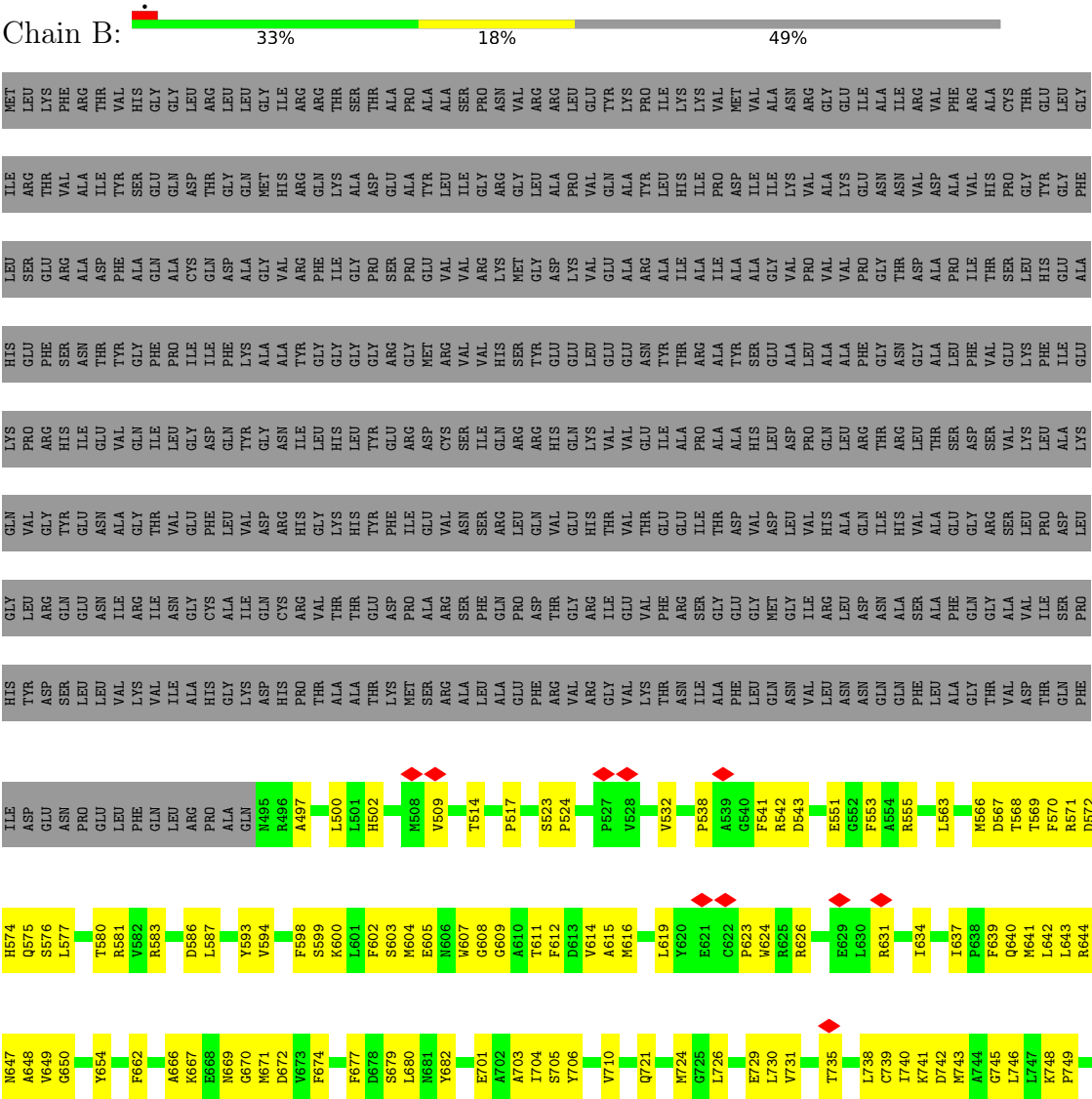
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

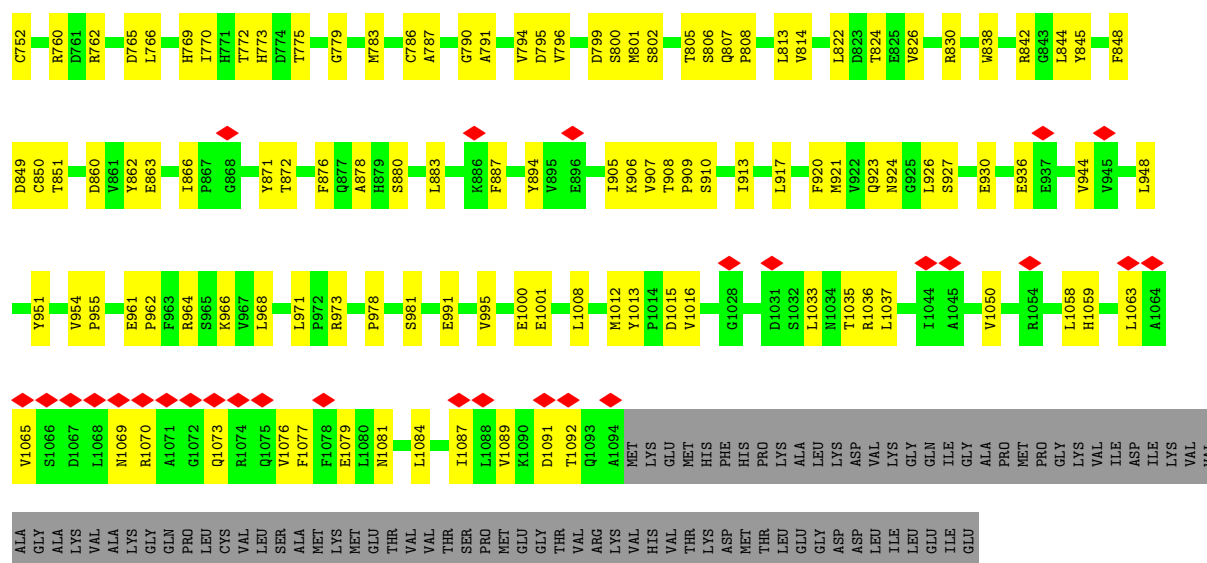
- Molecule 1: Pyruvate carboxylase, mitochondrial



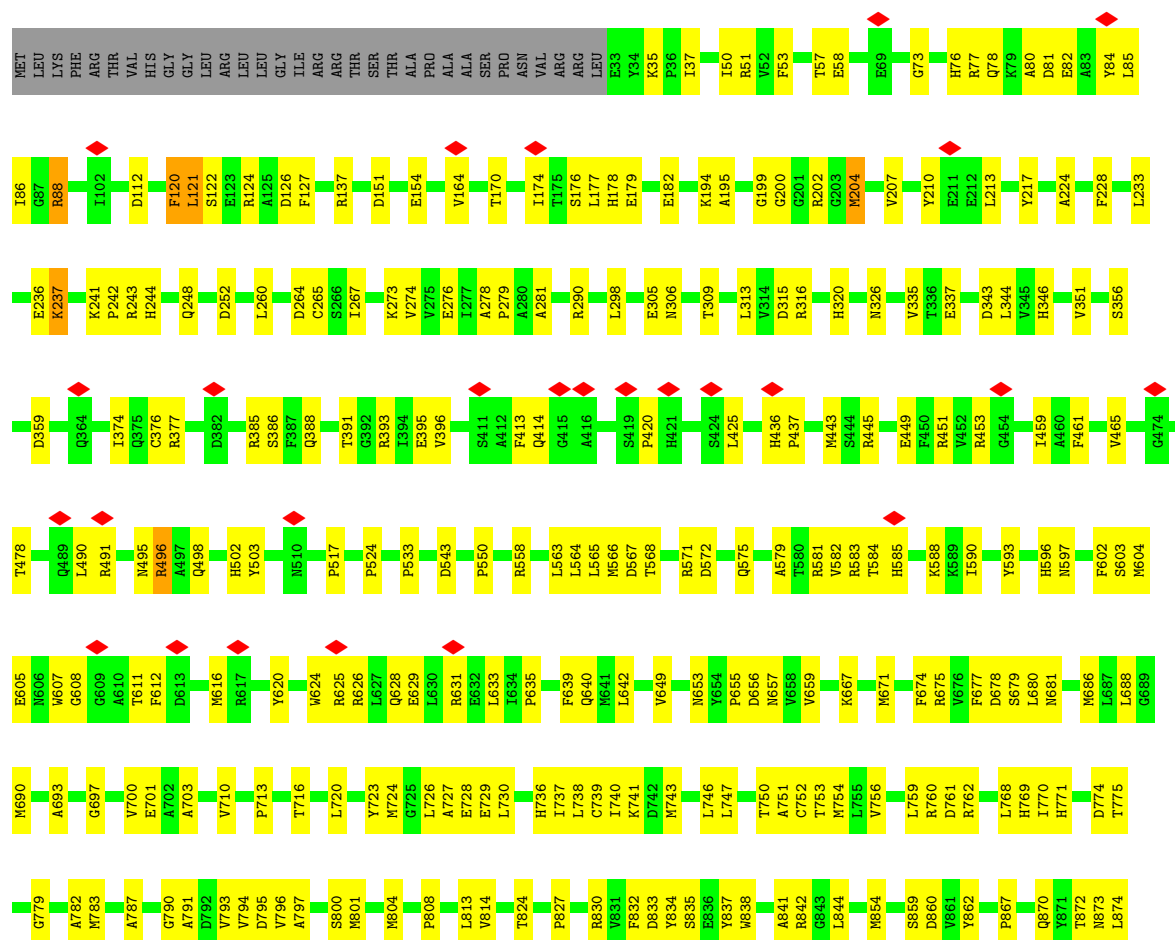


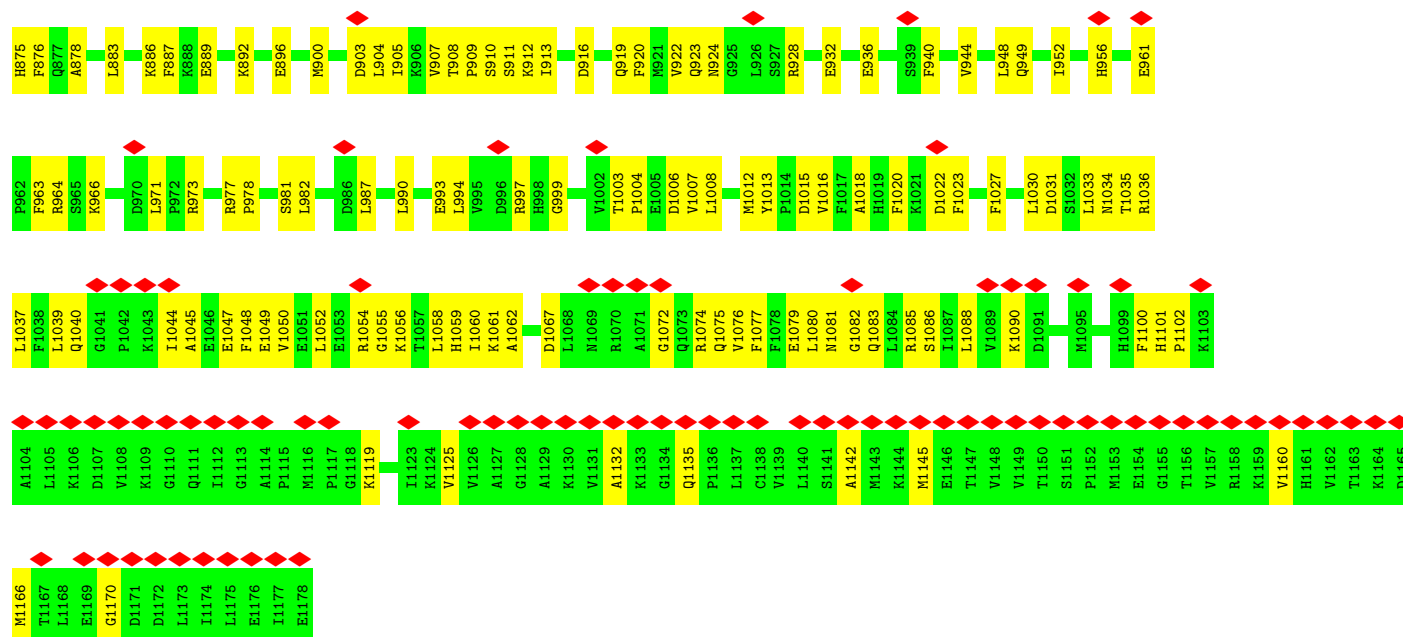
• Molecule 1: Pyruvate carboxylase, mitochondrial



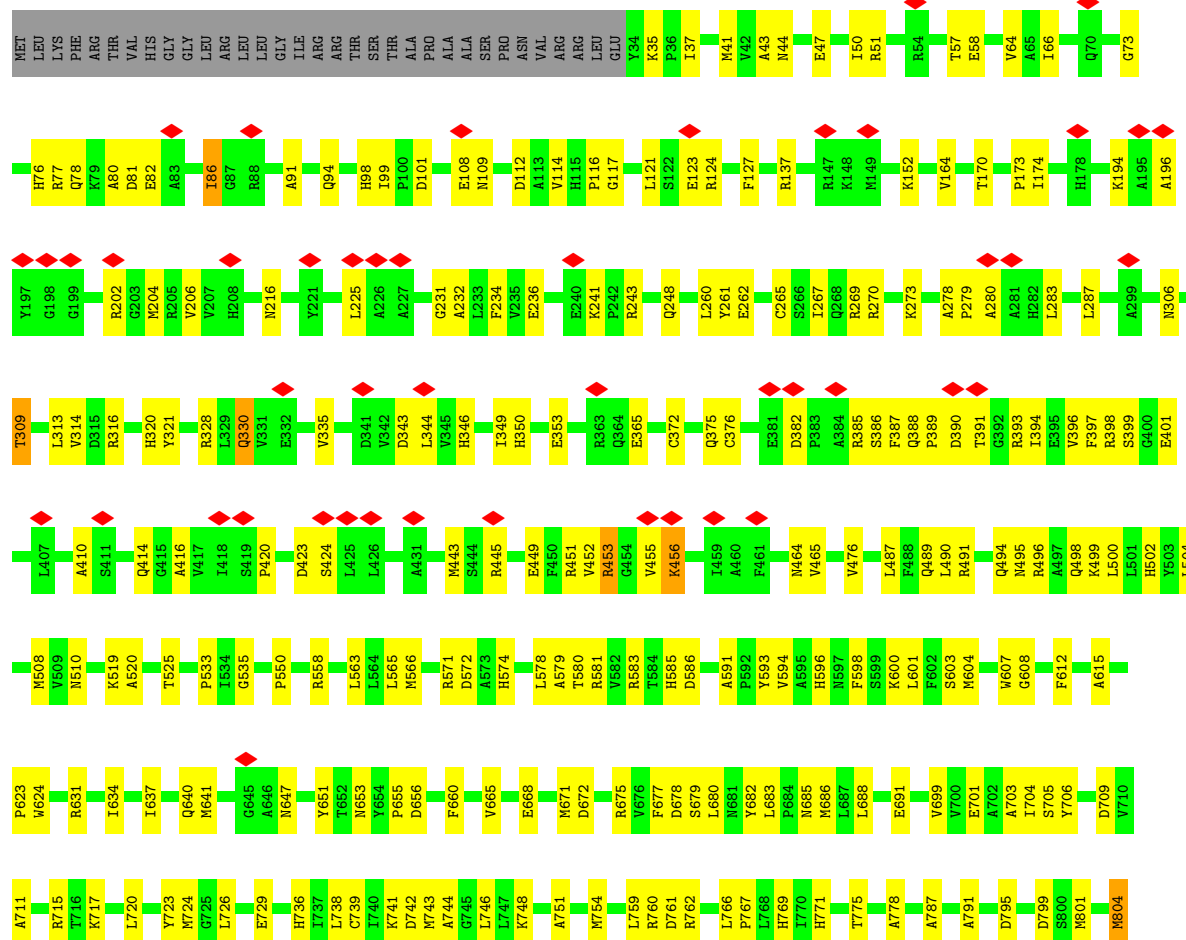


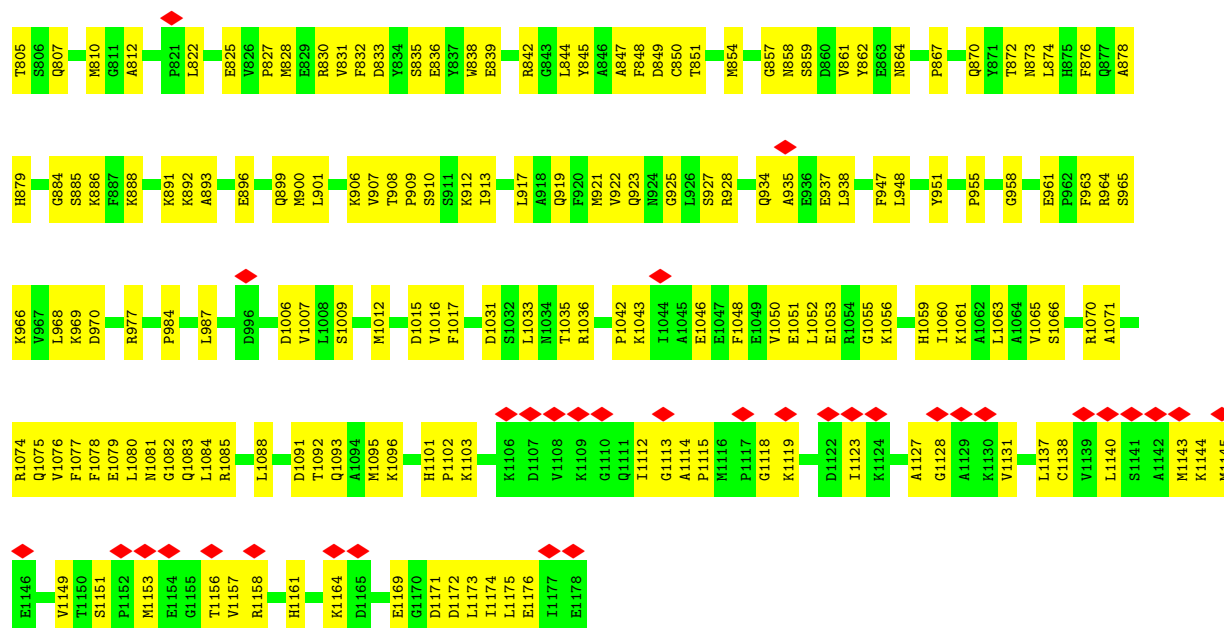
• Molecule 1: Pyruvate carboxylase, mitochondrial





• Molecule 1: Pyruvate carboxylase, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79353	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.132	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	343.2, 343.2, 343.2	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.15	0/4734	0.40	0/6425
1	B	0.15	0/4734	0.40	0/6425
1	C	0.25	0/9060	0.47	0/12277
1	D	0.24	0/9051	0.42	0/12265
All	All	0.22	0/27579	0.43	0/37392

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4625	0	4573	194	0
1	B	4625	0	4573	208	0
1	C	8869	0	8826	360	0
1	D	8860	0	8823	401	0
2	C	31	0	12	8	0
2	D	31	0	12	0	0
3	C	48	0	30	17	0
3	D	48	0	31	19	0
All	All	27137	0	26880	1075	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 20.

