



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:45 AM UTC

PDB ID : 7CRC / pdb_00007crc
EMDB ID : EMD-30450
Title : Cryo-EM structure of plant NLR RPP1 tetramer in complex with ATR1
Authors : Ma, S.C.; Lapin, D.; Liu, L.; Sun, Y.; Song, W.; Zhang, X.X.; Logemann, E.; Yu, D.L.; Wang, J.; Jirschitzka, J.; Han, Z.F.; SchulzeLefert, P.; Parker, J.E.; Chai, J.J.
Deposited on : 2020-08-13
Resolution : 3.02 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:

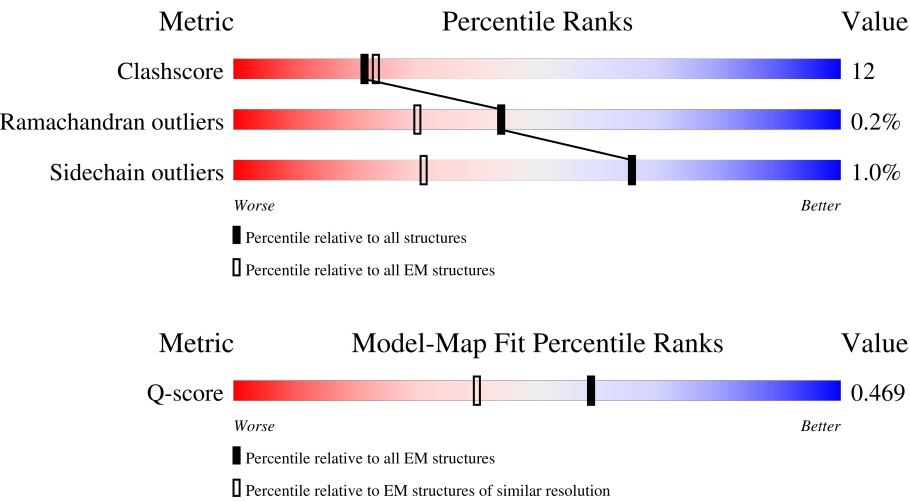
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.02 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.



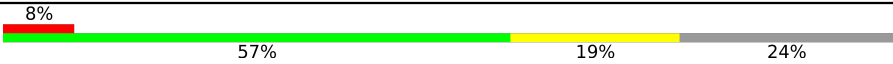
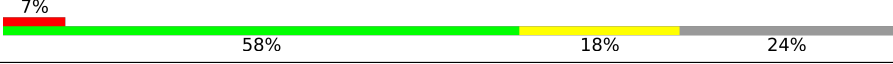
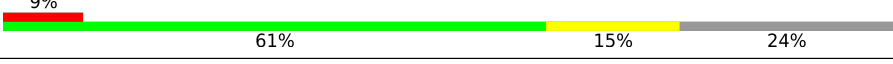
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	1221	11% 64% 26% • 9%
1	B	1221	11% 66% 25% 9%
1	C	1221	11% 61% 29% • 9%
1	D	1221	11% 65% 25% • 9%

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Mol	Chain	Length	Quality of chain
2	E	311	
2	F	311	
2	G	311	
2	H	311	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 43168 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.

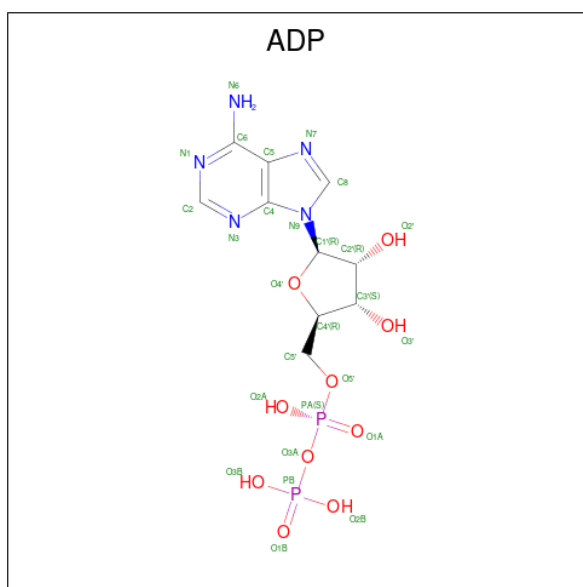
- Molecule 1 is a protein called NAD⁺ hydrolase (NADase).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1108	Total	C	N	O	S	0	0
			8850	5635	1516	1642	57		
1	B	1112	Total	C	N	O	S	0	0
			8886	5661	1523	1645	57		
1	C	1108	Total	C	N	O	S	0	0
			8844	5632	1513	1642	57		
1	D	1112	Total	C	N	O	S	0	0
			8886	5661	1523	1645	57		

- Molecule 2 is a protein called Avirulence protein ATR1.

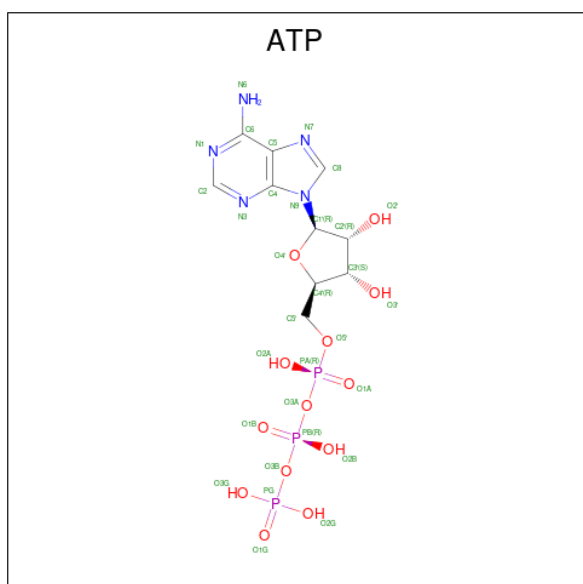
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	237	Total	C	N	O	S	1	0
			1883	1197	323	358	5		
2	H	237	Total	C	N	O	S	1	0
			1883	1197	323	358	5		
2	F	237	Total	C	N	O	S	1	0
			1883	1197	323	358	5		
2	G	237	Total	C	N	O	S	1	0
			1883	1197	323	358	5		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