All (1075) 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:1077:PHE:CE2	1:B:1063:LEU:HD21	1.21	1.59
1:C:1055:GLY:HA2	1:D:82:GLU:CD	1.29	1.53
1:A:1077:PHE:CZ	1:B:1063:LEU:HD11	1.52	1.44
1:A:1077:PHE:CE2	1:B:1063:LEU:CD2	2.07	1.36
1:B:1063:LEU:HD13	1:B:1077:PHE:CD2	1.64	1.32
3:C:2001:COA:S1P	1:D:57:THR:HG21	1.69	1.32
1:C:1081:ASN:HD22	1:D:77:ARG:NH1	1.31	1.29
1:C:1055:GLY:CA	1:D:82:GLU:CD	2.08	1.27
1:C:1055:GLY:HA2	1:D:82:GLU:OE1	1.38	1.23
1:D:388:GLN:HB2	1:D:1145:MET:CE	1.68	1.23
1:C:1055:GLY:HA2	1:D:82:GLU:OE2	1.35	1.22
1:C:1054:ARG:NH2	1:D:108:GLU:OE1	1.71	1.22
1:C:1081:ASN:O	1:D:78:GLN:OE1	1.58	1.21
1:B:576:SER:O	1:B:872:THR:HG21	1.39	1.20
1:D:396:VAL:HG21	1:D:1085:ARG:CZ	1.70	1.20
1:D:1078:PHE:O	1:D:1084:LEU:HD12	1.41	1.19
1:A:1077:PHE:CZ	1:B:1063:LEU:CD1	2.24	1.19
1:D:451:ARG:NH1	3:D:2001:COA:O8A	1.74	1.18
1:C:453:ARG:CD	1:C:498:GLN:HG2	1.74	1.18
1:B:1079:GLU:HA	1:B:1084:LEU:CD2	1.72	1.17
1:C:1055:GLY:CA	1:D:82:GLU:OE2	1.93	1.17
1:A:1077:PHE:CZ	1:B:1063:LEU:HD21	1.80	1.17
1:C:413:PHE:CE1	1:D:1082:GLY:O	1.97	1.17
1:C:1077:PHE:CE1	1:D:1063:LEU:HD21	1.80	1.15
1:A:1077:PHE:HZ	1:B:1063:LEU:CD1	1.61	1.14
1:C:395:GLU:CD	1:C:1088:LEU:HD23	1.71	1.14
3:C:2001:COA:N1A	1:D:81:ASP:HA	1.24	1.14
1:C:1077:PHE:CZ	1:D:1063:LEU:HD21	1.84	1.13
1:C:77:ARG:NH1	1:D:1059:HIS:ND1	1.96	1.12
1:B:1079:GLU:HA	1:B:1084:LEU:HD23	1.17	1.11
1:C:453:ARG:HD2	1:C:498:GLN:CG	1.80	1.10
1:B:1079:GLU:HG3	1:B:1084:LEU:HD22	1.29	1.10
3:C:2001:COA:N1A	1:D:81:ASP:CA	2.07	1.10
1:D:388:GLN:HB2	1:D:1145:MET:HE1	1.26	1.09
1:C:453:ARG:HD2	1:C:498:GLN:HG2	1.16	1.09
1:C:1054:ARG:NH2	1:D:109:ASN:OD1	1.86	1.08
1:D:388:GLN:CB	1:D:1145:MET:HE1	1.66	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:ARG:CG	1:D:498:GLN:HG3	1.83	1.06
1:D:393:ARG:NH2	1:D:1075:GLN:OE1	1.90	1.05
1:C:395:GLU:CD	1:C:1088:LEU:CD2	2.30	1.04
1:C:199:GLY:O	2:C:2000:ATP:PA	2.16	1.04
1:D:453:ARG:HG3	1:D:498:GLN:CG	1.88	1.03
1:D:453:ARG:HG3	1:D:498:GLN:HG3	1.41	1.03
1:C:393:ARG:HH12	1:C:1075:GLN:HG3	1.21	1.03
1:C:395:GLU:HG3	1:C:1088:LEU:CD2	1.88	1.03
1:C:395:GLU:HB3	1:C:1086:SER:O	1.59	1.02
3:C:2001:COA:S1P	1:D:57:THR:CG2	2.46	1.02
1:C:395:GLU:CG	1:C:1088:LEU:CD2	2.38	1.02
1:C:82:GLU:HB3	1:D:1055:GLY:HA3	1.42	1.01
1:C:1081:ASN:ND2	1:D:77:ARG:NH1	2.07	1.01
1:D:388:GLN:CB	1:D:1145:MET:CE	2.30	0.99
1:D:1079:GLU:HG3	1:D:1084:LEU:HD13	1.44	0.99
1:A:1077:PHE:HZ	1:B:1063:LEU:HD11	0.81	0.97
1:D:112:ASP:OD1	1:D:137:ARG:NH1	1.96	0.97
1:D:194:LYS:HE3	1:D:236:GLU:OE2	1.64	0.97
1:C:1059:HIS:HD2	1:D:77:ARG:NH1	1.61	0.97
1:C:82:GLU:CB	1:D:1055:GLY:HA3	1.93	0.96
1:C:1055:GLY:O	1:D:82:GLU:HA	1.64	0.96
1:C:1081:ASN:OD1	1:D:78:GLN:OE1	1.85	0.94
1:A:1077:PHE:CZ	1:B:1063:LEU:CD2	2.44	0.94
1:C:1081:ASN:HD22	1:D:77:ARG:HH11	1.12	0.94
1:D:388:GLN:HB2	1:D:1145:MET:HE2	1.48	0.94
1:D:451:ARG:NH1	3:D:2001:COA:H3B	1.81	0.93
1:C:453:ARG:CG	1:C:498:GLN:HG2	1.99	0.93
1:C:393:ARG:HD3	1:C:1088:LEU:HD21	1.50	0.92
1:D:389:PRO:HG2	1:D:1143:MET:HB3	1.51	0.92
1:B:1063:LEU:HD13	1:B:1077:PHE:HD2	1.20	0.92
1:D:396:VAL:CG2	1:D:1085:ARG:CZ	2.47	0.92
1:C:395:GLU:OE2	1:C:1088:LEU:CD2	2.18	0.92
1:B:1079:GLU:CA	1:B:1084:LEU:CD2	2.48	0.92
3:C:2001:COA:C2A	1:D:81:ASP:HA	2.00	0.91
1:C:1080:LEU:HG	1:D:78:GLN:NE2	1.85	0.91
1:C:413:PHE:HE1	1:D:1082:GLY:O	1.44	0.91
1:C:1059:HIS:CD2	1:D:77:ARG:NH1	2.39	0.91
1:C:393:ARG:HH12	1:C:1075:GLN:CG	1.84	0.90
1:C:1054:ARG:CZ	1:D:109:ASN:OD1	2.18	0.90
1:C:395:GLU:CG	1:C:1088:LEU:HD22	2.02	0.89
1:D:389:PRO:HG2	1:D:1143:MET:CB	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ARG:HG2	3:D:2001:COA:O8A	1.73	0.89
1:D:453:ARG:NE	1:D:498:GLN:HG3	1.87	0.89
1:C:1055:GLY:CA	1:D:82:GLU:OE1	2.16	0.88
1:C:1077:PHE:HZ	1:D:1063:LEU:HD11	1.37	0.88
1:C:1054:ARG:NH1	1:D:109:ASN:OD1	2.06	0.88
1:C:393:ARG:NH1	1:C:1075:GLN:CD	2.22	0.87
1:C:396:VAL:HG22	1:C:1085:ARG:HD2	1.55	0.87
1:B:1063:LEU:HD13	1:B:1077:PHE:CE2	2.09	0.86
1:D:453:ARG:CD	1:D:498:GLN:HG3	2.05	0.86
3:C:2001:COA:C2P	1:D:57:THR:HG21	2.04	0.86
1:C:393:ARG:NH1	1:C:1075:GLN:HG3	1.91	0.85
1:C:395:GLU:CG	1:C:1088:LEU:HD23	2.06	0.85
1:B:1063:LEU:CD1	1:B:1077:PHE:CD2	2.58	0.84
1:B:1079:GLU:CG	1:B:1084:LEU:HD22	2.07	0.84
1:B:1079:GLU:HG3	1:B:1084:LEU:CD2	2.08	0.83
1:C:948:LEU:O	1:C:964:ARG:NH1	2.12	0.83
1:C:199:GLY:O	2:C:2000:ATP:O3A	1.95	0.83
1:C:80:ALA:O	3:D:2001:COA:N6A	2.12	0.82
1:C:393:ARG:NH1	1:C:1075:GLN:CG	2.43	0.82
1:D:396:VAL:HG21	1:D:1085:ARG:NH2	1.95	0.82
1:D:451:ARG:HH12	3:D:2001:COA:H3B	1.41	0.82
1:D:453:ARG:HE	1:D:498:GLN:CG	1.94	0.81
1:C:82:GLU:CG	1:D:1055:GLY:HA3	2.12	0.80
1:D:453:ARG:HG3	1:D:498:GLN:CD	2.06	0.80
1:D:495:ASN:HB2	1:D:499:LYS:HE3	1.64	0.80
1:C:199:GLY:O	2:C:2000:ATP:O1A	1.99	0.80
1:D:872:THR:HG23	1:D:873:ASN:N	1.95	0.80
1:B:1079:GLU:CB	1:B:1084:LEU:CD2	2.60	0.80
1:C:1100:PHE:HB3	1:C:1101:HIS:HB2	1.62	0.79
1:B:779:GLY:O	1:B:783:MET:HB2	1.82	0.79
1:C:1077:PHE:CZ	1:D:1063:LEU:CD2	2.65	0.79
1:D:393:ARG:HD3	1:D:1088:LEU:CD1	2.13	0.78
1:C:693:ALA:O	1:C:697:GLY:N	2.15	0.78
1:D:241:LYS:HB2	1:D:316:ARG:HD2	1.64	0.78
1:D:844:LEU:HD23	1:D:1035:THR:HB	1.65	0.77
1:D:1061:LYS:HB3	1:D:1079:GLU:HB2	1.64	0.77
3:C:2001:COA:C6A	1:D:80:ALA:O	2.33	0.77
1:B:1079:GLU:CG	1:B:1084:LEU:CD2	2.63	0.77
1:D:278:ALA:HB2	1:D:335:VAL:HG12	1.66	0.76
1:C:1054:ARG:HH22	1:D:109:ASN:CG	1.92	0.76
1:D:451:ARG:HH11	3:D:2001:COA:P3B	2.08	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:ASP:HB3	1:C:604:MET:HE1	1.68	0.76
1:D:451:ARG:CD	3:D:2001:COA:O8A	2.34	0.76
1:A:877:GLN:HB3	1:A:881:MET:HE1	1.66	0.76
1:C:584:THR:HG22	1:C:626:ARG:HE	1.49	0.76
1:C:1055:GLY:HA3	1:D:82:GLU:OE2	1.84	0.76
1:B:787:ALA:HA	1:B:791:ALA:HB3	1.68	0.76
1:A:812:ALA:HB1	1:D:778:ALA:HB2	1.67	0.75
1:B:1079:GLU:CB	1:B:1084:LEU:HD21	2.16	0.75
1:C:395:GLU:CB	1:C:1086:SER:O	2.33	0.75
1:A:1075:GLN:NE2	1:A:1086:SER:OG	2.19	0.75
1:A:778:ALA:HB2	1:D:812:ALA:HB1	1.67	0.75
1:A:1077:PHE:HE2	1:B:1063:LEU:CD2	1.67	0.75
1:B:741:LYS:HE3	1:B:743:MET:HE2	1.67	0.75
1:B:894:TYR:HE2	1:B:906:LYS:HE3	1.52	0.74
1:D:1059:HIS:H	1:D:1081:ASN:ND2	1.86	0.74
1:D:393:ARG:HD3	1:D:1088:LEU:HD11	1.70	0.74
1:D:1079:GLU:HG3	1:D:1084:LEU:CD1	2.17	0.73
1:C:1080:LEU:HD12	1:C:1081:ASN:H	1.52	0.73
1:B:783:MET:HE2	1:B:794:VAL:HG13	1.69	0.73
1:D:453:ARG:NE	1:D:498:GLN:CG	2.50	0.73
1:D:804:MET:HG2	1:D:805:THR:HG23	1.70	0.73
1:D:35:LYS:CD	1:D:137:ARG:HH21	2.02	0.73
1:A:743:MET:SD	1:A:773:HIS:NE2	2.61	0.73
1:C:73:GLY:HA2	1:D:1081:ASN:O	1.87	0.73
1:C:1080:LEU:HG	1:D:78:GLN:HE22	1.49	0.72
1:C:77:ARG:NH2	1:D:1059:HIS:CE1	2.57	0.72
1:D:1078:PHE:O	1:D:1085:ARG:N	2.19	0.72
1:D:535:GLY:O	1:D:596:HIS:NE2	2.18	0.72
1:B:760:ARG:NH2	1:B:790:GLY:O	2.22	0.72
1:C:77:ARG:CZ	1:D:1059:HIS:CE1	2.72	0.72
1:D:451:ARG:CG	3:D:2001:COA:O8A	2.36	0.72
1:B:1063:LEU:CD1	1:B:1077:PHE:HD2	2.01	0.71
1:C:395:GLU:OE2	1:C:1088:LEU:HD22	1.90	0.71
1:C:908:THR:HB	1:C:909:PRO:HD3	1.72	0.71
1:C:1081:ASN:OD1	1:D:78:GLN:CD	2.33	0.71
1:C:747:LEU:HD21	1:C:752:CYS:HB2	1.72	0.71
1:A:530:PRO:HG3	1:A:833:ASP:HB3	1.72	0.71
1:D:398:ARG:NH2	1:D:1085:ARG:HH22	1.87	0.71
1:B:1079:GLU:CA	1:B:1084:LEU:HD23	2.08	0.71
1:D:558:ARG:O	1:D:558:ARG:NH1	2.24	0.71
1:D:453:ARG:HE	1:D:498:GLN:HG2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:HIS:HB3	1:B:580:THR:HA	1.72	0.71
1:C:728:GLU:OE1	1:C:762:ARG:NH1	2.24	0.71
3:C:2001:COA:HS1	1:D:57:THR:HG21	1.55	0.71
1:D:51:ARG:NH2	1:D:343:ASP:OD1	2.23	0.70
1:D:393:ARG:CD	1:D:1088:LEU:HD11	2.22	0.70
1:A:1077:PHE:CE1	1:B:1063:LEU:HD11	2.21	0.70
1:B:571:ARG:O	1:B:575:GLN:NE2	2.24	0.70
1:D:398:ARG:HH21	1:D:1085:ARG:HH22	1.39	0.70
1:D:451:ARG:HD2	3:D:2001:COA:O8A	1.91	0.70
1:D:907:VAL:HG12	1:D:908:THR:H	1.56	0.70
1:D:1078:PHE:C	1:D:1084:LEU:HD12	2.16	0.70
1:A:583:ARG:HH21	1:A:1031:ASP:HA	1.57	0.70
1:C:51:ARG:NH2	1:C:343:ASP:OD1	2.25	0.70
1:C:584:THR:OG1	1:C:1031:ASP:OD1	2.08	0.70
1:B:555:ARG:HH22	1:B:766:LEU:HD13	1.57	0.70
1:D:396:VAL:CG2	1:D:1085:ARG:NH1	2.55	0.70
1:D:1079:GLU:HA	1:D:1084:LEU:HA	1.74	0.70
1:D:44:ASN:ND2	1:D:116:PRO:O	2.25	0.70
1:B:679:SER:HB2	1:B:907:VAL:H	1.57	0.69
1:C:900:MET:HE3	1:C:928:ARG:HH22	1.58	0.69
1:C:77:ARG:NH1	1:D:1059:HIS:CE1	2.60	0.69
1:A:523:SER:O	1:A:1036:ARG:NH2	2.26	0.69
1:A:1077:PHE:CZ	1:B:1063:LEU:CG	2.75	0.68
1:C:913:ILE:HG23	1:C:944:VAL:HG22	1.74	0.68
1:D:872:THR:CG2	1:D:873:ASN:N	2.56	0.68
1:A:814:VAL:O	1:A:818:ARG:NH1	2.26	0.68
1:C:593:TYR:O	1:C:597:ASN:ND2	2.24	0.68
1:D:653:ASN:ND2	1:D:951:TYR:O	2.26	0.68
1:D:810:MET:HE2	1:D:831:VAL:HG22	1.74	0.68
1:D:1078:PHE:O	1:D:1084:LEU:CD1	2.32	0.68
1:C:377:ARG:HG3	1:C:425:LEU:HD13	1.75	0.68
1:C:1081:ASN:CG	1:D:78:GLN:OE1	2.36	0.68
1:D:58:GLU:OE1	1:D:346:HIS:NE2	2.23	0.67
1:A:842:ARG:NH2	1:A:851:THR:OG1	2.26	0.67
1:B:644:ARG:HE	1:B:908:THR:HG21	1.56	0.67
1:D:1112:ILE:HB	1:D:1175:LEU:HB2	1.75	0.67
1:A:571:ARG:HD3	1:A:608:GLY:HA3	1.77	0.67
1:C:451:ARG:HH11	3:C:2001:COA:P3B	2.16	0.67
1:B:927:SER:OG	1:B:930:GLU:OE1	2.13	0.67
1:B:814:VAL:HG22	1:B:824:THR:HG21	1.75	0.67
1:B:948:LEU:O	1:B:964:ARG:NH1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ALA:HB1	1:A:767:PRO:HG2	1.77	0.67
1:D:1102:PRO:HG2	1:D:1161:HIS:HE1	1.60	0.67
1:C:453:ARG:CD	1:C:498:GLN:CG	2.38	0.67
1:B:667:LYS:HE3	1:B:674:PHE:HE2	1.60	0.67
1:C:680:LEU:HD21	1:C:904:LEU:HD11	1.77	0.67
1:C:241:LYS:HB3	1:C:316:ARG:HH11	1.60	0.66
1:D:801:MET:HE3	1:D:838:TRP:HB3	1.77	0.66
1:D:631:ARG:NH1	1:D:672:ASP:OD2	2.29	0.66
1:A:538:PRO:O	1:A:636:ASN:ND2	2.28	0.66
1:B:581:ARG:HG2	1:B:619:LEU:HD11	1.78	0.66
1:C:1022:ASP:OD1	1:C:1023:PHE:N	2.28	0.66
1:B:648:ALA:H	1:B:654:TYR:HD2	1.44	0.66
3:C:2001:COA:H21	1:D:57:THR:HG21	1.77	0.66
1:A:780:VAL:HG11	1:D:778:ALA:HA	1.76	0.66
1:D:867:PRO:HG2	1:D:870:GLN:HB3	1.77	0.66
1:C:1077:PHE:CZ	1:D:1063:LEU:HD11	2.25	0.66
1:C:686:MET:HB3	1:C:690:MET:HE1	1.76	0.65
1:C:771:HIS:ND1	1:C:795:ASP:OD2	2.29	0.65
1:A:978:PRO:HA	1:A:981:SER:HB3	1.78	0.65
1:C:82:GLU:HG2	1:D:1055:GLY:HA3	1.79	0.65
1:B:631:ARG:NH2	1:B:634:ILE:O	2.23	0.65
1:D:248:GLN:HG2	1:D:260:LEU:HD12	1.77	0.65
1:A:625:ARG:NH2	1:A:1031:ASP:OD2	2.30	0.65
1:B:1069:ASN:HD21	1:B:1073:GLN:HB3	1.62	0.65
1:B:1079:GLU:HB3	1:B:1084:LEU:HD21	1.77	0.65
1:C:1013:TYR:HB3	1:C:1016:VAL:HG22	1.79	0.65
1:A:667:LYS:NZ	1:A:672:ASP:O	2.28	0.65
1:C:199:GLY:C	2:C:2000:ATP:O2B	2.39	0.65
1:C:1056:LYS:HD3	3:C:2001:COA:C6A	2.24	0.65
1:C:260:LEU:HD11	1:C:344:LEU:HD21	1.78	0.65
1:D:451:ARG:HG2	3:D:2001:COA:P3B	2.37	0.65
1:B:1063:LEU:CD1	1:B:1077:PHE:CE2	2.80	0.64
1:A:800:SER:OG	1:A:835:SER:O	2.15	0.64
1:B:752:CYS:SG	1:B:786:CYS:N	2.69	0.64
1:C:612:PHE:HB2	1:C:649:VAL:HG21	1.80	0.64
1:C:653:ASN:ND2	1:C:952:ILE:O	2.30	0.64
1:B:920:PHE:O	1:B:924:ASN:ND2	2.30	0.64
1:C:675:ARG:NH2	1:C:739:CYS:SG	2.70	0.64
1:C:655:PRO:HG3	1:C:982:LEU:HD22	1.80	0.64
1:D:389:PRO:CG	1:D:1143:MET:HB3	2.26	0.64
1:C:503:TYR:HD2	1:C:1027:PHE:HB3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:PRO:O	1:C:716:THR:OG1	2.16	0.64
1:C:1077:PHE:HZ	1:D:1063:LEU:CD1	2.10	0.64
1:A:920:PHE:O	1:A:924:ASN:HB2	1.98	0.64
1:C:396:VAL:CG2	1:C:1085:ARG:HD2	2.26	0.64
1:A:1075:GLN:NE2	1:A:1076:VAL:O	2.31	0.64
1:C:1061:LYS:HB3	1:C:1079:GLU:HG3	1.78	0.64
1:D:453:ARG:HB2	1:D:498:GLN:NE2	2.13	0.64
1:D:278:ALA:HB3	1:D:279:PRO:HD3	1.80	0.63
1:D:872:THR:CG2	1:D:873:ASN:H	2.11	0.63
1:A:942:ARG:NH2	1:A:943:SER:OG	2.31	0.63
1:C:35:LYS:HB2	1:C:137:ARG:HH22	1.64	0.63
1:C:1055:GLY:O	1:D:82:GLU:OE1	2.17	0.63
1:D:572:ASP:OD2	1:D:807:GLN:NE2	2.29	0.63
1:C:453:ARG:CG	1:C:498:GLN:CG	2.71	0.63
3:C:2001:COA:H2A	1:D:81:ASP:OD1	1.97	0.63
1:A:1049:GLU:OE1	1:A:1059:HIS:ND1	2.27	0.62
1:A:1090:LYS:NZ	1:A:1091:ASP:O	2.29	0.62
1:B:566:MET:HB2	1:B:602:PHE:HB3	1.81	0.62
1:D:935:ALA:HB3	1:D:966:LYS:HD3	1.80	0.62
1:A:532:VAL:HG11	1:A:593:TYR:HA	1.81	0.62
1:A:572:ASP:HB3	1:A:807:GLN:HE22	1.64	0.62
1:B:641:MET:HE2	1:B:671:MET:HG2	1.82	0.62
1:D:724:MET:HE1	1:D:759:LEU:HD22	1.81	0.62
1:A:535:GLY:O	1:A:596:HIS:NE2	2.23	0.62
1:B:566:MET:HE3	1:B:795:ASP:OD1	2.00	0.62
1:D:396:VAL:HG23	1:D:1085:ARG:NH1	2.14	0.62
1:A:608:GLY:HA2	1:A:642:LEU:HB3	1.82	0.62
1:A:677:PHE:HE2	1:A:907:VAL:HG11	1.65	0.62
1:C:756:VAL:HA	1:C:759:LEU:HG	1.82	0.62
1:C:1055:GLY:C	1:D:82:GLU:OE1	2.43	0.62
1:D:1123:ILE:HG23	1:D:1138:CYS:HA	1.80	0.62
1:C:77:ARG:CZ	1:D:1059:HIS:ND1	2.63	0.62
1:A:907:VAL:HG12	1:A:908:THR:H	1.65	0.61
1:D:309:THR:HG21	1:D:330:GLN:HG3	1.82	0.61
1:D:510:ASN:HB3	1:D:1093:GLN:HE22	1.65	0.61
1:C:524:PRO:HA	1:C:1036:ARG:HH12	1.66	0.61
1:D:206:VAL:O	1:D:216:ASN:ND2	2.34	0.61
1:D:594:VAL:HA	1:D:598:PHE:HD2	1.65	0.61
1:D:1079:GLU:CG	1:D:1084:LEU:HD13	2.26	0.61
1:C:787:ALA:HA	1:C:791:ALA:HB3	1.82	0.61
1:A:538:PRO:HG2	1:A:599:SER:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1080:LEU:HD23	1:D:1081:ASN:N	2.16	0.61
1:B:576:SER:O	1:B:872:THR:CG2	2.32	0.61
1:A:570:PHE:O	1:A:574:HIS:NE2	2.34	0.61
1:A:1091:ASP:OD1	1:A:1093:GLN:NE2	2.34	0.61
1:B:849:ASP:OD2	1:B:851:THR:OG1	2.19	0.61
1:C:1055:GLY:HA3	1:D:82:GLU:CD	2.22	0.61
1:D:382:ASP:OD2	1:D:385:ARG:NH1	2.33	0.61
1:C:730:LEU:HD13	1:C:738:LEU:HD11	1.82	0.60
1:C:1049:GLU:OE1	1:C:1059:HIS:ND1	2.33	0.60
1:D:91:ALA:HB3	1:D:94:GLN:HG2	1.83	0.60
1:A:835:SER:OG	1:D:858:ASN:ND2	2.34	0.60
1:B:704:ILE:O	1:B:741:LYS:N	2.32	0.60
1:B:775:THR:HA	1:B:805:THR:HA	1.82	0.60
1:C:199:GLY:O	2:C:2000:ATP:PB	2.60	0.60
1:C:498:GLN:O	1:C:502:HIS:ND1	2.34	0.60
1:D:741:LYS:HD2	1:D:743:MET:HE3	1.82	0.60
1:C:164:VAL:HG11	1:C:298:LEU:HD12	1.83	0.60
1:C:572:ASP:OD1	1:C:575:GLN:NE2	2.35	0.60
1:C:800:SER:O	1:C:842:ARG:NH1	2.34	0.60
1:A:550:PRO:HB3	1:A:699:VAL:HG22	1.84	0.60
1:C:170:THR:HG21	1:C:174:ILE:HG12	1.84	0.60
1:C:241:LYS:O	1:C:316:ARG:NH1	2.34	0.60
1:C:859:SER:OG	1:C:860:ASP:N	2.31	0.60
1:D:194:LYS:CE	1:D:236:GLU:OE2	2.44	0.60
1:C:608:GLY:N	1:C:611:THR:OG1	2.35	0.60
1:A:1077:PHE:CE2	1:B:1063:LEU:HD22	2.28	0.59
1:C:243:ARG:NH1	1:C:264:ASP:OD2	2.35	0.59
1:B:936:GLU:OE1	1:B:966:LYS:NZ	2.28	0.59
1:C:582:VAL:O	1:C:626:ARG:NH2	2.35	0.59
1:D:170:THR:HB	1:D:174:ILE:HD11	1.84	0.59
1:D:591:ALA:HB1	1:D:634:ILE:HD11	1.84	0.59
1:A:1077:PHE:HE2	1:B:1063:LEU:HD21	0.79	0.59
1:A:651:TYR:CG	1:A:912:LYS:HE2	2.38	0.59
1:B:583:ARG:NH2	1:B:1033:LEU:O	2.34	0.59
1:C:278:ALA:HB2	1:C:335:VAL:HB	1.84	0.59
1:B:779:GLY:O	1:B:783:MET:CB	2.50	0.59
1:C:566:MET:HG2	1:C:603:SER:H	1.68	0.59
1:C:688:LEU:HB2	1:C:977:ARG:HH21	1.67	0.59
1:C:963:PHE:HA	1:C:966:LYS:HD3	1.85	0.59
1:D:583:ARG:HH21	1:D:1031:ASP:HA	1.67	0.59
1:D:678:ASP:OD2	1:D:685:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:814:VAL:HG22	1:C:824:THR:HG21	1.84	0.59
1:D:1043:LYS:HB2	1:D:1046:GLU:HG2	1.83	0.59
1:C:453:ARG:HG3	1:C:498:GLN:CG	2.32	0.58
1:D:631:ARG:NH2	1:D:637:ILE:O	2.32	0.58
1:A:747:LEU:HD11	1:A:770:ILE:HD11	1.84	0.58
1:C:1059:HIS:HB2	1:C:1081:ASN:HB3	1.84	0.58
1:D:563:LEU:HD13	1:D:822:LEU:HD22	1.85	0.58
1:D:593:TYR:OH	1:D:833:ASP:HB2	2.03	0.58
1:D:680:LEU:HD13	1:D:955:PRO:HA	1.85	0.58
1:A:873:ASN:HA	1:A:876:PHE:CE2	2.38	0.58
1:B:1058:LEU:HA	1:B:1081:ASN:HD21	1.68	0.58
1:B:563:LEU:HD22	1:B:822:LEU:HD13	1.84	0.58
1:C:315:ASP:OD1	1:C:316:ARG:N	2.35	0.58
1:C:517:PRO:HB3	1:C:876:PHE:CE1	2.38	0.58
1:D:919:GLN:NE2	1:D:923:GLN:OE1	2.37	0.58
1:A:619:LEU:HB3	1:A:621:GLU:OE1	2.03	0.58
1:C:612:PHE:HB3	1:C:616:MET:HE1	1.86	0.58
1:A:583:ARG:HH22	1:A:1033:LEU:HB2	1.69	0.57
3:D:2001:COA:O5P	3:D:2001:COA:N8P	2.35	0.57
1:C:126:ASP:OD1	1:C:127:PHE:N	2.37	0.57
1:C:385:ARG:HG3	1:C:386:SER:H	1.69	0.57
1:D:385:ARG:HG3	1:D:386:SER:H	1.69	0.57
1:B:555:ARG:NH2	1:B:765:ASP:O	2.38	0.57
1:B:572:ASP:OD2	1:B:773:HIS:NE2	2.38	0.57
1:C:740:ILE:N	1:C:769:HIS:O	2.37	0.57
3:C:2001:COA:C5A	1:D:80:ALA:O	2.53	0.57
1:D:262:GLU:OE2	1:D:280:ALA:N	2.35	0.57
1:D:641:MET:HG2	1:D:671:MET:HE2	1.87	0.57
1:A:499:LYS:HB3	1:A:1027:PHE:HA	1.87	0.57
1:B:524:PRO:HA	1:B:1036:ARG:HH12	1.68	0.57
1:B:739:CYS:SG	1:B:740:ILE:N	2.77	0.57
1:B:978:PRO:HA	1:B:981:SER:HB3	1.85	0.57
1:B:608:GLY:HA2	1:B:642:LEU:HB3	1.87	0.57
1:D:558:ARG:HB2	1:D:767:PRO:HG3	1.87	0.57
1:D:775:THR:HG23	1:D:805:THR:HG22	1.85	0.57
1:B:894:TYR:CE2	1:B:906:LYS:HE3	2.36	0.57
1:C:451:ARG:HG2	3:C:2001:COA:O7A	2.04	0.57
1:C:243:ARG:HH22	1:C:281:ALA:HB3	1.69	0.57
1:C:1054:ARG:NH2	1:D:108:GLU:CD	2.61	0.57
1:D:423:ASP:OD1	1:D:424:SER:N	2.36	0.57
1:D:585:HIS:NE2	1:D:1051:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:LEU:HA	1:D:686:MET:HE2	1.86	0.57
1:D:711:ALA:HA	1:D:754:MET:HE1	1.85	0.57
1:C:701:GLU:HB3	1:C:737:ILE:HB	1.87	0.57
1:D:44:ASN:HD22	1:D:117:GLY:HA3	1.70	0.57
1:C:73:GLY:CA	1:D:1081:ASN:O	2.53	0.57
1:D:909:PRO:O	1:D:913:ILE:HG12	2.04	0.57
1:C:680:LEU:HD13	1:C:905:ILE:HD11	1.87	0.56
1:C:949:GLN:O	1:C:964:ARG:NH2	2.31	0.56
1:D:394:ILE:HG12	1:D:455:VAL:HG11	1.86	0.56
1:D:1101:HIS:NE2	1:D:1172:ASP:OD1	2.30	0.56
1:C:919:GLN:HA	1:C:922:VAL:HG12	1.87	0.56
1:D:265:CYS:SG	1:D:273:LYS:HD3	2.45	0.56
1:D:934:GLN:HB2	1:D:937:GLU:HB2	1.86	0.56
1:A:818:ARG:NH2	1:A:823:ASP:OD1	2.33	0.56
1:A:855:LYS:HE3	1:D:851:THR:HG21	1.87	0.56
1:B:644:ARG:NE	1:B:908:THR:HG21	2.20	0.56
1:B:908:THR:HB	1:B:909:PRO:HD3	1.86	0.56
1:C:743:MET:HG3	1:C:867:PRO:HA	1.87	0.56
1:D:50:ILE:HD11	1:D:76:HIS:HA	1.87	0.56
1:B:607:TRP:HB2	1:B:641:MET:HB2	1.86	0.56
1:A:855:LYS:HE2	1:D:842:ARG:HG2	1.88	0.56
1:C:80:ALA:O	3:D:2001:COA:C6A	2.53	0.56
1:D:706:TYR:N	1:D:741:LYS:O	2.37	0.56
1:A:909:PRO:O	1:A:912:LYS:HG2	2.05	0.56
1:B:742:ASP:OD1	1:B:745:GLY:N	2.39	0.56
1:C:750:THR:HA	1:C:753:THR:HG22	1.88	0.56
1:D:504:LEU:HD12	1:D:1042:PRO:HD3	1.87	0.56
1:C:563:LEU:HD11	1:C:794:VAL:HG23	1.87	0.56
1:D:1161:HIS:HB2	1:D:1176:GLU:HB2	1.88	0.56
1:A:945:VAL:O	1:A:949:GLN:HB2	2.05	0.56
1:C:1003:THR:OG1	1:C:1006:ASP:OD2	2.15	0.56
1:B:604:MET:HB3	1:B:639:PHE:HD1	1.71	0.55
1:B:650:GLY:HA2	1:B:1012:MET:HE1	1.87	0.55
1:C:588:LYS:NZ	1:C:1031:ASP:OD2	2.37	0.55
1:C:1003:THR:HB	1:C:1004:PRO:HD2	1.88	0.55
1:C:224:ALA:HA	1:C:228:PHE:HD2	1.70	0.55
1:C:517:PRO:HB3	1:C:876:PHE:HE1	1.70	0.55
1:D:550:PRO:HB2	1:D:736:HIS:CD2	2.41	0.55
1:C:593:TYR:OH	1:C:833:ASP:OD1	2.24	0.55
1:C:747:LEU:HD22	1:C:782:ALA:HB1	1.88	0.55
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:872:THR:HG23	1:D:873:ASN:H	1.66	0.55
1:C:50:ILE:HD11	1:C:76:HIS:HA	1.89	0.55
1:C:199:GLY:C	2:C:2000:ATP:PB	2.90	0.55
1:D:723:TYR:HA	1:D:726:LEU:HD12	1.88	0.55
1:A:1091:ASP:OD1	1:A:1092:THR:N	2.39	0.55
1:D:850:CYS:O	1:D:854:MET:N	2.31	0.55
1:A:564:LEU:O	1:A:794:VAL:HG22	2.07	0.55
1:C:395:GLU:HG3	1:C:1088:LEU:HD23	1.69	0.55
1:C:724:MET:HE3	1:C:762:ARG:HH21	1.70	0.55
1:B:1091:ASP:OD1	1:B:1092:THR:N	2.40	0.55
1:C:178:HIS:NE2	1:C:182:GLU:OE2	2.40	0.55
1:A:948:LEU:HB3	1:A:968:LEU:HD21	1.87	0.55
1:B:724:MET:HG2	1:B:762:ARG:HH21	1.71	0.55
1:D:533:PRO:HG2	1:D:596:HIS:CD2	2.41	0.55
1:D:1127:ALA:HB1	1:D:1175:LEU:HD21	1.89	0.55
1:A:1069:ASN:OD1	1:A:1070:ARG:N	2.40	0.54
1:B:600:LYS:HD2	1:B:826:VAL:HG22	1.88	0.54
1:C:1044:ILE:HD13	1:C:1062:ALA:HB1	1.89	0.54
1:D:948:LEU:HD22	1:D:964:ARG:HG3	1.88	0.54
1:D:1063:LEU:HD23	1:D:1077:PHE:HB3	1.89	0.54
1:D:1080:LEU:HD23	1:D:1081:ASN:H	1.72	0.54
1:B:1000:GLU:HG2	1:B:1001:GLU:OE1	2.06	0.54
1:C:391:THR:HG21	1:C:420:PRO:HB3	1.89	0.54
1:C:396:VAL:HB	1:C:453:ARG:HB2	1.89	0.54
1:B:682:TYR:HE1	1:B:954:VAL:HG12	1.73	0.54
1:B:1050:VAL:HB	1:B:1058:LEU:HD11	1.88	0.54
1:D:35:LYS:HB3	1:D:137:ARG:NH2	2.22	0.54
1:D:35:LYS:HD2	1:D:137:ARG:HH21	1.72	0.54
1:D:121:LEU:HD23	1:D:124:ARG:HG3	1.89	0.54
1:D:394:ILE:HD12	1:D:416:ALA:HB3	1.89	0.54
1:C:1082:GLY:HA2	1:D:73:GLY:O	2.07	0.54
1:D:35:LYS:HD3	1:D:137:ARG:NH2	2.22	0.54
1:A:576:SER:O	1:A:872:THR:HG21	2.08	0.54
1:B:570:PHE:CD1	1:B:604:MET:HE2	2.42	0.54
1:A:1015:ASP:OD1	1:A:1016:VAL:N	2.40	0.54
1:C:827:PRO:HB2	1:C:830:ARG:HE	1.72	0.54
1:D:508:MET:HE3	1:D:1042:PRO:HD2	1.88	0.54
1:A:854:MET:HE1	1:A:857:GLY:HA2	1.88	0.54
1:D:715:ARG:HE	1:D:717:LYS:H	1.56	0.54
1:C:585:HIS:HA	1:C:588:LYS:HE2	1.89	0.54
1:B:1069:ASN:OD1	1:B:1070:ARG:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1059:HIS:CD2	1:D:77:ARG:CZ	2.90	0.54
1:C:37:ILE:HG23	1:C:112:ASP:HB3	1.90	0.53
1:C:265:CYS:SG	1:C:276:GLU:HG3	2.48	0.53
1:C:681:ASN:C	1:C:956:HIS:HB2	2.33	0.53
1:C:783:MET:HE1	1:C:808:PRO:HD2	1.90	0.53
1:C:1077:PHE:CZ	1:D:1063:LEU:CG	2.92	0.53
1:D:47:GLU:HB3	1:D:410:ALA:HB2	1.89	0.53
1:B:608:GLY:N	1:B:611:THR:OG1	2.41	0.53
1:D:604:MET:O	1:D:640:GLN:N	2.41	0.53
1:D:660:PHE:HZ	1:D:691:GLU:HG3	1.72	0.53
1:B:509:VAL:HG21	1:B:1089:VAL:HG21	1.90	0.53
1:B:538:PRO:HG2	1:B:599:SER:HB3	1.89	0.53
1:B:581:ARG:HB2	1:B:848:PHE:CE2	2.44	0.53
1:C:564:LEU:HB2	1:C:793:VAL:HG22	1.90	0.53
1:D:921:MET:O	1:D:925:GLY:N	2.40	0.53
1:C:1034:ASN:OD1	1:C:1035:THR:N	2.35	0.53
1:C:451:ARG:NH1	3:C:2001:COA:P3B	2.81	0.53
1:D:390:ASP:OD2	1:D:456:LYS:HB2	2.07	0.53
1:D:896:GLU:HB2	1:D:928:ARG:HD2	1.89	0.53
1:B:514:THR:HG21	1:B:581:ARG:NH1	2.24	0.53
1:B:568:THR:OG1	1:B:807:GLN:OE1	2.23	0.53
1:C:82:GLU:OE1	1:C:84:TYR:OH	2.25	0.53
1:C:453:ARG:HG3	1:C:498:GLN:HG2	1.89	0.53
1:B:667:LYS:HE3	1:B:674:PHE:CE2	2.42	0.53
1:D:37:ILE:HG23	1:D:112:ASP:HB3	1.90	0.53
1:D:908:THR:OG1	1:D:909:PRO:HD3	2.08	0.53
1:A:814:VAL:HA	1:A:824:THR:HG21	1.90	0.53
1:A:828:MET:HE1	1:D:862:TYR:HD2	1.74	0.53
1:A:874:LEU:HG	1:A:887:PHE:HE1	1.74	0.53
1:A:909:PRO:HA	1:A:912:LYS:HE3	1.91	0.53
1:A:998:HIS:CE1	1:A:1021:LYS:HB2	2.44	0.53
1:B:523:SER:O	1:B:1036:ARG:NH2	2.42	0.53
1:D:1113:GLY:HA2	1:D:1174:ILE:H	1.73	0.53
1:D:1131:VAL:HG21	1:D:1151:SER:H	1.74	0.53
1:A:544:ILE:HA	1:A:547:ARG:HH21	1.74	0.52
1:A:593:TYR:OH	1:A:833:ASP:HB2	2.09	0.52
1:A:667:LYS:HE2	1:A:674:PHE:CD2	2.43	0.52
1:A:949:GLN:NE2	1:A:972:PRO:O	2.33	0.52
1:B:567:ASP:OD1	1:B:568:THR:N	2.43	0.52
1:C:1059:HIS:CD2	1:D:77:ARG:HH12	2.25	0.52
1:D:1115:PRO:HA	1:D:1171:ASP:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:PHE:HB3	1:A:601:LEU:HD23	1.90	0.52
1:A:760:ARG:NH1	1:A:766:LEU:O	2.39	0.52
1:B:667:LYS:NZ	1:B:672:ASP:O	2.42	0.52
1:C:386:SER:OG	1:C:388:GLN:OE1	2.27	0.52
1:A:683:LEU:HA	1:A:686:MET:HE2	1.91	0.52
1:D:864:ASN:ND2	1:D:891:LYS:HD2	2.25	0.52
1:A:565:LEU:HD12	1:A:794:VAL:HG23	1.91	0.52
1:B:614:VAL:HG22	1:B:619:LEU:HD13	1.92	0.52
1:A:640:GLN:OE1	1:A:675:ARG:N	2.42	0.52
1:A:817:THR:HG22	1:A:823:ASP:HA	1.92	0.52
1:C:51:ARG:NH2	1:C:337:GLU:OE2	2.42	0.52
1:C:964:ARG:HH21	1:C:973:ARG:CZ	2.23	0.52
1:C:1132:ALA:HB3	1:C:1135:GLN:HG2	1.92	0.52
1:D:265:CYS:SG	1:D:273:LYS:HG2	2.50	0.51
1:D:705:SER:HA	1:D:741:LYS:HB3	1.92	0.51
1:A:738:LEU:HD23	1:A:739:CYS:N	2.25	0.51
1:B:644:ARG:HH11	1:B:649:VAL:HA	1.75	0.51
1:D:769:HIS:NE2	1:D:795:ASP:OD1	2.37	0.51
1:D:900:MET:HE3	1:D:928:ARG:HG3	1.91	0.51
1:A:593:TYR:O	1:A:597:ASN:ND2	2.42	0.51
1:A:997:ARG:HD3	1:A:1021:LYS:HZ3	1.73	0.51
1:B:623:PRO:HA	1:B:626:ARG:HB3	1.91	0.51
1:C:565:LEU:HD11	1:C:813:LEU:HD22	1.91	0.51
1:C:566:MET:HE1	1:C:568:THR:HG23	1.92	0.51
2:C:2000:ATP:H5'1	2:C:2000:ATP:H8	1.75	0.51
1:B:1065:VAL:HG23	1:B:1076:VAL:HG12	1.92	0.51
1:C:242:PRO:HD2	1:C:478:THR:HB	1.91	0.51
1:C:1061:LYS:HB3	1:C:1079:GLU:CG	2.40	0.51
1:A:622:CYS:H	1:A:625:ARG:NH2	2.08	0.51
1:B:666:ALA:O	1:B:671:MET:HB3	2.10	0.51
1:D:335:VAL:HG21	1:D:375:GLN:HB2	1.92	0.51
1:A:571:ARG:HH22	1:A:743:MET:HE1	1.76	0.51
1:C:720:LEU:HA	1:C:723:TYR:HD2	1.75	0.51
1:A:563:LEU:HD21	1:A:794:VAL:HG11	1.93	0.51
1:A:581:ARG:HD3	1:A:619:LEU:HD21	1.93	0.51
1:A:842:ARG:HH21	1:A:851:THR:HG1	1.54	0.51
1:B:677:PHE:CZ	1:B:705:SER:HB3	2.46	0.51
1:C:1003:THR:N	1:C:1006:ASP:OD2	2.40	0.51
1:D:571:ARG:HD3	1:D:608:GLY:HA3	1.92	0.51
1:D:600:LYS:NZ	1:D:825:GLU:O	2.33	0.51
1:A:667:LYS:HE2	1:A:674:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:PRO:O	1:A:913:ILE:HG12	2.11	0.51
1:C:841:ALA:HA	1:C:844:LEU:HD13	1.93	0.51
1:A:1009:SER:HA	1:A:1012:MET:HE2	1.92	0.51
1:C:703:ALA:HB1	1:C:741:LYS:HG2	1.93	0.51
1:C:994:LEU:O	1:C:999:GLY:N	2.44	0.51
1:D:399:SER:OG	1:D:401:GLU:OE1	2.20	0.51
1:D:1006:ASP:OD1	1:D:1007:VAL:N	2.44	0.51
1:D:1128:GLY:HA2	1:D:1157:VAL:HG11	1.93	0.51
1:A:779:GLY:O	1:A:783:MET:CB	2.59	0.51
1:B:616:MET:HE3	1:B:616:MET:HA	1.93	0.51
1:B:909:PRO:O	1:B:913:ILE:HG12	2.11	0.50
1:C:265:CYS:SG	1:C:273:LYS:HD2	2.51	0.50
1:C:395:GLU:CD	1:C:1088:LEU:HD22	2.15	0.50
1:C:590:ILE:HG21	1:C:834:TYR:HE1	1.76	0.50
1:C:604:MET:O	1:C:640:GLN:N	2.40	0.50
1:D:123:GLU:OE1	1:D:328:ARG:HD3	2.10	0.50
1:D:314:VAL:HA	1:D:320:HIS:HA	1.93	0.50
1:B:1015:ASP:OD1	1:B:1016:VAL:N	2.45	0.50
1:C:1079:GLU:HB2	1:C:1083:GLN:O	2.11	0.50
1:D:566:MET:HG2	1:D:603:SER:O	2.12	0.50
1:D:771:HIS:ND1	1:D:795:ASP:OD2	2.37	0.50
1:B:951:TYR:O	1:B:978:PRO:HG2	2.11	0.50
1:C:883:LEU:HB3	1:C:886:LYS:HB2	1.93	0.50
1:D:878:ALA:HB1	1:D:884:GLY:HA3	1.92	0.50
1:C:309:THR:HB	1:C:326:ASN:HB2	1.94	0.50
1:C:920:PHE:O	1:C:923:GLN:HG3	2.11	0.50
1:D:828:MET:HB3	1:D:832:PHE:CZ	2.47	0.50
1:B:575:GLN:O	1:B:872:THR:OG1	2.23	0.50
1:D:1080:LEU:N	1:D:1083:GLN:O	2.45	0.50
1:A:593:TYR:OH	1:A:830:ARG:O	2.25	0.50
1:A:761:ASP:OD1	1:A:762:ARG:N	2.45	0.50
1:A:868:GLY:O	1:A:872:THR:HG23	2.12	0.50
1:A:1068:LEU:HG	1:A:1074:ARG:HE	1.75	0.50
1:B:524:PRO:HA	1:B:1036:ARG:HH22	1.77	0.50
1:D:64:VAL:HA	1:D:82:GLU:HB2	1.94	0.50
1:A:500:LEU:HD23	1:A:504:LEU:HD23	1.93	0.50
1:B:796:VAL:HG13	1:B:808:PRO:O	2.12	0.50
1:C:566:MET:HG3	1:C:602:PHE:HD2	1.76	0.50
1:D:896:GLU:HA	1:D:899:GLN:HB2	1.94	0.50
1:C:207:VAL:HG11	1:C:213:LEU:HD13	1.93	0.49
1:C:997:ARG:HH12	1:C:1018:ALA:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LYS:HD3	1:D:137:ARG:HH21	1.71	0.49
1:D:593:TYR:OH	1:D:830:ARG:O	2.26	0.49
1:B:566:MET:N	1:B:794:VAL:O	2.35	0.49
1:C:290:ARG:HD3	1:C:320:HIS:CE1	2.47	0.49
1:C:584:THR:HG22	1:C:626:ARG:NE	2.23	0.49
1:C:801:MET:HE1	1:C:838:TRP:CG	2.46	0.49
1:D:393:ARG:HD2	1:D:1088:LEU:HD11	1.94	0.49
1:B:706:TYR:HE1	1:B:710:VAL:HB	1.77	0.49
1:C:80:ALA:C	3:D:2001:COA:H62A	2.19	0.49
1:C:583:ARG:HH22	1:C:1031:ASP:H	1.60	0.49
1:D:583:ARG:HH22	1:D:1033:LEU:HB2	1.77	0.49
1:D:799:ASP:HB3	1:D:835:SER:HB2	1.93	0.49
1:A:816:CYS:HA	1:D:748:LYS:HD2	1.94	0.49
1:A:1077:PHE:HZ	1:B:1063:LEU:CG	2.17	0.49
1:B:680:LEU:HA	1:B:905:ILE:HG13	1.93	0.49
1:B:1079:GLU:CG	1:B:1084:LEU:HD21	2.38	0.49
1:C:1081:ASN:ND2	1:D:77:ARG:HH11	1.93	0.49
1:D:196:ALA:HB3	1:D:232:ALA:HB3	1.94	0.49
1:D:578:LEU:HG	1:D:579:ALA:H	1.77	0.49
1:A:901:LEU:HD12	1:A:947:PHE:HE2	1.77	0.49
1:C:756:VAL:HG21	1:C:790:GLY:HA3	1.94	0.49
1:D:525:THR:O	1:D:1036:ARG:NH2	2.45	0.49
1:D:558:ARG:HE	1:D:760:ARG:CZ	2.26	0.49
1:D:937:GLU:OE1	1:D:937:GLU:N	2.45	0.49
1:A:737:ILE:HG12	1:A:767:PRO:HB2	1.95	0.49
1:A:828:MET:HE2	1:A:832:PHE:CZ	2.48	0.49
1:B:593:TYR:OH	1:B:830:ARG:O	2.31	0.49
1:A:801:MET:SD	1:A:838:TRP:HB3	2.53	0.49
1:B:801:MET:HE1	1:B:838:TRP:CG	2.47	0.49
1:B:920:PHE:HA	1:B:923:GLN:HG2	1.95	0.49
1:B:1059:HIS:N	1:B:1081:ASN:OD1	2.46	0.49
1:C:896:GLU:HB3	1:C:928:ARG:HH21	1.78	0.49
1:A:501:LEU:HD23	1:A:504:LEU:HD21	1.95	0.49
1:C:73:GLY:O	1:D:1082:GLY:CA	2.61	0.49
1:C:177:LEU:HB2	1:C:217:TYR:CE2	2.48	0.49
1:C:459:ILE:HD12	1:C:459:ILE:H	1.77	0.49
1:C:604:MET:HB3	1:C:639:PHE:HD1	1.77	0.49
1:C:656:ASP:OD1	1:C:657:ASN:N	2.46	0.49
1:B:609:GLY:HA2	1:B:644:ARG:HH22	1.78	0.49
1:C:878:ALA:O	1:C:883:LEU:N	2.46	0.49
1:D:397:PHE:N	1:D:414:GLN:OE1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:675:ARG:HA	1:D:701:GLU:HB3	1.95	0.49
1:D:927:SER:OG	1:D:928:ARG:N	2.46	0.49
1:D:1070:ARG:NH1	1:D:1071:ALA:HB3	2.28	0.49
1:D:1114:ALA:N	1:D:1172:ASP:O	2.46	0.49
1:B:1079:GLU:HA	1:B:1084:LEU:HD22	1.83	0.48
1:D:265:CYS:SG	1:D:273:LYS:CD	3.01	0.48
1:A:576:SER:HA	1:A:869:GLY:HA2	1.95	0.48
1:C:57:THR:HG21	3:D:2001:COA:H32	1.94	0.48
1:C:667:LYS:HD2	1:C:671:MET:O	2.13	0.48
1:B:746:LEU:HD22	1:B:862:TYR:CD2	2.48	0.48
1:C:58:GLU:OE2	1:C:346:HIS:NE2	2.46	0.48
1:C:210:TYR:HA	1:C:213:LEU:HB3	1.94	0.48
1:C:356:SER:OG	1:C:359:ASP:OD2	2.23	0.48
1:C:990:LEU:O	1:C:993:GLU:HG3	2.14	0.48
1:C:1035:THR:O	1:C:1039:LEU:HG	2.13	0.48
1:D:519:LYS:HE2	1:D:519:LYS:HA	1.94	0.48
1:D:801:MET:HE1	1:D:842:ARG:HB2	1.95	0.48
1:D:1103:LYS:NZ	1:D:1169:GLU:OE2	2.46	0.48
1:A:1015:ASP:O	1:A:1019:HIS:ND1	2.41	0.48
1:C:77:ARG:HH22	1:D:1059:HIS:CE1	2.31	0.48
1:C:82:GLU:HG2	1:D:1055:GLY:CA	2.42	0.48
1:D:398:ARG:NH2	3:D:2001:COA:O9A	2.29	0.48
1:D:804:MET:HA	1:D:857:GLY:H	1.77	0.48
1:A:1008:LEU:HG	1:A:1012:MET:HE1	1.95	0.48
1:B:568:THR:HG22	1:B:605:GLU:HG3	1.94	0.48
1:B:577:LEU:HD13	1:B:850:CYS:SG	2.53	0.48
1:B:796:VAL:HG21	1:B:813:LEU:HD21	1.96	0.48
1:C:916:ASP:O	1:C:919:GLN:HG3	2.14	0.48
1:C:1119:LYS:HA	1:C:1170:GLY:HA2	1.96	0.48
1:D:565:LEU:HG	1:D:601:LEU:HD12	1.95	0.48
1:D:1151:SER:OG	1:D:1153:MET:O	2.31	0.48
1:A:504:LEU:O	1:A:508:MET:HG2	2.13	0.48
1:B:775:THR:HG23	1:B:805:THR:HG22	1.96	0.48
1:D:870:GLN:HE22	1:D:874:LEU:HD22	1.79	0.48
1:A:583:ARG:NH1	1:A:1038:PHE:HB2	2.28	0.48
1:B:968:LEU:HD11	1:B:973:ARG:HG2	1.96	0.48
1:C:81:ASP:C	3:D:2001:COA:H62A	2.22	0.48
1:C:604:MET:HB3	1:C:639:PHE:CD1	2.48	0.48
1:C:873:ASN:HA	1:C:876:PHE:HB3	1.95	0.48
1:A:675:ARG:HD3	1:A:741:LYS:HD2	1.95	0.48
1:B:603:SER:HA	1:B:637:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ARG:HD3	1:C:608:GLY:HA3	1.96	0.48
1:D:385:ARG:HG3	1:D:386:SER:N	2.28	0.48
1:D:1091:ASP:OD1	1:D:1092:THR:N	2.47	0.48
1:D:1161:HIS:CD2	1:D:1173:LEU:HB3	2.49	0.48
1:A:742:ASP:OD2	1:A:746:LEU:N	2.45	0.48
1:A:828:MET:HE2	1:A:832:PHE:HZ	1.77	0.48
1:B:643:LEU:HD12	1:B:662:PHE:HE2	1.79	0.48
1:C:82:GLU:HB3	1:D:1055:GLY:CA	2.29	0.48
1:C:751:ALA:HA	1:C:754:MET:SD	2.53	0.48
1:C:1008:LEU:HD23	1:C:1012:MET:HE3	1.96	0.48
1:D:677:PHE:CE2	1:D:907:VAL:HG11	2.48	0.48
1:A:948:LEU:O	1:A:964:ARG:NE	2.42	0.47
1:B:604:MET:HB3	1:B:639:PHE:CD1	2.47	0.47
1:A:667:LYS:HG3	1:A:696:ALA:HB1	1.97	0.47
1:A:779:GLY:O	1:A:783:MET:HB2	2.14	0.47
1:C:1015:ASP:OD1	1:C:1015:ASP:N	2.47	0.47
1:C:558:ARG:HH22	1:C:760:ARG:HD2	1.78	0.47
1:D:1033:LEU:HD23	1:D:1050:VAL:HG21	1.97	0.47
1:D:1118:GLY:C	1:D:1119:LYS:HD3	2.39	0.47
1:D:453:ARG:CG	1:D:498:GLN:CG	2.60	0.47
1:D:720:LEU:O	1:D:724:MET:HG2	2.14	0.47
1:A:1068:LEU:HD22	1:A:1072:GLY:HA2	1.97	0.47
1:B:680:LEU:HD11	1:B:955:PRO:HB3	1.96	0.47
1:D:283:LEU:HD12	1:D:287:LEU:HD23	1.96	0.47
1:D:787:ALA:HA	1:D:791:ALA:HB3	1.96	0.47
1:D:969:LYS:HG3	1:D:970:ASP:H	1.79	0.47
1:D:987:LEU:H	1:D:987:LEU:HD23	1.79	0.47
1:D:1065:VAL:HG23	1:D:1076:VAL:HG22	1.96	0.47
1:A:648:ALA:HB1	1:A:662:PHE:CD2	2.49	0.47
1:A:680:LEU:O	1:A:682:TYR:N	2.45	0.47
1:A:1068:LEU:HG	1:A:1074:ARG:HH21	1.80	0.47
1:C:244:HIS:HB3	1:C:313:LEU:HD12	1.95	0.47
1:C:677:PHE:HZ	1:C:907:VAL:HG21	1.80	0.47
1:D:550:PRO:HB3	1:D:699:VAL:HA	1.95	0.47
1:D:1140:LEU:HD11	1:D:1174:ILE:HG21	1.97	0.47
1:A:1034:ASN:HB2	1:A:1037:LEU:HG	1.97	0.47
1:B:726:LEU:O	1:B:729:GLU:HG2	2.13	0.47
1:C:677:PHE:CZ	1:C:907:VAL:HG21	2.49	0.47
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.80	0.47
1:C:978:PRO:HA	1:C:981:SER:HB3	1.97	0.47
1:D:265:CYS:SG	1:D:273:LYS:CG	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1102:PRO:HG2	1:D:1161:HIS:CE1	2.44	0.47
1:A:797:ALA:HB2	1:A:807:GLN:HB2	1.96	0.47
1:D:498:GLN:O	1:D:502:HIS:ND1	2.34	0.47
1:B:573:ALA:HB1	1:B:801:MET:HB3	1.97	0.47
1:B:794:VAL:HG12	1:B:796:VAL:HG23	1.97	0.47
1:C:176:SER:HB2	1:C:179:GLU:HG2	1.97	0.47
1:C:395:GLU:O	1:C:414:GLN:NE2	2.33	0.47
1:D:335:VAL:CG2	1:D:375:GLN:HB2	2.45	0.47
1:B:571:ARG:HG3	1:B:607:TRP:C	2.40	0.46
1:B:917:LEU:HD12	1:B:944:VAL:HG22	1.97	0.46
1:C:77:ARG:NH2	1:D:1059:HIS:HE1	2.11	0.46
1:C:194:LYS:HD3	1:C:204:MET:HE1	1.97	0.46
1:D:391:THR:HG21	1:D:420:PRO:HB3	1.96	0.46
1:B:639:PHE:HB3	1:B:671:MET:HE1	1.97	0.46
1:B:649:VAL:HG23	1:B:1012:MET:SD	2.55	0.46
1:B:721:GLN:HA	1:B:724:MET:HE2	1.97	0.46
1:D:376:CYS:SG	1:D:443:MET:HE3	2.55	0.46
1:A:612:PHE:CD1	1:A:623:PRO:HG2	2.49	0.46
1:C:624:TRP:HB3	1:C:628:GLN:HE22	1.81	0.46
1:C:1067:ASP:HA	1:C:1074:ARG:HH21	1.80	0.46
1:C:1067:ASP:HA	1:C:1074:ARG:NH2	2.30	0.46
3:C:2001:COA:H21	1:D:57:THR:CG2	2.44	0.46
1:D:464:ASN:HD21	1:D:489:GLN:HB2	1.79	0.46
1:C:827:PRO:HG2	1:C:830:ARG:HH21	1.80	0.46
1:D:243:ARG:O	1:D:314:VAL:HG12	2.14	0.46
1:D:1066:SER:O	1:D:1074:ARG:NH1	2.45	0.46
1:A:992:LYS:HA	1:A:995:VAL:HG12	1.97	0.46
1:B:770:ILE:CG2	1:B:783:MET:HE1	2.45	0.46
1:C:1055:GLY:C	1:D:82:GLU:CD	2.82	0.46
1:D:578:LEU:HD21	1:D:848:PHE:HE1	1.79	0.46
1:B:612:PHE:HD1	1:B:623:PRO:HG2	1.80	0.46