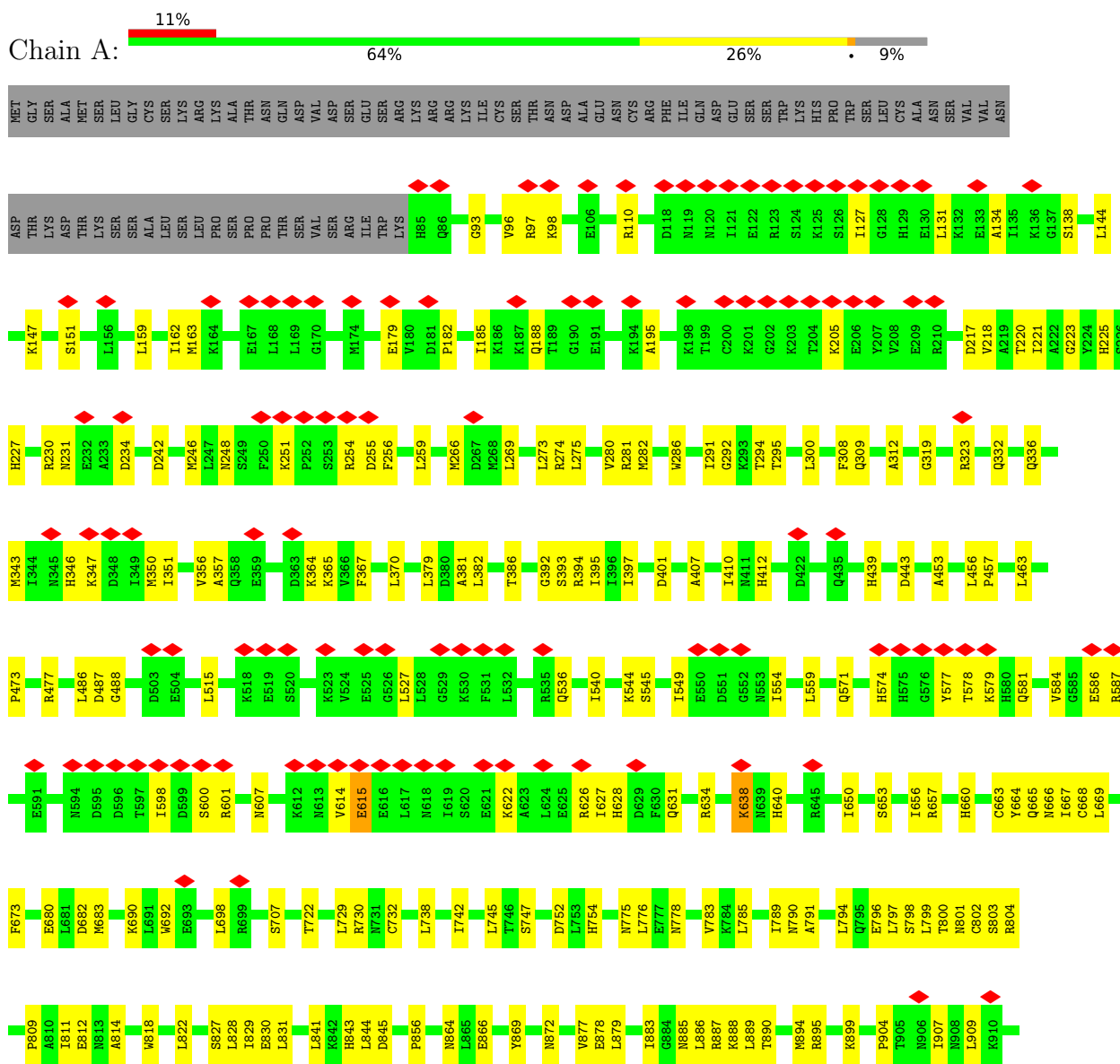


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0

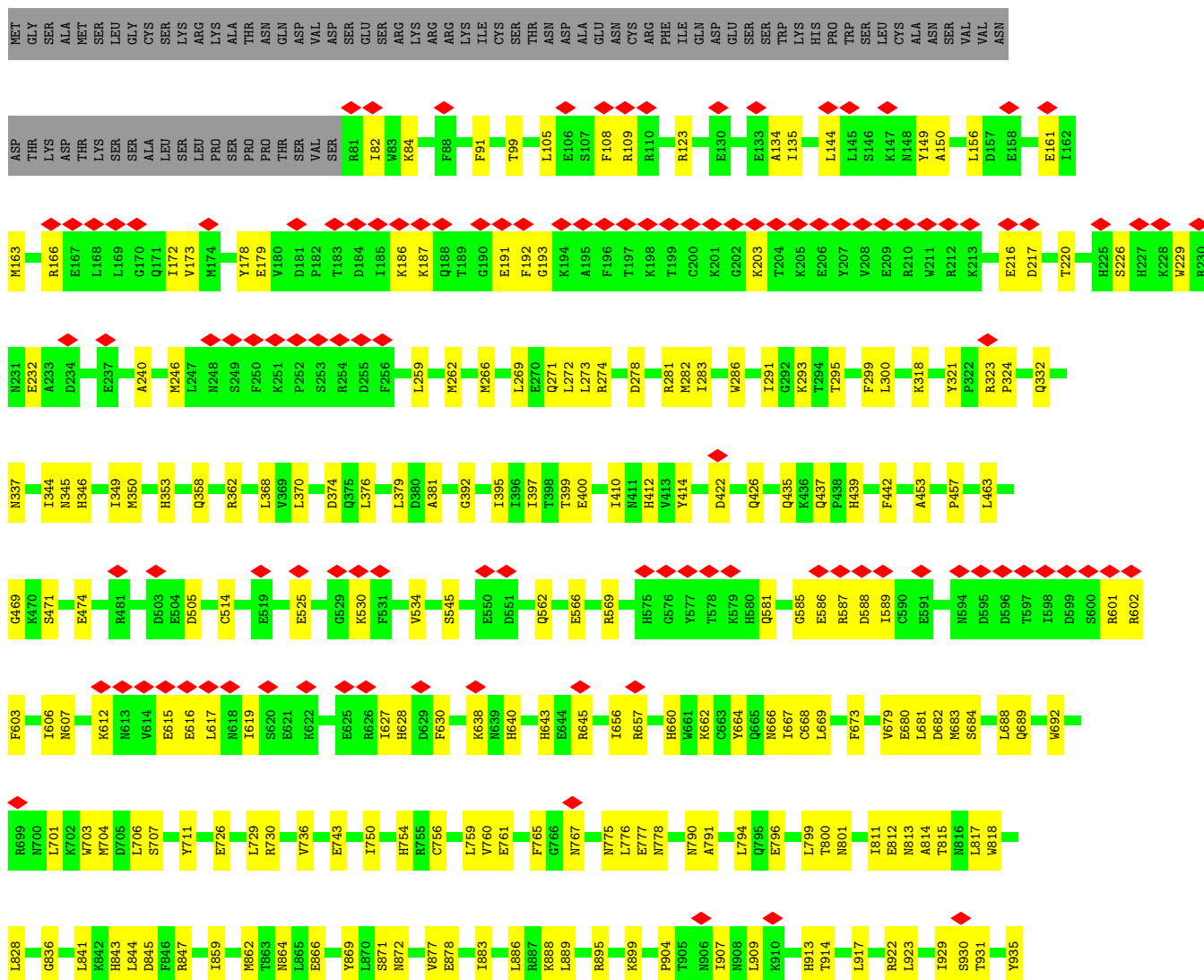
3 Residue-property plots

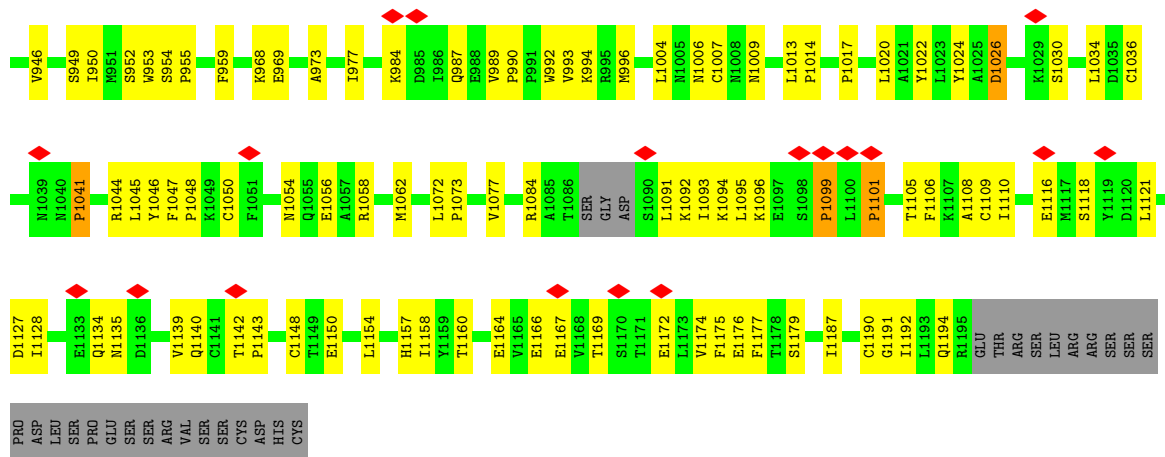
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: NAD⁺ hydrolase (NADase)