1:D:453:ARG:CB	1:D:498:GLN:HG3	2.42	0.46
1:A:888:LYS:HA	1:A:891:LYS:HE2	1.98	0.46
1:C:248:GLN:HG2	1:C:260:LEU:HD12	1.98	0.46
1:C:453:ARG:CB	1:C:498:GLN:HG2	2.45	0.46
3:C:2001:COA:C2A	1:D:81:ASP:OD1	2.63	0.46
1:A:501:LEU:HA	1:A:504:LEU:HG	1.98	0.46
1:B:961:GLU:N	1:B:962:PRO:HD2	2.31	0.46
1:B:1077:PHE:CZ	1:B:1084:LEU:HB3	2.51	0.46
1:C:870:GLN:NE2	1:C:874:LEU:HB2	2.31	0.46
1:C:910:SER:HA	1:C:913:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:955:PRO:HG2	1:D:958:GLY:C	2.41	0.46
1:D:679:SER:HB2	1:D:909:PRO:HD2	1.98	0.46
1:D:827:PRO:HG2	1:D:830:ARG:HE	1.81	0.46
1:B:749:PRO:O	1:B:752:CYS:HB3	2.16	0.46
1:C:909:PRO:O	1:C:912:LYS:HG2	2.16	0.46
1:D:520:ALA:HB3	1:D:847:ALA:HA	1.98	0.46
1:B:1069:ASN:ND2	1:B:1070:ARG:HH11	2.14	0.45
1:D:99:ILE:HG12	1:D:127:PHE:HD1	1.81	0.45
1:D:225:LEU:HD22	1:D:231:GLY:HA3	1.98	0.45
1:C:605:GLU:HA	1:C:640:GLN:O	2.16	0.45
1:C:940:PHE:HB3	1:C:944:VAL:HB	1.98	0.45
1:D:350:HIS:HA	1:D:353:GLU:OE2	2.16	0.45
1:D:453:ARG:CB	1:D:498:GLN:NE2	2.80	0.45
1:A:782:ALA:O	1:A:786:CYS:HB2	2.16	0.45
1:A:859:SER:O	1:A:860:ASP:HB2	2.16	0.45
1:A:722:TYR:CE2	1:A:726:LEU:HD11	2.52	0.45
1:A:746:LEU:HD11	1:A:862:TYR:HA	1.97	0.45
1:B:800:SER:O	1:B:842:ARG:NH1	2.45	0.45
1:C:961:GLU:CD	1:C:961:GLU:H	2.24	0.45
1:D:456:LYS:HD2	1:D:456:LYS:HA	1.67	0.45
1:A:710:VAL:HG11	1:A:755:LEU:HD21	1.97	0.45
1:A:828:MET:HE1	1:D:862:TYR:CD2	2.52	0.45
1:A:855:LYS:HG2	1:D:839:GLU:OE1	2.17	0.45
1:B:563:LEU:HB2	1:B:822:LEU:HB3	1.99	0.45
1:C:385:ARG:HG3	1:C:386:SER:N	2.29	0.45
1:C:393:ARG:HD3	1:C:1088:LEU:CD2	2.32	0.45
1:C:503:TYR:CZ	1:C:1030:LEU:HD11	2.52	0.45
1:D:680:LEU:HD11	1:D:682:TYR:HB2	1.98	0.45
1:D:1015:ASP:OD1	1:D:1016:VAL:N	2.48	0.45
1:A:566:MET:HE3	1:A:795:ASP:OD1	2.16	0.45
1:A:820:THR:HG22	1:A:822:LEU:H	1.81	0.45
1:B:532:VAL:HG11	1:B:593:TYR:HA	1.98	0.45
1:B:567:ASP:HB3	1:B:604:MET:SD	2.57	0.45
1:B:748:LYS:HE2	1:B:862:TYR:CE2	2.52	0.45
1:C:796:VAL:HG21	1:C:813:LEU:HD13	1.99	0.45
1:A:504:LEU:HD12	1:A:505:GLY:N	2.31	0.45
1:A:741:LYS:NZ	1:A:743:MET:HE2	2.32	0.45
1:B:570:PHE:CZ	1:B:587:LEU:HD12	2.52	0.45
1:B:742:ASP:O	1:B:772:THR:HA	2.16	0.45
1:B:1012:MET:HE3	1:B:1013:TYR:CE2	2.52	0.45
1:C:1047:GLU:OE2	1:C:1059:HIS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LYS:CB	1:D:137:ARG:NH2	2.80	0.45
1:D:744:ALA:O	1:D:861:VAL:HG11	2.17	0.45
1:A:1061:LYS:HD2	1:A:1079:GLU:HB3	1.99	0.45
1:B:604:MET:O	1:B:640:GLN:N	2.41	0.45
1:B:878:ALA:HB1	1:B:883:LEU:HB2	1.97	0.45
1:C:923:GLN:NE2	1:C:924:ASN:OD1	2.50	0.45
1:D:742:ASP:OD2	1:D:746:LEU:N	2.50	0.45
1:D:934:GLN:O	1:D:938:LEU:HG	2.17	0.45
1:D:1048:PHE:CZ	1:D:1060:ILE:HB	2.52	0.45
1:A:506:HIS:O	1:A:510:ASN:ND2	2.50	0.45
1:B:677:PHE:HE2	1:B:907:VAL:HG21	1.82	0.45
1:B:1033:LEU:HD11	1:B:1037:LEU:HB3	1.98	0.45
1:C:195:ALA:HA	1:C:233:LEU:HD23	1.99	0.45
1:C:674:PHE:O	1:C:700:VAL:HA	2.17	0.45
1:C:1058:LEU:HD13	1:C:1080:LEU:HD13	1.99	0.45
1:D:586:ASP:OD2	1:D:845:TYR:OH	2.18	0.45
1:A:677:PHE:CE2	1:A:907:VAL:HG11	2.48	0.44
1:A:760:ARG:NH2	1:A:768:LEU:HD23	2.32	0.44
1:A:1006:ASP:HB3	1:A:1017:PHE:CZ	2.52	0.44
1:B:677:PHE:HZ	1:B:705:SER:HB3	1.82	0.44
1:C:908:THR:CB	1:C:909:PRO:HD3	2.45	0.44
1:A:855:LYS:HG3	1:D:842:ARG:HD3	1.99	0.44
1:C:566:MET:HE3	1:C:795:ASP:HB3	1.98	0.44
1:C:590:ILE:HG13	1:C:837:TYR:CE2	2.53	0.44
1:D:280:ALA:HB1	1:D:283:LEU:HB2	1.98	0.44
1:D:677:PHE:HB3	1:D:703:ALA:HB3	1.99	0.44
1:D:688:LEU:O	1:D:691:GLU:HG2	2.16	0.44
1:D:43:ALA:HA	1:D:66:ILE:HD11	1.99	0.44
1:D:387:PHE:HB3	1:D:1144:LYS:HZ2	1.81	0.44
1:A:504:LEU:HA	1:A:507:VAL:HG22	1.98	0.44
1:B:731:VAL:HA	1:B:735:THR:HG22	1.99	0.44
1:B:860:ASP:OD1	1:B:863:GLU:HB2	2.17	0.44
1:C:77:ARG:CZ	1:D:1059:HIS:HE1	2.30	0.44
1:C:524:PRO:HA	1:C:1036:ARG:NH1	2.32	0.44
1:D:558:ARG:HD2	1:D:558:ARG:HA	1.63	0.44
1:D:655:PRO:HB3	1:D:984:PRO:HA	1.98	0.44
1:D:917:LEU:O	1:D:921:MET:HG3	2.17	0.44
1:B:551:GLU:OE1	1:B:555:ARG:NH1	2.50	0.44
1:B:1069:ASN:ND2	1:B:1073:GLN:HB3	2.30	0.44
1:C:739:CYS:HA	1:C:769:HIS:HB2	2.00	0.44
1:D:760:ARG:NH1	1:D:766:LEU:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:GLN:HB3	1:A:923:GLN:HE22	1.82	0.44
1:C:710:VAL:HB	1:C:720:LEU:HG	1.99	0.44
1:D:1009:SER:HA	1:D:1012:MET:HE2	2.00	0.44
1:A:854:MET:HE1	1:A:857:GLY:CA	2.48	0.44
1:A:908:THR:HB	1:A:909:PRO:HD3	1.99	0.44
1:C:575:GLN:O	1:C:872:THR:HG21	2.17	0.44
1:C:625:ARG:HA	1:C:628:GLN:OE1	2.18	0.44
1:D:66:ILE:HB	1:D:86:ILE:HG12	2.00	0.44
1:D:558:ARG:HD3	1:D:767:PRO:HA	1.99	0.44
1:A:907:VAL:HG12	1:A:908:THR:N	2.30	0.44
1:B:844:LEU:HD13	1:B:1035:THR:HB	1.99	0.44
1:C:88:ARG:HE	1:C:88:ARG:HB2	1.59	0.44
1:C:1081:ASN:ND2	1:D:77:ARG:HH12	2.04	0.44
1:C:1102:PRO:HG2	1:C:1166:MET:HE1	1.99	0.44
1:C:761:ASP:OD1	1:C:762:ARG:N	2.51	0.44
1:D:886:LYS:HD2	1:D:886:LYS:O	2.18	0.44
1:B:517:PRO:HB3	1:B:880:SER:HA	1.99	0.43
1:C:81:ASP:HA	1:D:1056:LYS:NZ	2.34	0.43
1:C:854:MET:SD	1:C:875:HIS:CE1	3.11	0.43
1:D:453:ARG:CG	1:D:498:GLN:CD	2.86	0.43
1:D:833:ASP:O	1:D:836:GLU:HG3	2.18	0.43
1:D:864:ASN:HD21	1:D:891:LYS:HD2	1.82	0.43
1:D:1059:HIS:H	1:D:1081:ASN:HD21	1.63	0.43
1:C:1045:ALA:HA	1:C:1061:LYS:NZ	2.33	0.43
1:D:726:LEU:HA	1:D:729:GLU:OE2	2.18	0.43
1:D:879:HIS:CE1	1:D:885:SER:HA	2.53	0.43
1:A:550:PRO:HB2	1:A:736:HIS:NE2	2.32	0.43
1:A:780:VAL:HG23	1:A:813:LEU:HD22	2.00	0.43
1:C:413:PHE:CE1	1:D:1082:GLY:C	2.86	0.43
1:D:260:LEU:HD11	1:D:344:LEU:HD11	2.00	0.43
1:D:267:ILE:HD13	1:D:476:VAL:HG11	1.99	0.43
1:D:873:ASN:HA	1:D:876:PHE:HB3	1.99	0.43
1:A:742:ASP:CG	1:A:746:LEU:H	2.26	0.43
1:A:919:GLN:HA	1:A:922:VAL:HG22	2.01	0.43
1:B:924:ASN:HB2	1:B:926:LEU:HG	2.00	0.43
1:C:567:ASP:OD1	1:C:797:ALA:HA	2.18	0.43
1:D:349:ILE:O	1:D:353:GLU:HG3	2.18	0.43
1:D:1006:ASP:HB2	1:D:1017:PHE:CZ	2.52	0.43
1:A:655:PRO:HG3	1:A:984:PRO:HA	2.00	0.43
1:A:738:LEU:HB3	1:A:766:LEU:HD21	2.00	0.43
1:A:901:LEU:HD11	1:A:948:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ASP:OD2	1:B:845:TYR:OH	2.30	0.43
1:C:571:ARG:HG3	1:C:607:TRP:O	2.18	0.43
1:C:952:ILE:O	1:C:978:PRO:HG2	2.18	0.43
1:C:1048:PHE:CE2	1:C:1060:ILE:HD13	2.54	0.43
1:C:1125:VAL:HG11	1:C:1160:VAL:HG11	2.01	0.43
1:B:574:HIS:HB3	1:B:580:THR:HG23	2.01	0.43
1:C:727:ALA:HA	1:C:730:LEU:HG	2.01	0.43
1:D:260:LEU:O	1:D:261:TYR:CG	2.72	0.43
1:D:1006:ASP:HB2	1:D:1017:PHE:CE1	2.53	0.43
1:B:906:LYS:HA	1:B:910:SER:OG	2.18	0.43
1:C:53:PHE:CE2	1:C:80:ALA:HB2	2.54	0.43
1:C:436:HIS:HB3	1:C:437:PRO:HD3	2.01	0.43
1:C:675:ARG:HH21	1:C:703:ALA:HB2	1.83	0.43
1:C:678:ASP:OD1	1:C:679:SER:N	2.52	0.43
1:D:194:LYS:HB3	1:D:234:PHE:HB2	2.00	0.43
1:D:280:ALA:HB1	1:D:283:LEU:HD23	1.99	0.43
1:D:828:MET:HB3	1:D:832:PHE:CE2	2.53	0.43
1:A:704:ILE:HD11	1:A:730:LEU:HD12	2.01	0.43
1:B:569:THR:HG22	1:B:604:MET:HE1	2.00	0.43
1:B:641:MET:CE	1:B:671:MET:HG2	2.47	0.43
1:B:644:ARG:HG3	1:B:647:ASN:O	2.19	0.43
1:C:775:THR:HA	1:C:804:MET:O	2.19	0.43
1:D:269:ARG:HD2	1:D:387:PHE:CE2	2.54	0.43
1:D:709:ASP:OD1	1:D:709:ASP:N	2.50	0.43
1:B:555:ARG:NH2	1:B:766:LEU:HA	2.34	0.43
1:B:948:LEU:HD22	1:B:964:ARG:HB3	2.01	0.43
1:C:496:ARG:O	1:C:498:GLN:N	2.52	0.43
1:C:936:GLU:HA	1:C:966:LYS:HB3	2.00	0.43
1:D:269:ARG:NH2	1:D:270:ARG:HE	2.16	0.43
1:A:841:ALA:HA	1:A:844:LEU:HD23	2.01	0.43
1:A:1075:GLN:HG2	1:A:1087:ILE:O	2.19	0.43
1:B:570:PHE:HB2	1:B:605:GLU:O	2.19	0.43
1:C:607:TRP:CD1	1:C:611:THR:HG21	2.54	0.43
1:C:800:SER:HB2	1:C:838:TRP:HB3	2.01	0.43
1:D:948:LEU:HD11	1:D:963:PHE:CE2	2.54	0.43
1:D:1059:HIS:H	1:D:1081:ASN:HD22	1.65	0.43
1:A:721:GLN:HA	1:A:724:MET:HG3	2.00	0.42
1:C:830:ARG:HA	1:C:833:ASP:OD2	2.19	0.42
1:C:867:PRO:HG2	1:C:911:SER:HB3	1.99	0.42
1:D:761:ASP:OD1	1:D:762:ARG:N	2.52	0.42
1:D:961:GLU:OE1	1:D:965:SER:OG	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:ASP:OD1	1:A:809:SER:HB2	2.19	0.42
1:A:1077:PHE:CE1	1:B:1063:LEU:CD1	2.92	0.42
1:B:799:ASP:OD1	1:B:802:SER:OG	2.37	0.42
1:C:78:GLN:HG2	1:D:1080:LEU:HD21	2.00	0.42
1:C:461:PHE:O	1:C:465:VAL:HG23	2.20	0.42
1:C:832:PHE:O	1:C:835:SER:N	2.51	0.42
1:D:387:PHE:O	1:D:1144:LYS:HD2	2.19	0.42
1:B:883:LEU:HB3	1:B:887:PHE:HB2	2.00	0.42
1:C:376:CYS:SG	1:C:443:MET:HE3	2.59	0.42
1:C:445:ARG:NH1	1:C:449:GLU:OE1	2.51	0.42
1:C:656:ASP:HB3	1:C:977:ARG:HH12	1.84	0.42
1:C:750:THR:O	1:C:753:THR:HG22	2.19	0.42
1:C:949:GLN:NE2	1:C:971:LEU:HB2	2.33	0.42
1:C:1056:LYS:NZ	1:C:1058:LEU:HB3	2.34	0.42
1:D:574:HIS:HB3	1:D:580:THR:HA	2.00	0.42
1:A:1043:LYS:NZ	1:A:1044:ILE:HG12	2.34	0.42
1:B:669:ASN:OD1	1:B:670:GLY:N	2.53	0.42
1:C:200:GLY:HA2	2:C:2000:ATP:O2B	2.19	0.42
1:D:279:PRO:HG2	1:D:372:CYS:SG	2.59	0.42
1:D:607:TRP:HZ2	1:D:612:PHE:HD1	1.67	0.42
1:B:624:TRP:HE1	1:B:1008:LEU:HD11	1.84	0.42
1:D:739:CYS:HB2	1:D:769:HIS:HB3	2.01	0.42
1:D:948:LEU:O	1:D:968:LEU:HD11	2.18	0.42
1:D:1156:THR:OG1	1:D:1158:ARG:NH1	2.52	0.42
1:A:631:ARG:NH2	1:A:637:ILE:O	2.29	0.42
1:A:774:ASP:OD2	1:A:808:PRO:HA	2.20	0.42
1:A:1023:PHE:HA	1:A:1026:THR:HG22	2.02	0.42
1:A:1078:PHE:O	1:A:1084:LEU:HG	2.20	0.42
1:B:964:ARG:HH21	1:B:973:ARG:HD3	1.84	0.42
1:C:675:ARG:NH2	1:C:741:LYS:HE2	2.35	0.42
1:D:173:PRO:HB3	1:D:232:ALA:HB1	2.01	0.42
1:D:906:LYS:HA	1:D:910:SER:HB2	2.00	0.42
1:A:572:ASP:HB3	1:A:807:GLN:NE2	2.31	0.42
1:A:586:ASP:OD2	1:A:845:TYR:OH	2.22	0.42
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.54	0.42
1:A:719:SER:OG	1:A:720:LEU:N	2.50	0.42
1:A:998:HIS:ND1	1:A:1021:LYS:HD2	2.35	0.42
1:B:566:MET:HG2	1:B:603:SER:H	1.84	0.42
1:B:615:ALA:HA	1:B:619:LEU:HB2	2.01	0.42
1:C:1080:LEU:HD23	1:C:1085:ARG:NH2	2.34	0.42
1:A:571:ARG:HH21	1:A:605:GLU:CD	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ARG:NH2	1:A:605:GLU:OE2	2.53	0.42
1:A:1042:PRO:HB3	1:A:1048:PHE:CE1	2.54	0.42
1:B:703:ALA:HB1	1:B:741:LYS:HB2	2.00	0.42
1:B:968:LEU:HD21	1:B:971:LEU:O	2.20	0.42
1:B:991:GLU:O	1:B:995:VAL:HG23	2.19	0.42
1:C:82:GLU:OE2	1:D:1053:GLU:OE1	2.38	0.42
1:C:374:ILE:HD11	1:C:436:HIS:CE1	2.55	0.42
1:C:1050:VAL:HG12	1:C:1052:LEU:HD22	2.02	0.42
1:C:1142:ALA:HB3	1:C:1145:MET:O	2.20	0.42
1:D:194:LYS:O	1:D:234:PHE:N	2.52	0.42
1:D:704:ILE:HD11	1:D:738:LEU:HD11	2.02	0.42
1:B:517:PRO:HG2	1:B:876:PHE:CE1	2.54	0.42
1:C:533:PRO:HG2	1:C:596:HIS:ND1	2.35	0.42
1:D:651:TYR:CE1	1:D:912:LYS:HD3	2.55	0.42
1:D:665:VAL:O	1:D:668:GLU:HG2	2.19	0.42
1:D:1095:MET:O	1:D:1096:LYS:HD2	2.19	0.42
1:A:563:LEU:HD11	1:A:794:VAL:HG13	2.02	0.42
1:B:543:ASP:N	1:B:543:ASP:OD1	2.53	0.42
1:C:278:ALA:HB3	1:C:279:PRO:HD3	2.02	0.42
1:C:453:ARG:HD2	1:C:498:GLN:CB	2.44	0.42
1:C:874:LEU:HG	1:C:887:PHE:HE1	1.84	0.42
1:D:1164:LYS:HA	1:D:1164:LYS:HD3	1.88	0.42
3:D:2001:COA:O6A	3:D:2001:COA:OAP	2.37	0.42
1:A:498:GLN:OE1	1:A:1085:ARG:NH1	2.53	0.41
1:B:968:LEU:HG	1:B:971:LEU:HB2	2.01	0.41
1:C:579:ALA:HB3	1:C:581:ARG:HD3	2.02	0.41
1:C:1076:VAL:O	1:C:1086:SER:HA	2.19	0.41
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.35	0.41
1:C:252:ASP:HA	1:C:351:VAL:HG21	2.02	0.41
1:C:413:PHE:CD1	1:D:1082:GLY:O	2.65	0.41
1:D:1137:LEU:HB2	1:D:1149:VAL:H	1.85	0.41
1:A:604:MET:HE3	1:A:639:PHE:CD1	2.55	0.41
1:A:688:LEU:HD13	1:A:691:GLU:OE2	2.20	0.41
1:B:497:ALA:O	1:B:500:LEU:HG	2.20	0.41
1:B:594:VAL:HG23	1:B:598:PHE:HD2	1.86	0.41
1:B:801:MET:SD	1:B:801:MET:N	2.94	0.41
1:B:921:MET:SD	1:B:926:LEU:HB2	2.60	0.41
1:C:151:ASP:HB3	1:C:154:GLU:OE1	2.20	0.41
1:C:583:ARG:NH1	1:C:1031:ASP:HA	2.35	0.41
1:A:542:ARG:NH2	1:A:670:GLY:O	2.51	0.41
1:A:654:TYR:OH	1:A:1012:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:THR:HG21	1:A:822:LEU:HD12	2.02	0.41
1:B:674:PHE:O	1:B:701:GLU:HB3	2.21	0.41
1:C:237:LYS:H	1:C:237:LYS:HG2	1.45	0.41
1:C:760:ARG:HH22	1:C:768:LEU:HB2	1.86	0.41
1:C:774:ASP:CG	1:C:779:GLY:H	2.28	0.41
1:C:1033:LEU:HB3	1:C:1037:LEU:HB2	2.01	0.41
1:D:396:VAL:HA	1:D:414:GLN:HE22	1.86	0.41
1:D:842:ARG:NH2	1:D:851:THR:HB	2.35	0.41
1:A:1003:THR:OG1	1:A:1006:ASP:OD2	2.31	0.41
1:B:566:MET:SD	1:B:605:GLU:HG2	2.61	0.41
1:C:121:LEU:HA	1:C:121:LEU:HD12	1.78	0.41
1:C:248:GLN:HB3	1:C:260:LEU:HB2	2.02	0.41
1:C:726:LEU:HA	1:C:729:GLU:CD	2.45	0.41
1:D:41:MET:HE2	1:D:114:VAL:HG12	2.02	0.41
1:D:98:HIS:ND1	1:D:101:ASP:HB2	2.35	0.41
1:D:387:PHE:HB3	1:D:1144:LYS:NZ	2.35	0.41
1:D:858:ASN:OD1	1:D:859:SER:N	2.54	0.41
1:B:642:LEU:HD13	1:B:741:LYS:NZ	2.36	0.41
1:B:677:PHE:CE2	1:B:907:VAL:HG21	2.55	0.41
1:C:73:GLY:O	1:D:1082:GLY:HA3	2.21	0.41
1:C:961:GLU:HA	1:C:964:ARG:HG2	2.03	0.41
1:D:464:ASN:ND2	1:D:489:GLN:HB2	2.35	0.41
1:B:568:THR:HA	1:B:605:GLU:HB2	2.02	0.41
1:B:730:LEU:HD11	1:B:738:LEU:HD13	2.02	0.41
1:D:451:ARG:CZ	3:D:2001:COA:O8A	2.59	0.41
1:D:751:ALA:HA	1:D:754:MET:HE2	2.03	0.41
1:D:888:LYS:O	1:D:892:LYS:N	2.53	0.41
1:B:577:LEU:HD23	1:B:806:SER:HB2	2.02	0.41
1:C:566:MET:HB2	1:C:602:PHE:HB3	2.02	0.41
1:C:631:ARG:HH12	1:C:635:PRO:HB3	1.85	0.41
1:D:269:ARG:HH22	1:D:270:ARG:NE	2.18	0.41
1:D:453:ARG:HH22	1:D:495:ASN:HA	1.86	0.41
1:D:615:ALA:HB3	1:D:623:PRO:HG3	2.02	0.41
1:A:553:PHE:O	1:A:557:VAL:HG23	2.21	0.41
1:A:801:MET:HE1	1:A:838:TRP:CD2	2.56	0.41
1:A:828:MET:HG2	1:A:832:PHE:CZ	2.56	0.41
1:A:1037:LEU:HA	1:A:1041:GLY:HA2	2.02	0.41
1:A:1075:GLN:HB2	1:A:1088:LEU:HD13	2.02	0.41
1:B:541:PHE:HB3	1:B:553:PHE:CE1	2.56	0.41
1:B:542:ARG:NH1	1:B:672:ASP:OD2	2.53	0.41
1:B:594:VAL:HG23	1:B:598:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:LYS:CE	1:B:743:MET:HE2	2.44	0.41
1:B:866:ILE:HG21	1:B:871:TYR:HD1	1.86	0.41
1:C:550:PRO:HB2	1:C:736:HIS:CD2	2.56	0.41
1:C:710:VAL:CB	1:C:720:LEU:HG	2.51	0.41
1:C:729:GLU:HG2	1:C:730:LEU:N	2.36	0.41
1:C:770:ILE:HD12	1:C:791:ALA:HB2	2.02	0.41
1:D:313:LEU:O	1:D:321:TYR:N	2.49	0.41
1:D:465:VAL:HG22	1:D:487:LEU:HD21	2.02	0.41
3:D:2001:COA:H2B	3:D:2001:COA:H8A	1.59	0.41
1:C:583:ARG:HH12	1:C:1031:ASP:HA	1.86	0.41
1:C:659:VAL:HB	1:C:688:LEU:HD21	2.02	0.41
1:C:723:TYR:HA	1:C:726:LEU:HB2	2.03	0.41
1:C:889:GLU:HA	1:C:892:LYS:HD3	2.02	0.41
1:C:987:LEU:HB2	1:C:1007:VAL:HG11	2.02	0.41
1:A:558:ARG:HA	1:A:558:ARG:HD2	1.84	0.40
1:B:624:TRP:CZ2	1:B:1008:LEU:HD11	2.56	0.40
1:C:608:GLY:HA2	1:C:642:LEU:HB3	2.04	0.40
1:C:629:GLU:O	1:C:633:LEU:HG	2.21	0.40
1:D:365:GLU:H	1:D:365:GLU:CD	2.28	0.40
1:D:496:ARG:HD2	1:D:1052:LEU:HD21	2.02	0.40
1:D:647:ASN:HD22	1:D:651:TYR:C	2.29	0.40
1:D:901:LEU:HD11	1:D:947:PHE:HE2	1.85	0.40
1:A:701:GLU:HG2	1:A:737:ILE:HB	2.03	0.40
1:A:770:ILE:HG23	1:A:783:MET:HE1	2.03	0.40
1:C:620:TYR:C	1:C:1020:PHE:HE1	2.28	0.40
1:C:746:LEU:CD2	1:C:862:TYR:HA	2.51	0.40
1:C:896:GLU:O	1:C:900:MET:HG2	2.22	0.40
1:C:900:MET:HG3	1:C:932:GLU:OE2	2.21	0.40
1:C:903:ASP:N	1:C:903:ASP:OD1	2.53	0.40
1:D:35:LYS:CD	1:D:137:ARG:NH2	2.75	0.40
1:D:581:ARG:HB2	1:D:848:PHE:CE1	2.57	0.40
1:D:624:TRP:CD1	1:D:624:TRP:H	2.39	0.40
1:D:893:ALA:HA	1:D:896:GLU:OE2	2.21	0.40
1:D:909:PRO:O	1:D:912:LYS:HG2	2.22	0.40
1:A:661:LYS:HA	1:A:664:GLU:HG2	2.03	0.40
1:B:948:LEU:HD23	1:B:948:LEU:HA	1.96	0.40
1:C:120:PHE:HD1	1:C:120:PHE:HA	1.81	0.40
1:B:502:HIS:CE1	1:B:1087:ILE:HG21	2.56	0.40
1:B:770:ILE:HG23	1:B:783:MET:HE1	2.04	0.40
1:C:267:ILE:HG22	1:C:274:VAL:HB	2.03	0.40
1:C:543:ASP:N	1:C:543:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:ARG:NH2	1:C:790:GLY:O	2.37	0.40
1:C:1039:LEU:HD12	1:C:1040:GLN:HB2	2.04	0.40
1:C:1072:GLY:O	1:C:1090:LYS:HD2	2.21	0.40
1:D:845:TYR:O	1:D:849:ASP:HB2	2.21	0.40
1:A:683:LEU:O	1:A:687:LEU:HD23	2.21	0.40
1:A:827:PRO:HB2	1:A:830:ARG:HG3	2.04	0.40
1:B:644:ARG:HD3	1:B:647:ASN:CG	2.47	0.40
1:B:739:CYS:HA	1:B:769:HIS:O	2.20	0.40
1:C:739:CYS:SG	1:C:740:ILE:N	2.95	0.40
1:C:801:MET:HE1	1:C:838:TRP:CD2	2.56	0.40
1:D:500:LEU:O	1:D:504:LEU:HD23	2.22	0.40
1:D:900:MET:HE1	1:D:921:MET:SD	2.61	0.40
1:D:919:GLN:HA	1:D:922:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/1178 (51%)	555 (93%)	43 (7%)	0	100	100
1	B	478/1178 (41%)	443 (93%)	35 (7%)	0	100	100
1	C	275/1178 (23%)	256 (93%)	19 (7%)	0	100	100
1	D	903/1178 (77%)	835 (92%)	67 (7%)	1 (0%)	48	80
All	All	2254/4712 (48%)	2089 (93%)	164 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	804	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/968 (51%)	493 (100%)	0	100	100
1	B	493/968 (51%)	493 (100%)	0	100	100
1	C	942/968 (97%)	925 (98%)	17 (2%)	51	67
1	D	941/968 (97%)	925 (98%)	16 (2%)	53	68
All	All	2869/3872 (74%)	2836 (99%)	33 (1%)	61	72

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	85	LEU
1	C	86	ILE
1	C	88	ARG
1	C	120	PHE
1	C	121	LEU
1	C	122	SER
1	C	124	ARG
1	C	202	ARG
1	C	204	MET
1	C	236	GLU
1	C	237	LYS
1	C	305	GLU
1	C	306	ASN
1	C	490	LEU
1	C	491	ARG
1	C	495	ASN
1	C	496	ARG
1	D	86	ILE
1	D	152	LYS
1	D	164	VAL
1	D	202	ARG
1	D	204	MET
1	D	306	ASN
1	D	309	THR

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Mol	Chain	Res	Type
1	D	330	GLN
1	D	445	ARG
1	D	449	GLU
1	D	452	VAL
1	D	453	ARG
1	D	456	LYS
1	D	490	LEU
1	D	491	ARG
1	D	494	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	899	GLN
1	A	923	GLN
1	A	956	HIS
1	A	1075	GLN
1	B	597	ASN
1	B	771	HIS
1	B	899	GLN
1	B	924	ASN
1	B	956	HIS
1	C	208	HIS
1	C	348	GLN
1	C	484	ASN
1	C	510	ASN
1	C	773	HIS
1	C	879	HIS
1	C	988	GLN
1	C	1040	GLN
1	D	244	HIS
1	D	248	GLN
1	D	259	HIS
1	D	268	GLN
1	D	364	GLN
1	D	470	GLN
1	D	489	GLN
1	D	498	GLN
1	D	506	HIS
1	D	510	ASN
1	D	736	HIS