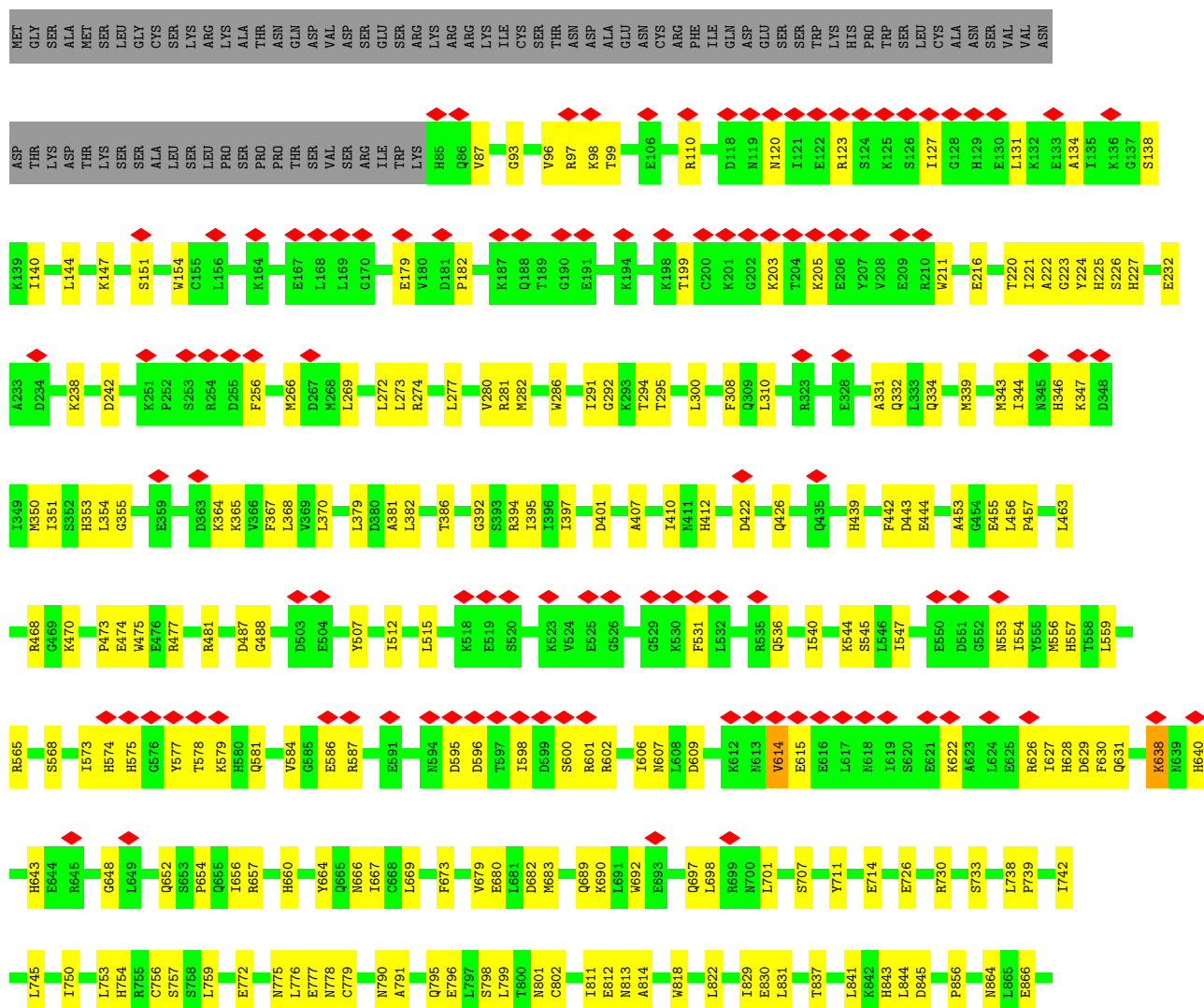


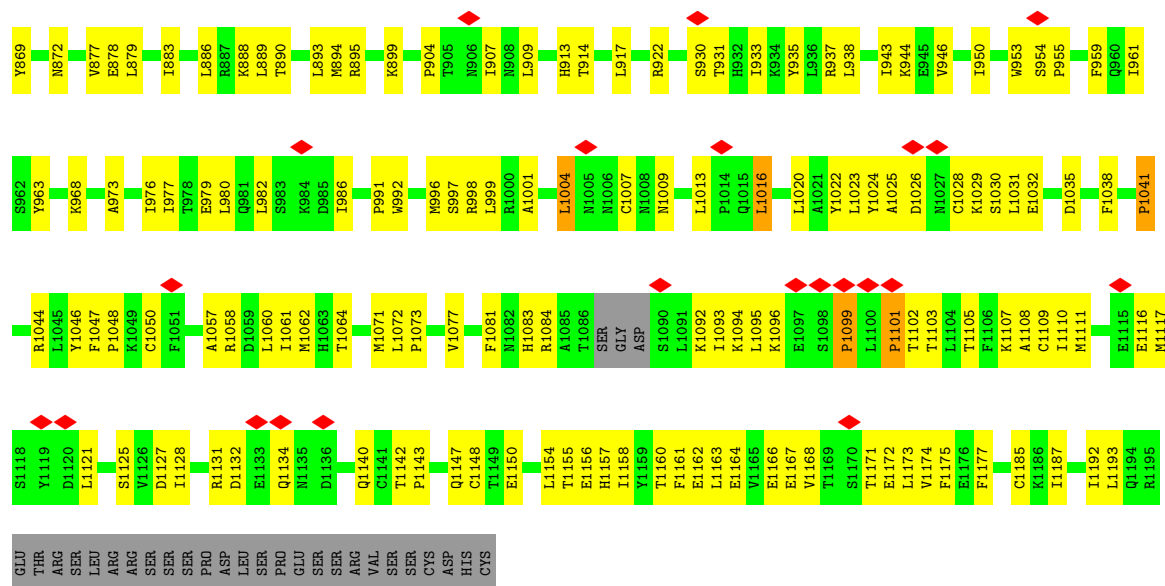
- Molecule 1: NAD⁺ hydrolase (NADase)



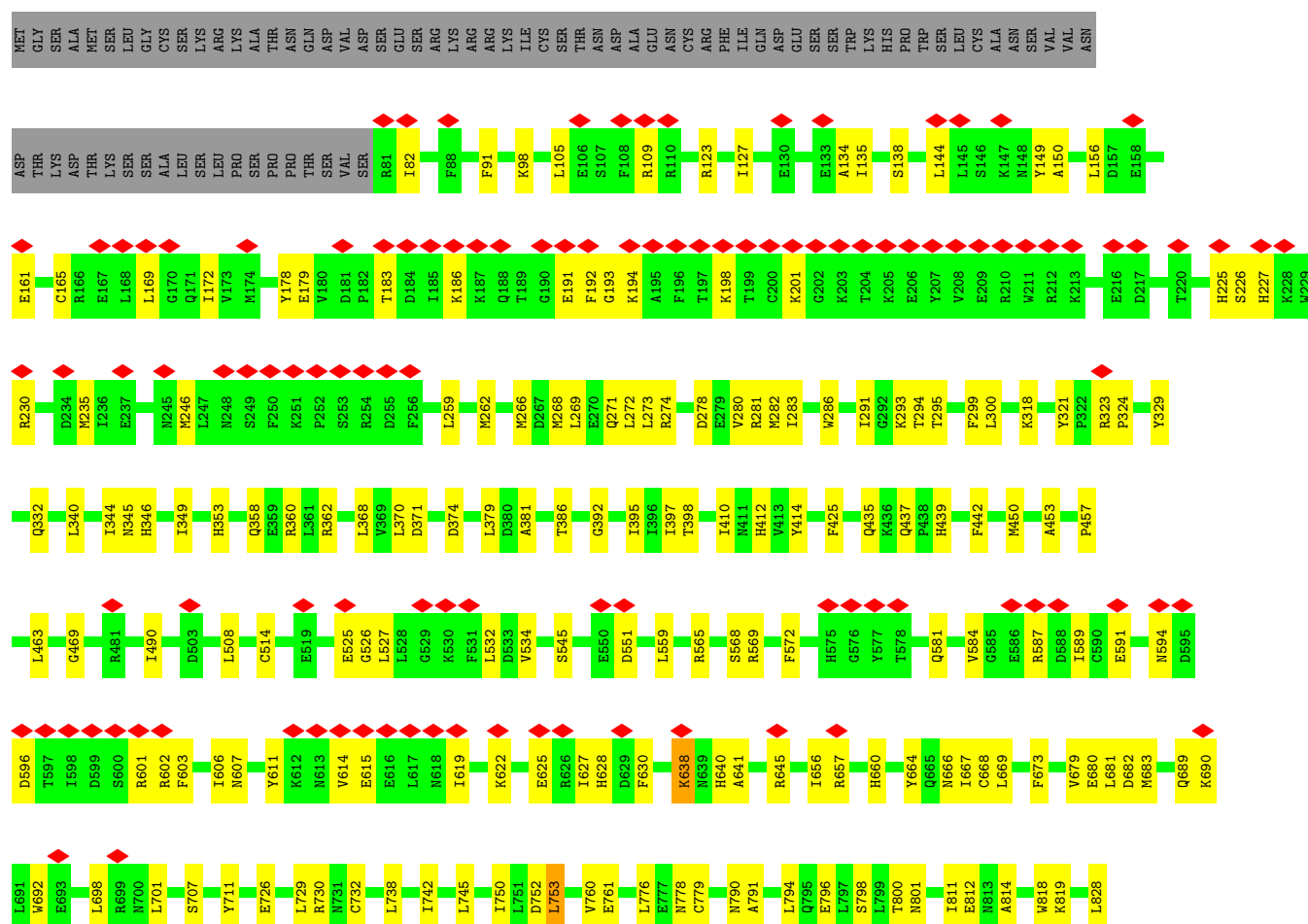


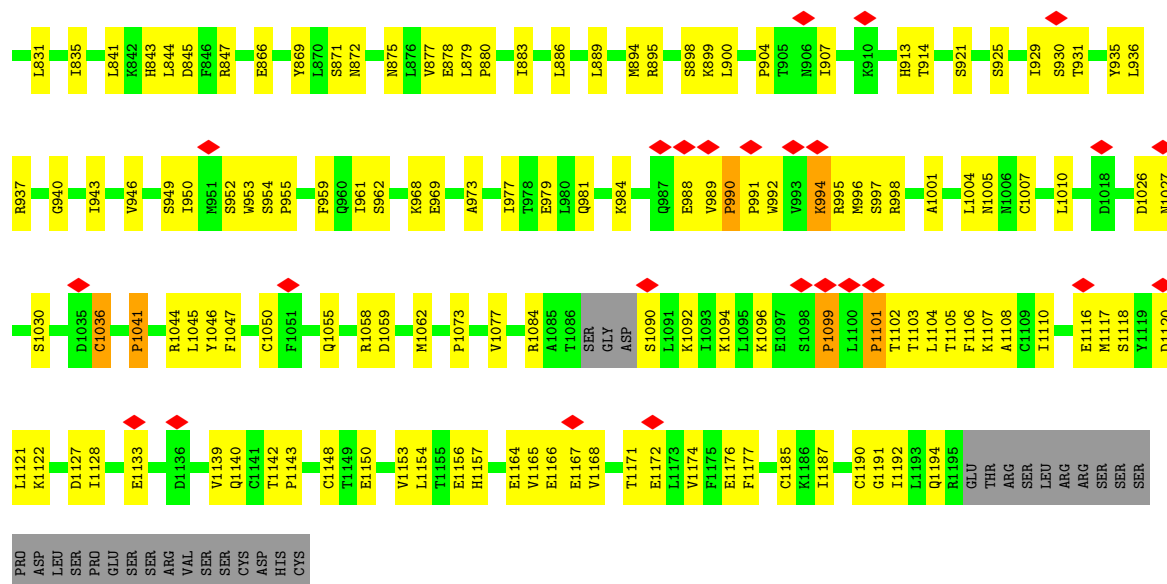
• Molecule 1: NAD⁺ hydrolase (NADase)



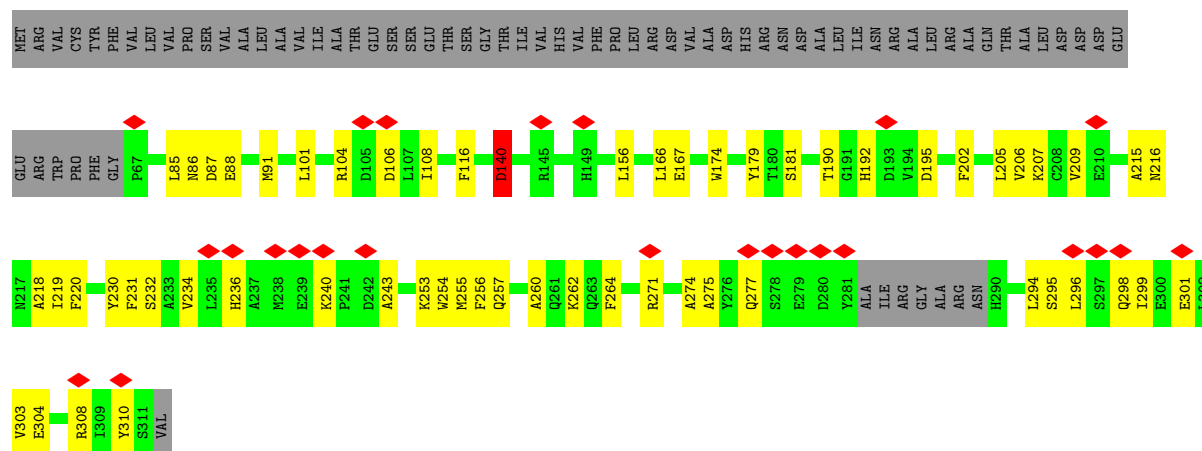


• Molecule 1: NAD⁺ hydrolase (NADase)



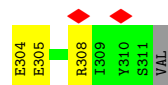


• Molecule 2: Avirulence protein ATR1



• Molecule 2: Avirulence protein ATR1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	323232	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 ($e^-/\text{\AA}^2$)	23.542	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	395.24402, 395.24402, 395.24402	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.33	0/9016	0.54	5/12175 (0.0%)
1	B	0.30	0/9054	0.52	4/12227 (0.0%)
1	C	0.34	0/9010	0.55	5/12168 (0.0%)
1	D	0.30	0/9054	0.51	5/12227 (0.0%)
2	E	0.24	0/1931	0.43	1/2615 (0.0%)
2	F	0.29	0/1931	0.45	0/2615
2	G	0.26	0/1931	0.41	1/2615 (0.0%)
2	H	0.27	0/1931	0.43	0/2615
All	All	0.31	0/43858	0.51	21/59257 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1026	ASP	N-CA-C	8.50	120.16	111.07
1	A	1099	PRO	N-CA-CB	8.21	111.87	103.25
1	B	1099	PRO	N-CA-CB	8.21	111.87	103.25
1	D	1099	PRO	N-CA-CB	7.93	111.58	103.25