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Mol	Chain	Res	Type
1	D	870	GLN
1	D	1081	ASN
1	D	1111	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	ATP	D	2002	-	32,33,33	0.28	0	48,52,52	0.28	0
2	ATP	C	2000	-	32,33,33	0.55	0	48,52,52	0.54	0
3	COA	D	2001	-	47,50,50	3.18	18 (38%)	69,75,75	2.61	15 (21%)
3	COA	C	2001	-	47,50,50	3.20	18 (38%)	69,75,75	2.67	16 (23%)

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
2	ATP	D	2002	-	-	6/22/38/38	0/3/3/3
2	ATP	C	2000	-	-	8/22/38/38	0/3/3/3
3	COA	D	2001	-	-	17/48/64/64	0/3/3/3
3	COA	C	2001	-	-	17/48/64/64	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2001	COA	O4B-C1B	7.77	1.60	1.42
3	C	2001	COA	O4B-C1B	7.63	1.59	1.42
3	D	2001	COA	C9P-N8P	6.98	1.50	1.33
3	C	2001	COA	C9P-N8P	6.94	1.49	1.33
3	C	2001	COA	P2A-O3A	6.58	1.66	1.59
3	D	2001	COA	C5P-N4P	6.45	1.48	1.33
3	C	2001	COA	C3B-C4B	-6.43	1.36	1.52
3	C	2001	COA	C2B-C1B	-6.43	1.33	1.53
3	D	2001	COA	C3B-C4B	-6.43	1.36	1.52
3	C	2001	COA	C5P-N4P	6.42	1.48	1.33
3	D	2001	COA	C2B-C1B	-6.41	1.33	1.53
3	D	2001	COA	P2A-O3A	6.40	1.66	1.59
3	D	2001	COA	C6A-N6A	5.33	1.47	1.34
3	C	2001	COA	C6A-N6A	5.09	1.47	1.34
3	C	2001	COA	C2B-C3B	5.05	1.64	1.53
3	D	2001	COA	C2B-C3B	4.85	1.63	1.53
3	C	2001	COA	P1A-O3A	4.45	1.64	1.59
3	C	2001	COA	O4B-C4B	4.39	1.54	1.45
3	D	2001	COA	O4B-C4B	4.31	1.54	1.45
3	D	2001	COA	OAP-CAP	-4.29	1.34	1.42
3	D	2001	COA	P1A-O3A	4.26	1.64	1.59
3	C	2001	COA	OAP-CAP	-4.18	1.34	1.42
3	C	2001	COA	P3B-O3B	3.95	1.66	1.59
3	D	2001	COA	P3B-O3B	3.94	1.66	1.59
3	C	2001	COA	CCP-CBP	3.56	1.58	1.52
3	D	2001	COA	CCP-CBP	3.41	1.58	1.52
3	C	2001	COA	C2A-N3A	3.12	1.39	1.33
3	C	2001	COA	C5A-C4A	-3.10	1.33	1.39
3	C	2001	COA	O9P-C9P	-3.09	1.17	1.23
3	D	2001	COA	O9P-C9P	-2.91	1.17	1.23
3	D	2001	COA	C5A-C4A	-2.85	1.34	1.39
3	D	2001	COA	C2A-N3A	2.64	1.38	1.33
3	D	2001	COA	P1A-O5B	2.29	1.68	1.59
3	D	2001	COA	C7P-C6P	2.28	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2001	COA	C7P-C6P	2.20	1.58	1.51
3	C	2001	COA	P1A-O5B	2.20	1.68	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2001	COA	C1B-N9A-C8A	-10.49	103.81	127.09
3	D	2001	COA	C1B-N9A-C8A	-10.11	104.65	127.09
3	C	2001	COA	C4A-N9A-C1B	9.02	147.73	126.63
3	D	2001	COA	C4A-N9A-C1B	8.91	147.48	126.63
3	D	2001	COA	N6A-C6A-N1A	-8.45	99.57	118.38
3	C	2001	COA	N6A-C6A-N1A	-8.22	100.08	118.38
3	D	2001	COA	C5A-C6A-N6A	6.78	140.08	123.29
3	C	2001	COA	C5A-C6A-N6A	6.13	138.47	123.29
3	D	2001	COA	N3A-C2A-N1A	-5.55	120.17	128.58
3	C	2001	COA	C5A-C4A-N3A	-5.27	119.45	126.72
3	C	2001	COA	N3A-C2A-N1A	-5.14	120.80	128.58
3	D	2001	COA	C5A-C4A-N3A	-5.04	119.78	126.72
3	C	2001	COA	N9A-C8A-N7A	-4.46	107.60	113.94
3	D	2001	COA	N9A-C8A-N7A	-4.22	107.95	113.94
3	D	2001	COA	C2A-N3A-C4A	3.44	120.23	111.83
3	C	2001	COA	C2A-N3A-C4A	3.41	120.17	111.83
3	C	2001	COA	C3B-C2B-C1B	3.40	107.37	99.89
3	C	2001	COA	N3A-C4A-N9A	3.36	132.88	127.17
3	D	2001	COA	N3A-C4A-N9A	2.97	132.22	127.17
3	D	2001	COA	C5A-N7A-C8A	2.94	108.06	103.45
3	C	2001	COA	C5A-N7A-C8A	2.81	107.87	103.45
3	C	2001	COA	C4A-N9A-C8A	2.59	108.46	105.74
3	C	2001	COA	C7P-N8P-C9P	-2.58	117.91	122.55
3	C	2001	COA	CAP-C9P-N8P	2.31	120.88	116.48
3	C	2001	COA	C7P-C6P-C5P	-2.31	108.54	112.39
3	D	2001	COA	C3B-C2B-C1B	2.29	104.93	99.89
3	C	2001	COA	P3B-O3B-C3B	-2.17	117.64	123.43
3	D	2001	COA	C4A-C5A-N7A	-2.16	108.11	110.58
3	D	2001	COA	C4A-N9A-C8A	2.03	107.87	105.74
3	D	2001	COA	C7P-C6P-C5P	-2.02	109.03	112.39
3	D	2001	COA	C5A-C4A-N9A	2.01	108.00	105.81