1	C	1099	PRO	N-CA-CB	7.85	111.49	103.25
1	D	1101	PRO	N-CA-CB	7.57	111.20	103.25
1	B	1101	PRO	N-CA-CB	7.47	111.10	103.25
1	C	1101	PRO	N-CA-CB	7.25	110.86	103.25
1	A	1101	PRO	N-CA-CB	6.97	110.57	103.25
1	B	1041	PRO	N-CA-CB	6.89	110.48	103.25
1	D	1041	PRO	N-CA-CB	6.87	110.46	103.25
1	C	1041	PRO	N-CA-CB	6.79	110.38	103.25
1	A	1041	PRO	N-CA-CB	6.70	110.28	103.25
1	D	1036	CYS	N-CA-C	6.42	118.94	109.69
2	E	140	ASP	N-CA-C	-6.38	104.42	111.82
1	D	753	LEU	N-CA-C	-6.25	100.98	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	LYS	N-CA-C	-6.14	105.10	112.59
2	G	140	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	1116	GLU	N-CA-C	-5.04	107.63	112.97
1	C	638	LYS	CA-C-N	-5.00	114.11	123.01
1	C	638	LYS	C-N-CA	-5.00	114.11	123.01

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	8850	0	8964	228	0
1	B	8886	0	9002	210	0
1	C	8844	0	8953	256	0
1	D	8886	0	9002	209	0
2	E	1883	0	1816	42	0
2	F	1883	0	1816	32	0
2	G	1883	0	1816	39	0
2	H	1883	0	1816	33	0
3	A	27	0	12	3	0
3	B	27	0	12	2	0
3	C	27	0	12	3	0
3	D	27	0	12	2	0
4	B	31	0	12	1	0
4	D	31	0	12	1	0
All	All	43168	0	43257	1007	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 12.

All (1007) 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:350:MET:HE3	1:A:351:ILE:H	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:MET:HE3	1:C:351:ILE:H	1.39	0.86
1:D:226:SER:HA	1:D:235:MET:HE1	1.58	0.84
1:C:310:LEU:HG	1:C:343:MET:HE2	1.59	0.82
1:A:473:PRO:HB2	1:A:477:ARG:HH12	1.44	0.82
1:A:1128:ILE:HD13	1:A:1163:LEU:HD21	1.62	0.81
1:A:159:LEU:HD11	1:A:218:VAL:HG21	1.62	0.80
1:A:1071:MET:HG2	1:A:1151:ILE:HD11	1.67	0.77
1:B:836:GLY:HA2	1:B:862:MET:HE2	1.66	0.76
1:B:899:LYS:HG2	1:B:922:ARG:HH21	1.52	0.75
1:A:909:LEU:H	1:A:931:THR:HG22	1.52	0.74
1:D:172:ILE:HD13	1:D:246:MET:HE1	1.70	0.74
1:C:996:MET:HG3	1:C:999:LEU:HD21	1.68	0.73
1:C:1058:ARG:HG2	1:C:1062:MET:HE1	1.70	0.73
1:D:707:SER:HB2	1:D:730:ARG:HB3	1.70	0.73
1:D:525:GLU:HA	1:D:534:VAL:HG21	1.69	0.73
1:C:577:TYR:OH	1:D:569:ARG:NH1	2.22	0.72
1:D:914:THR:HG22	1:D:935:TYR:HB2	1.71	0.72
1:A:364:LYS:HA	1:B:82:ILE:HG23	1.69	0.72
1:D:601:ARG:HH21	1:D:628:HIS:HA	1.53	0.72
1:C:473:PRO:HB2	1:C:477:ARG:HH21	1.54	0.72
2:G:271:ARG:HH21	2:G:275:ALA:HA	1.55	0.71
1:A:1154:LEU:HB2	1:A:1157:HIS:HD2	1.56	0.71
1:A:273:LEU:O	1:A:394:ARG:NH1	2.23	0.71
1:B:581:GLN:OE1	1:B:602:ARG:NH1	2.22	0.71
1:B:368:LEU:HB3	1:B:395:ILE:HG22	1.72	0.71
1:B:525:GLU:HA	1:B:534:VAL:HG21	1.73	0.70
2:G:301:GLU:O	2:G:305:GLU:N	2.24	0.70
1:D:883:ILE:HG23	1:D:886:LEU:HD12	1.73	0.70
2:F:125:THR:HG23	2:F:128:GLU:H	1.57	0.70
2:F:295:SER:H	2:F:298:GLN:NE2	1.90	0.70
1:C:368:LEU:HB3	1:C:395:ILE:HG22	1.72	0.70
1:C:1077:VAL:O	1:C:1084:ARG:NH2	2.25	0.70
1:B:638:LYS:HG3	2:F:241:PRO:HA	1.73	0.70
2:H:125:THR:HG23	2:H:128:GLU:H	1.56	0.69
1:C:977:ILE:HG21	1:C:996:MET:HE2	1.74	0.69
1:A:778:ASN:OD1	1:A:801:ASN:ND2	2.24	0.69
1:B:1077:VAL:O	1:B:1084:ARG:NH2	2.25	0.69
1:A:890:THR:O	1:A:913:HIS:N	2.26	0.69
1:A:1077:VAL:O	1:A:1084:ARG:NH2	2.26	0.69
1:D:581:GLN:OE1	1:D:602:ARG:NH2	2.26	0.69
1:A:110:ARG:O	1:D:345:ASN:ND2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:TRP:O	1:C:98:LYS:NZ	2.26	0.68
1:B:345:ASN:ND2	1:C:110:ARG:O	2.26	0.68
1:B:640:HIS:ND1	1:B:640:HIS:O	2.24	0.68
1:B:959:PHE:HD2	1:B:977:ILE:HA	1.59	0.68
1:B:660:HIS:NE2	1:B:680:GLU:OE2	2.27	0.68
1:A:904:PRO:HB2	1:A:907:ILE:HD13	1.76	0.67
1:A:401:ASP:HB3	1:A:544:LYS:HD3	1.75	0.67
1:C:1154:LEU:HB2	1:C:1157:HIS:HD2	1.59	0.67
1:A:255:ASP:HB2	1:D:353:HIS:HB2	1.76	0.67
1:A:577:TYR:OH	1:B:569:ARG:NH1	2.27	0.67
1:D:619:ILE:HD11	1:D:645:ARG:HB3	1.75	0.67
1:A:453:ALA:HB2	1:A:463:LEU:HD12	1.77	0.67
1:C:280:VAL:HB	1:C:386:THR:HG23	1.75	0.67
1:B:150:ALA:HA	1:B:156:LEU:HD21	1.77	0.67
1:A:221:ILE:O	4:B:1302:ATP:N6	2.27	0.66
1:A:1119:TYR:HA	1:A:1154:LEU:HD21	1.76	0.66
2:F:240:LYS:HB2	2:F:243:ALA:HB2	1.78	0.66
1:B:1154:LEU:HB2	1:B:1157:HIS:HD2	1.60	0.66
1:D:1077:VAL:O	1:D:1084:ARG:NH2	2.29	0.66
1:B:869:TYR:HH	2:F:125:THR:HG1	1.42	0.66
1:D:370:LEU:HB2	1:D:397:ILE:HG22	1.78	0.66
1:A:883:ILE:HG23	1:A:886:LEU:HD12	1.77	0.65
1:B:847:ARG:HG3	1:B:871:SER:HB2	1.78	0.65
1:B:914:THR:HG22	1:B:935:TYR:HB2	1.77	0.65
1:D:1150:GLU:N	1:D:1150:GLU:OE1	2.29	0.65
1:A:571:GLN:O	1:A:581:GLN:NE2	2.29	0.65
1:D:954:SER:HB2	1:D:955:PRO:HD3	1.79	0.65
1:C:401:ASP:HB3	1:C:544:LYS:HD3	1.77	0.65
1:C:914:THR:HG22	1:C:935:TYR:HB2	1.79	0.64
1:A:1085:ALA:HB3	1:A:1093:ILE:HD13	1.77	0.64
1:A:1150:GLU:N	1:A:1150:GLU:OE1	2.31	0.64
1:D:614:VAL:HA	1:D:641:ALA:HB2	1.78	0.64
1:B:946:VAL:HG11	1:B:973:ALA:HB2	1.79	0.64
2:E:209:VAL:HG11	2:E:215:ALA:HB2	1.79	0.64