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2000	ATP	PB-O3B-PG-O3G
2	C	2000	ATP	C5'-O5'-PA-O1A
2	C	2000	ATP	C5'-O5'-PA-O2A
2	C	2000	ATP	C5'-O5'-PA-O3A
2	D	2002	ATP	C5'-O5'-PA-O1A
2	D	2002	ATP	C5'-O5'-PA-O2A
2	D	2002	ATP	C5'-O5'-PA-O3A
3	C	2001	COA	C2B-C1B-N9A-C4A
3	C	2001	COA	C2B-C1B-N9A-C8A
3	C	2001	COA	CCP-O6A-P2A-O3A
3	C	2001	COA	CCP-O6A-P2A-O5A
3	C	2001	COA	C5P-C6P-C7P-N8P
3	C	2001	COA	S1P-C2P-C3P-N4P
3	D	2001	COA	CCP-O6A-P2A-O3A
3	D	2001	COA	CCP-O6A-P2A-O4A
3	D	2001	COA	CCP-O6A-P2A-O5A
3	D	2001	COA	OAP-CAP-CBP-CCP
3	D	2001	COA	C9P-CAP-CBP-CCP
3	D	2001	COA	OAP-CAP-CBP-CDP
3	D	2001	COA	C9P-CAP-CBP-CDP
3	D	2001	COA	OAP-CAP-CBP-CEP
3	D	2001	COA	C9P-CAP-CBP-CEP
3	D	2001	COA	S1P-C2P-C3P-N4P
3	C	2001	COA	O4B-C4B-C5B-O5B
3	D	2001	COA	C4B-C5B-O5B-P1A
3	C	2001	COA	P2A-O3A-P1A-O5B
3	D	2001	COA	P1A-O3A-P2A-O6A
3	C	2001	COA	C5B-O5B-P1A-O1A
3	C	2001	COA	C5B-O5B-P1A-O3A
3	C	2001	COA	CCP-O6A-P2A-O4A
3	D	2001	COA	C5B-O5B-P1A-O1A
3	D	2001	COA	C5B-O5B-P1A-O2A
3	D	2001	COA	C5B-O5B-P1A-O3A
2	C	2000	ATP	PB-O3B-PG-O1G
2	C	2000	ATP	PB-O3A-PA-O2A
3	C	2001	COA	C3B-O3B-P3B-O9A
2	D	2002	ATP	PA-O3A-PB-O3B
3	C	2001	COA	C4B-C3B-O3B-P3B
3	C	2001	COA	C3B-O3B-P3B-O7A
3	D	2001	COA	C5P-C6P-C7P-N8P
2	D	2002	ATP	PA-O3A-PB-O1B
3	C	2001	COA	CBP-CCP-O6A-P2A
3	C	2001	COA	O5P-C5P-C6P-C7P

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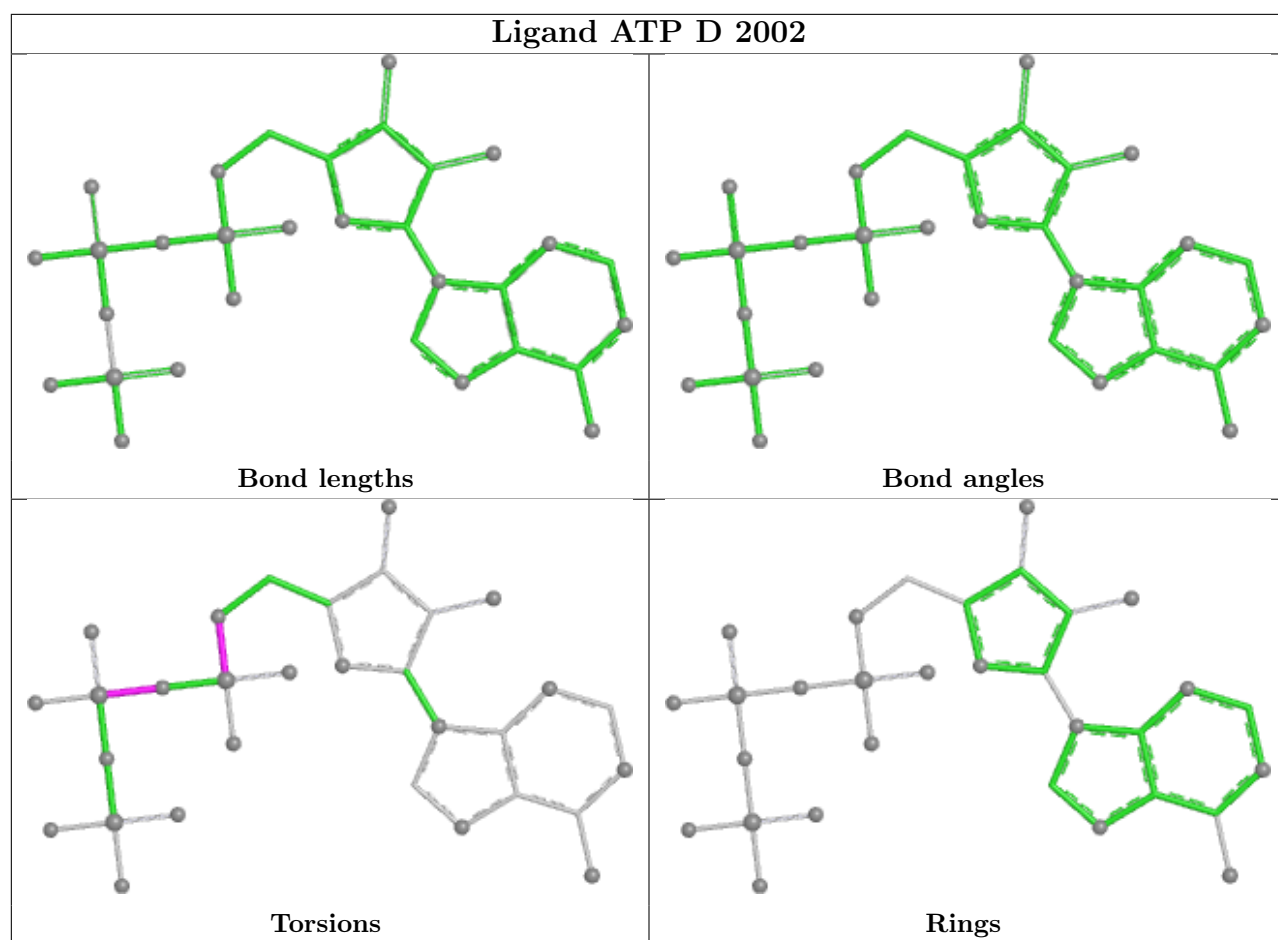
Mol	Chain	Res	Type	Atoms
3	D	2001	COA	N8P-C9P-CAP-OAP
2	C	2000	ATP	PG-O3B-PB-O2B
2	C	2000	ATP	PA-O3A-PB-O2B
2	D	2002	ATP	PA-O3A-PB-O2B
3	C	2001	COA	P2A-O3A-P1A-O2A

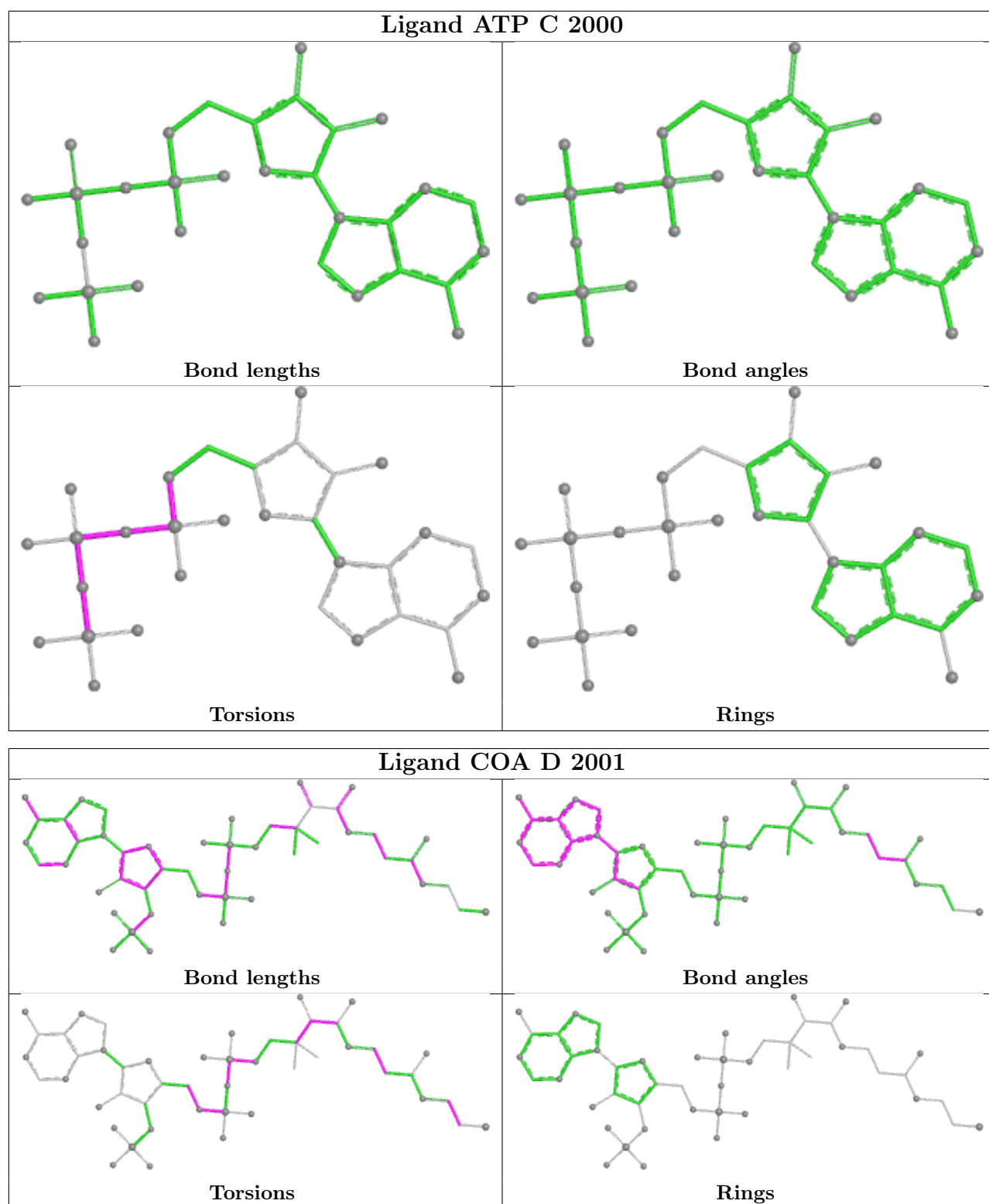
There are no ring outliers.

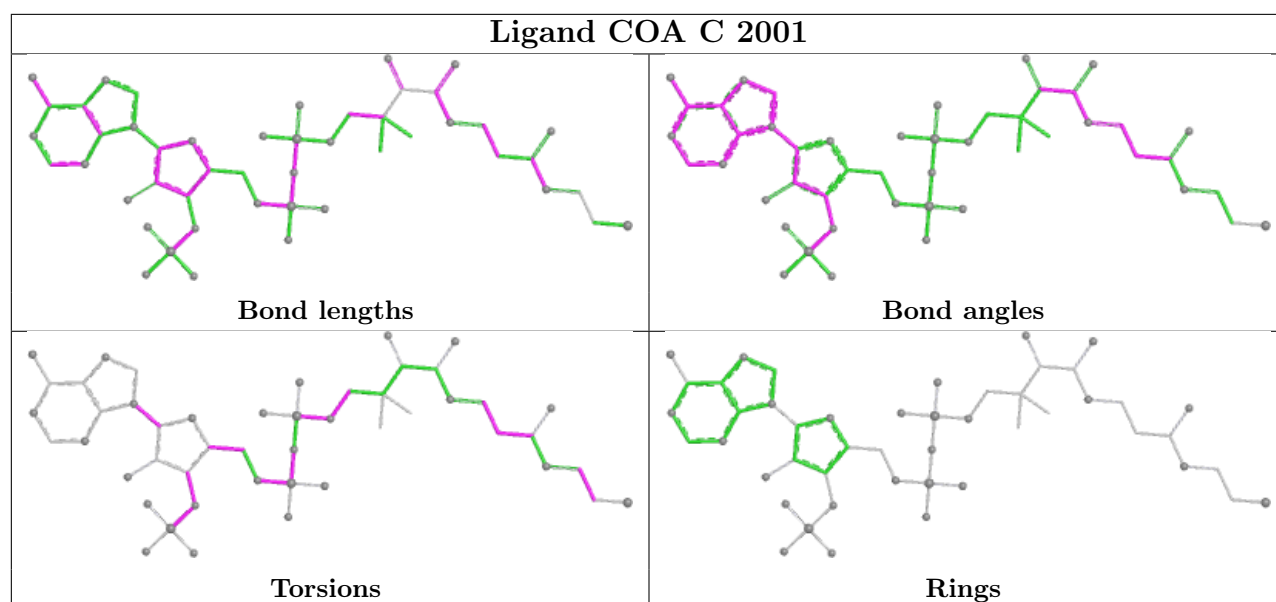
3 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2000	ATP	8	0
3	D	2001	COA	19	0
3	C	2001	COA	17	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

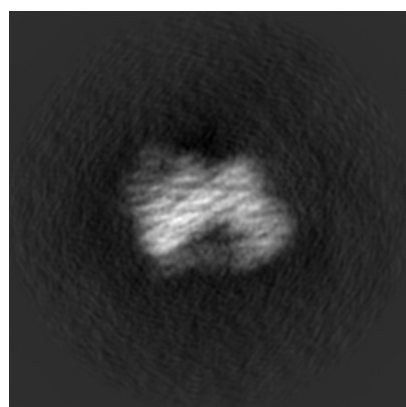
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32779. These allow visual inspection of the internal detail of the map and identification of artifacts.

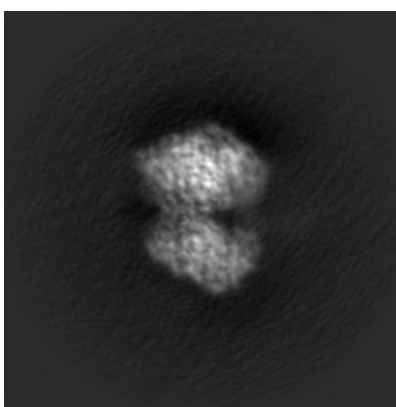
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

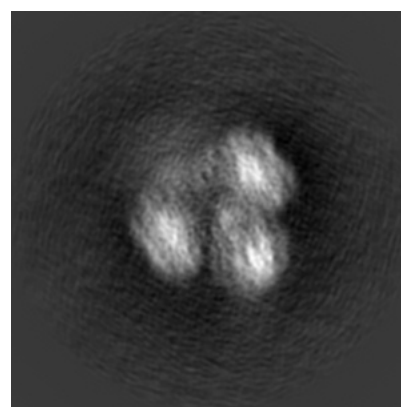
6.1.1 Primary map



X



Y

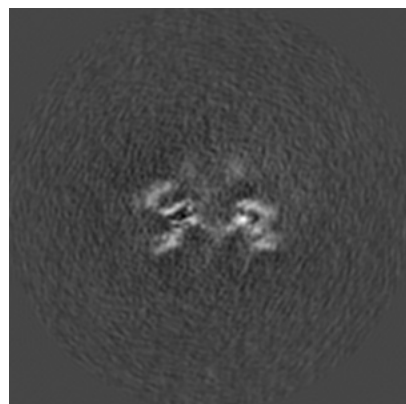


Z

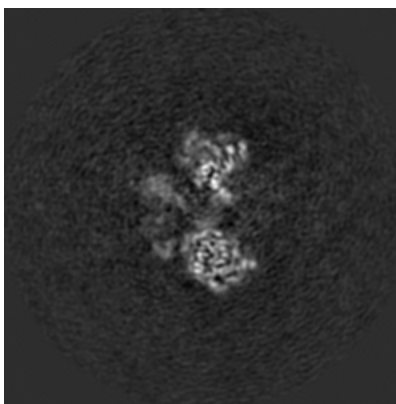
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

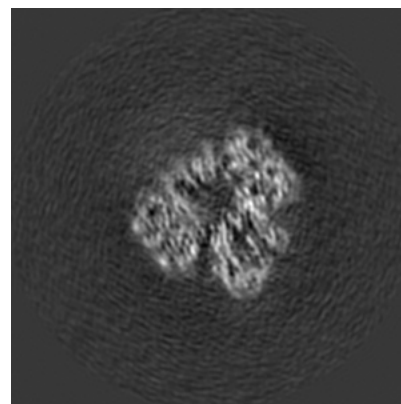
6.2.1 Primary map



X Index: 156



Y Index: 156

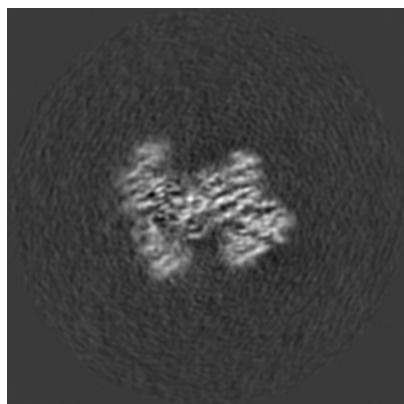


Z Index: 156

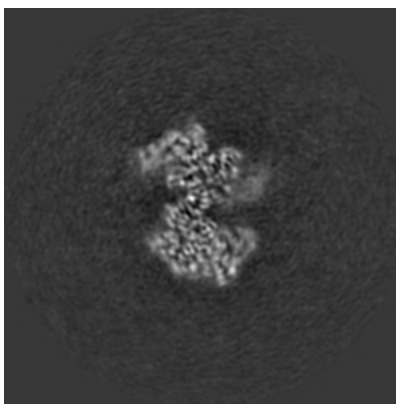
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

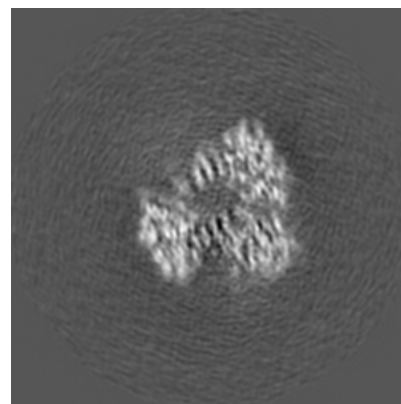
6.3.1 Primary map



X Index: 191



Y Index: 129

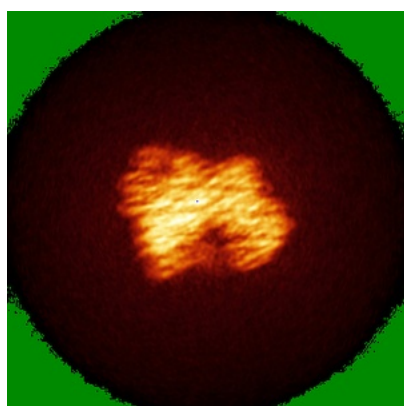


Z Index: 149

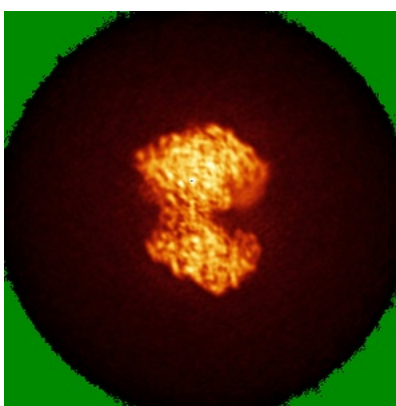
The images above show the largest variance slices of the map in three orthogonal directions.