1:D:660:HIS:NE2	1:D:680:GLU:OE2	2.30	0.64
1:D:1044:ARG:NH1	1:D:1148:CYS:SG	2.71	0.64
1:C:1150:GLU:OE1	1:C:1150:GLU:N	2.30	0.64
1:D:742:ILE:HA	1:D:745:LEU:HD13	1.79	0.64
1:C:790:ASN:ND2	1:C:812:GLU:OE2	2.31	0.63
1:D:968:LYS:HD2	1:D:991:PRO:HB2	1.80	0.63
1:C:742:ILE:HA	1:C:745:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1142:THR:OG1	1:D:1143:PRO:HD3	1.98	0.63
1:B:993:VAL:HA	1:B:996:MET:HE3	1.81	0.63
2:G:125:THR:HG23	2:G:128:GLU:H	1.63	0.63
1:D:1154:LEU:HB2	1:D:1157:HIS:HD2	1.63	0.63
1:A:864:ASN:OD1	1:A:888:LYS:NZ	2.26	0.63
1:A:985:ASP:OD1	1:A:1009:ASN:ND2	2.25	0.63
1:C:332:GLN:HG3	1:C:381:ALA:HB2	1.80	0.63
1:B:954:SER:HB2	1:B:955:PRO:HD3	1.81	0.63
1:A:954:SER:HB2	1:A:955:PRO:HD3	1.81	0.63
1:D:1047:PHE:HB3	1:D:1050:CYS:SG	2.37	0.63
1:A:248:ASN:HB3	1:D:360:ARG:HH21	1.64	0.63
1:A:601:ARG:HD2	1:A:601:ARG:O	1.98	0.62
1:B:282:MET:HE2	1:B:395:ILE:HD11	1.80	0.62
1:C:864:ASN:OD1	1:C:888:LYS:NZ	2.26	0.62
2:G:271:ARG:O	2:G:275:ALA:N	2.29	0.62
1:C:595:ASP:O	1:C:622:LYS:NZ	2.33	0.62
1:A:332:GLN:HG3	1:A:381:ALA:HB2	1.80	0.62
1:A:742:ILE:HA	1:A:745:LEU:HD13	1.81	0.62
1:B:321:TYR:O	1:B:323:ARG:NH1	2.33	0.62
1:D:572:PHE:HE1	1:D:602:ARG:HE	1.46	0.62
1:D:847:ARG:HG3	1:D:871:SER:HB2	1.81	0.62
1:A:231:ASN:ND2	1:A:234:ASP:OD2	2.32	0.62
1:A:266:MET:HE3	1:A:266:MET:HA	1.81	0.62
1:A:811:ILE:HG21	1:A:814:ALA:HB2	1.82	0.62
1:C:1172:GLU:O	1:C:1173:LEU:HD23	2.00	0.62
2:G:240:LYS:HB2	2:G:243:ALA:HB2	1.82	0.62
1:B:790:ASN:ND2	1:B:812:GLU:OE2	2.33	0.62
1:C:890:THR:O	1:C:913:HIS:N	2.33	0.62
2:H:240:LYS:HB2	2:H:243:ALA:HB2	1.82	0.62
1:A:790:ASN:ND2	1:A:812:GLU:OE2	2.32	0.61
1:C:127:ILE:HB	1:C:131:LEU:HD22	1.80	0.61
1:D:149:TYR:HB3	1:D:192:PHE:HE2	1.63	0.61
1:D:959:PHE:HD2	1:D:977:ILE:HA	1.63	0.61
1:C:811:ILE:HG21	1:C:814:ALA:HB2	1.82	0.61
2:F:296:LEU:HA	2:F:299:ILE:HD12	1.82	0.61
2:E:271:ARG:O	2:E:275:ALA:N	2.33	0.61
1:C:453:ALA:HB2	1:C:463:LEU:HD12	1.82	0.61
1:C:904:PRO:HB2	1:C:907:ILE:HD13	1.82	0.61
1:C:883:ILE:HG23	1:C:886:LEU:HD12	1.83	0.61
1:B:969:GLU:N	1:B:969:GLU:OE1	2.33	0.61
2:E:240:LYS:HB2	2:E:243:ALA:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:883:ILE:HG23	1:B:886:LEU:HD12	1.82	0.61
1:C:347:LYS:HD2	1:C:347:LYS:O	2.01	0.61
1:C:843:HIS:NE2	1:C:845:ASP:OD1	2.34	0.61
2:G:254:TRP:HA	2:G:257:GLN:HE22	1.65	0.61
2:G:295:SER:O	2:G:299:ILE:HG12	2.01	0.61
1:D:150:ALA:HA	1:D:156:LEU:HD21	1.81	0.61
1:C:954:SER:HB2	1:C:955:PRO:HD3	1.81	0.61
1:C:266:MET:HA	1:C:266:MET:HE3	1.82	0.61
1:D:179:GLU:H	1:D:226:SER:HB3	1.66	0.61
1:A:319:GLY:HA2	1:A:323:ARG:HH22	1.65	0.61
1:A:1093:ILE:HB	1:A:1175:PHE:HB2	1.82	0.61
1:C:754:HIS:NE2	1:C:777:GLU:OE1	2.34	0.61
1:C:339:MET:O	1:C:343:MET:HB2	2.01	0.60
1:C:707:SER:HB2	1:C:730:ARG:HB3	1.84	0.60
2:F:236:HIS:O	2:F:240:LYS:NZ	2.28	0.60
1:D:879:LEU:HD12	1:D:880:PRO:HD2	1.82	0.60
1:A:439:HIS:CD2	1:A:443:ASP:HB2	2.37	0.60
2:E:254:TRP:HA	2:E:257:GLN:HE22	1.66	0.60
1:D:790:ASN:ND2	1:D:812:GLU:OE2	2.33	0.60
1:C:1105:THR:HG22	1:C:1164:GLU:HG2	1.83	0.60
1:D:601:ARG:NH2	1:D:628:HIS:HA	2.16	0.60
1:D:601:ARG:NH2	1:D:627:ILE:O	2.34	0.60
1:A:707:SER:HB2	1:A:730:ARG:HB3	1.82	0.60
2:H:86:ASN:OD1	2:H:87:ASP:N	2.34	0.60
1:A:692:TRP:HH2	1:A:698:LEU:HD21	1.66	0.60
1:B:1058:ARG:HG2	1:B:1062:MET:HE3	1.84	0.60
1:C:1131:ARG:O	1:C:1174:VAL:HB	2.01	0.60
2:F:86:ASN:OD1	2:F:87:ASP:N	2.34	0.60
1:A:1047:PHE:HB3	1:A:1050:CYS:SG	2.42	0.60
2:G:236:HIS:O	2:G:240:LYS:NZ	2.31	0.60
1:D:321:TYR:O	1:D:323:ARG:NH1	2.34	0.59