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

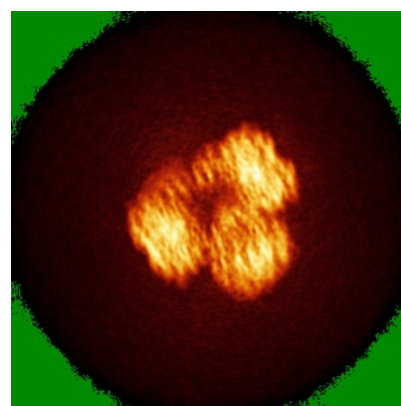
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

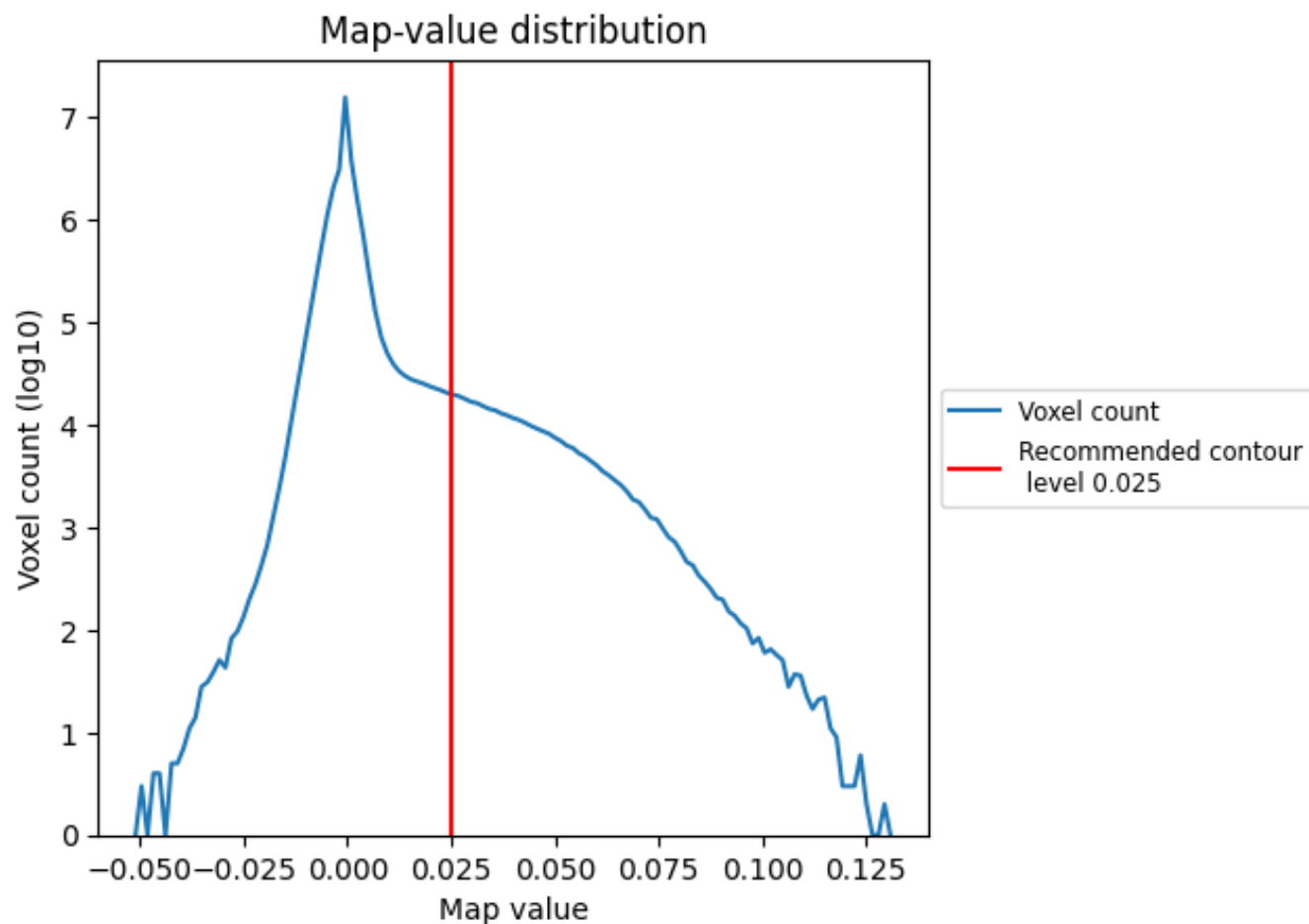
6.6 Mask visualisation

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

7 Map analysis [i](#)

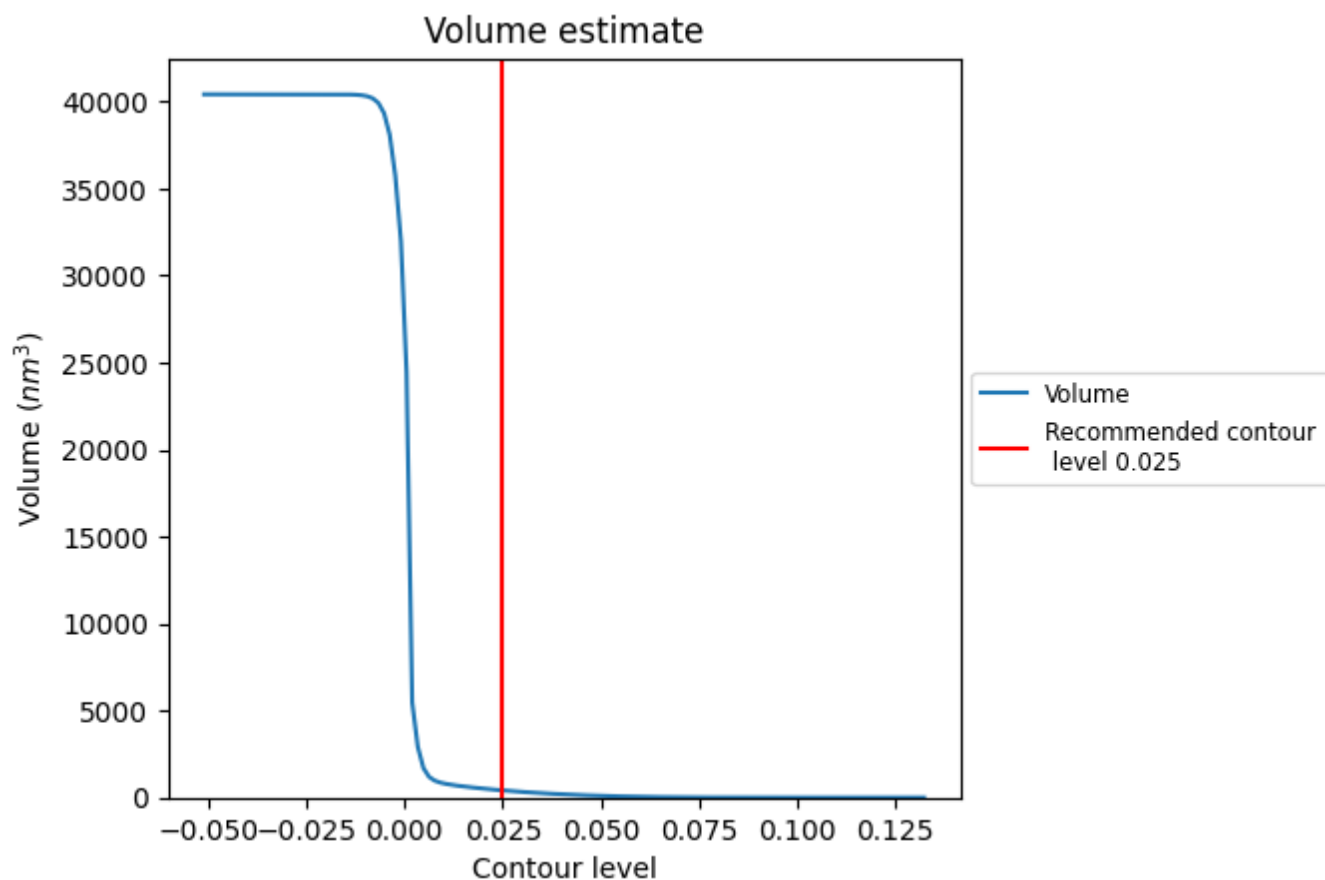
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

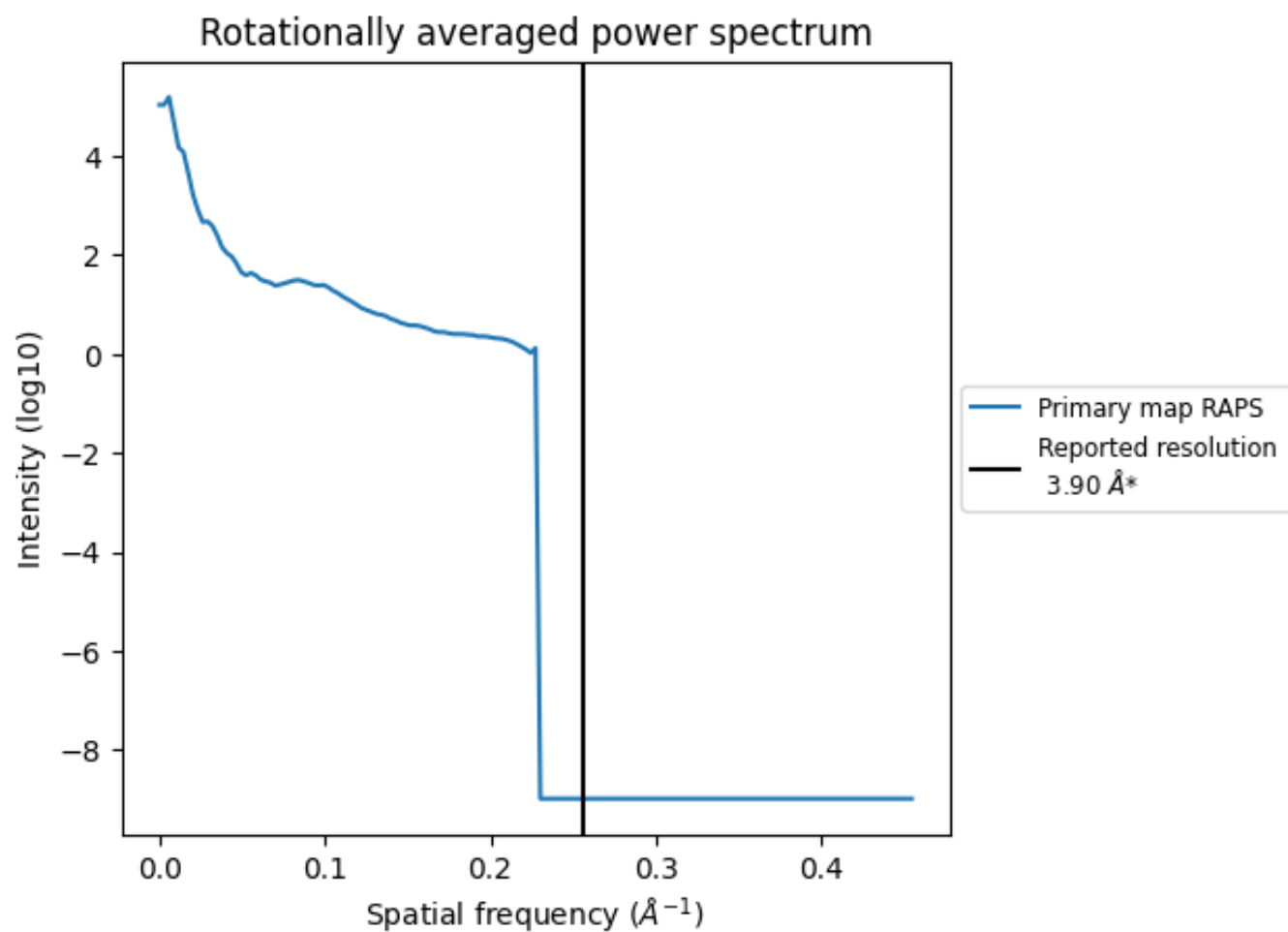
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm^3 ; this corresponds to an approximate mass of 372 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32779 and PDB model 7WTD. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

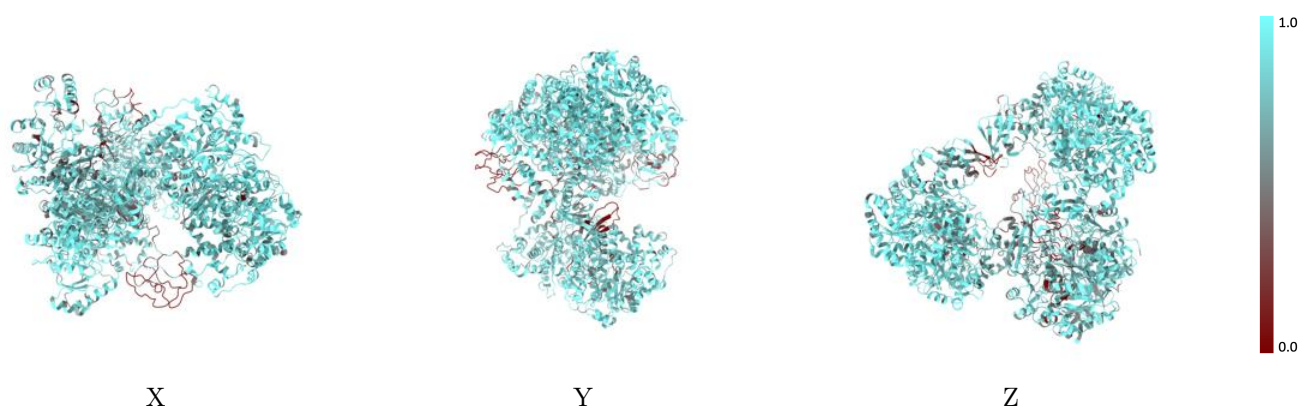
This section was not generated.

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



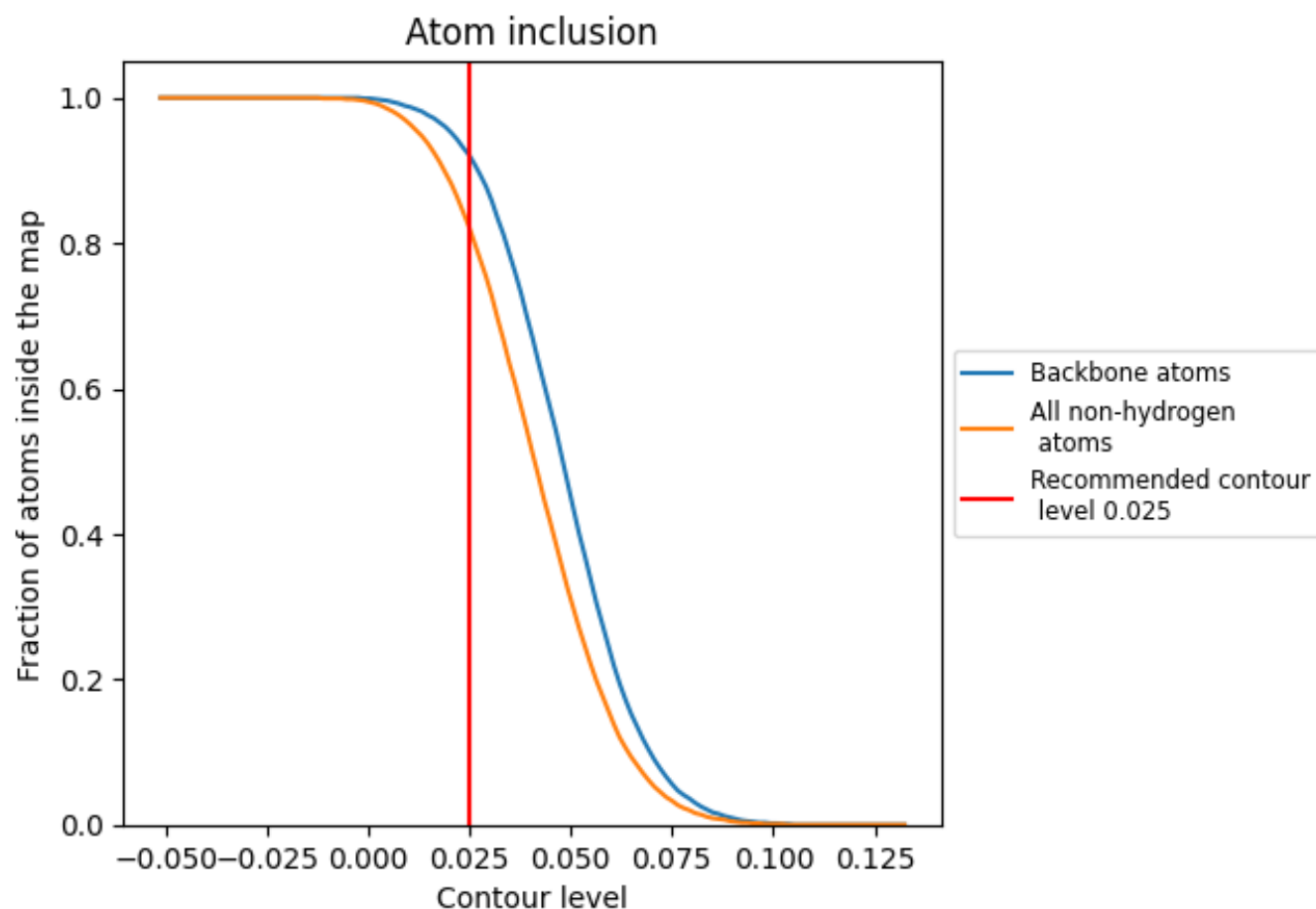
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.2260
A	0.8630	0.2300
B	0.8380	0.2370
C	0.7890	0.2200
D	0.8250	0.2230