1:D:1190:CYS:SG	1:D:1191:GLY:N	2.75	0.59
1:C:1134:GLN:HB3	1:C:1172:GLU:HG2	1.84	0.59
1:B:681:LEU:HD11	1:B:683:MET:HE3	1.85	0.59
1:D:611:TYR:HB2	1:D:638:LYS:HD3	1.83	0.59
1:A:586:GLU:HG3	1:A:587:ARG:HD3	1.84	0.59
1:B:1047:PHE:HB3	1:B:1050:CYS:SG	2.41	0.59
1:C:1155:THR:OG1	1:C:1156:GLU:OE1	2.17	0.59
1:A:996:MET:HG3	1:A:999:LEU:HD21	1.82	0.59
1:A:1140:GLN:HG3	1:A:1167:GLU:OE2	2.03	0.59
1:B:344:ILE:HG22	1:B:346:HIS:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:135:VAL:HG13	2:G:140:ASP:HB2	1.83	0.59
1:B:989:VAL:HG12	1:B:1014:PRO:HG3	1.84	0.59
2:H:236:HIS:O	2:H:240:LYS:NZ	2.31	0.59
1:D:282:MET:HE2	1:D:395:ILE:HD11	1.85	0.59
1:D:344:ILE:HG22	1:D:346:HIS:H	1.67	0.59
1:B:318:LYS:O	1:B:323:ARG:NH2	2.35	0.58
1:C:1140:GLN:HE22	1:C:1166:GLU:H	1.52	0.58
2:E:257:GLN:HA	2:E:260:ALA:HB3	1.84	0.58
1:B:1091:LEU:HD11	1:B:1190:CYS:HB3	1.85	0.58
1:C:587:ARG:HH12	1:C:615:GLU:H	1.49	0.58
2:H:101:LEU:HD12	2:H:108:ILE:HD13	1.85	0.58
2:E:108:ILE:HD12	2:E:166:LEU:HD21	1.85	0.58
1:D:690:LYS:HD2	1:D:690:LYS:O	2.04	0.58
1:A:487:ASP:OD1	1:A:488:GLY:N	2.37	0.58
1:C:282:MET:HE2	1:C:395:ILE:HD11	1.85	0.58
1:D:1118:SER:HB3	1:D:1121:LEU:HG	1.86	0.58
1:A:791:ALA:HB3	1:A:811:ILE:HG23	1.85	0.58
1:B:1150:GLU:N	1:B:1150:GLU:OE1	2.36	0.58
1:B:1022:TYR:HB3	1:B:1024:TYR:HE1	1.69	0.58
1:A:843:HIS:NE2	1:A:845:ASP:OD1	2.37	0.57
1:D:843:HIS:NE2	1:D:845:ASP:OD1	2.37	0.57
1:A:1172:GLU:O	1:A:1173:LEU:HD23	2.04	0.57
1:A:217:ASP:O	1:A:220:THR:OG1	2.21	0.57
1:C:1044:ARG:NH1	1:C:1148:CYS:SG	2.78	0.57
2:G:257:GLN:HA	2:G:260:ALA:HB3	1.86	0.57
1:D:657:ARG:HE	1:D:679:VAL:HG21	1.70	0.57
1:C:946:VAL:HG11	1:C:973:ALA:HB2	1.87	0.57
1:C:1092:LYS:HD3	1:C:1094:LYS:HE3	1.87	0.57
1:A:280:VAL:HB	1:A:386:THR:HB	1.85	0.57
1:C:487:ASP:OD1	1:C:488:GLY:N	2.37	0.57
1:C:943:ILE:HG13	1:C:944:LYS:H	1.69	0.56
1:C:344:ILE:HB	1:C:346:HIS:HB2	1.87	0.56
1:C:640:HIS:O	1:C:640:HIS:ND1	2.38	0.56
1:B:660:HIS:HE2	1:B:680:GLU:CD	2.12	0.56
2:G:86:ASN:OD1	2:G:87:ASP:N	2.38	0.56
1:A:1071:MET:HA	1:A:1158:ILE:O	2.06	0.56
1:C:96:VAL:HG21	1:C:144:LEU:HD22	1.87	0.56
1:A:584:VAL:HG22	1:A:607:ASN:HB3	1.88	0.56
1:C:581:GLN:OE1	1:C:602:ARG:NH2	2.39	0.56
1:C:778:ASN:OD1	1:C:801:ASN:ND2	2.39	0.56
2:G:231:PHE:HA	2:G:234:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:LYS:O	1:D:323:ARG:NH2	2.36	0.56
1:D:514:CYS:O	1:D:607:ASN:ND2	2.32	0.56
1:D:1045:LEU:HB3	1:D:1047:PHE:HE1	1.70	0.56
1:C:470:LYS:HB2	1:C:475:TRP:CD1	2.40	0.56
2:F:167:GLU:OE2	2:F:207:LYS:NZ	2.39	0.56
1:A:600:SER:HB3	1:A:626:ARG:NH2	2.21	0.56
1:B:843:HIS:NE2	1:B:845:ASP:OD1	2.39	0.56
1:C:669:LEU:HD21	1:C:683:MET:HE1	1.88	0.56
1:C:1047:PHE:HB3	1:C:1050:CYS:SG	2.46	0.56
1:D:946:VAL:HG11	1:D:973:ALA:HB2	1.87	0.56
1:A:96:VAL:HG21	1:A:144:LEU:HD22	1.88	0.56
1:B:1013:LEU:HD12	1:B:1034:LEU:HD22	1.88	0.56
1:C:796:GLU:HG2	1:C:818:TRP:HE3	1.71	0.56
2:G:209:VAL:HG11	2:G:215:ALA:HB2	1.88	0.56
1:A:473:PRO:HB2	1:A:477:ARG:NH1	2.16	0.55
1:B:266:MET:HE3	1:B:299:PHE:HD2	1.71	0.55
1:D:134:ALA:O	1:D:138:SER:OG	2.24	0.55
1:C:664:TYR:CE2	1:C:666:ASN:HB3	2.42	0.55
1:D:453:ALA:HB2	1:D:463:LEU:HD12	1.88	0.55
1:D:875:ASN:H	1:D:899:LYS:HG3	1.71	0.55
1:A:127:ILE:HB	1:A:131:LEU:HD22	1.89	0.55
1:A:872:ASN:N	1:A:895:ARG:O	2.31	0.55
1:B:1073:PRO:HA	1:B:1157:HIS:ND1	2.21	0.55
2:G:101:LEU:HB3	2:G:108:ILE:HD11	1.87	0.55
1:D:959:PHE:CE1	1:D:961:ILE:HD11	2.42	0.55
1:B:179:GLU:H	1:B:226:SER:HB3	1.70	0.55
1:C:295:THR:HG21	3:C:1301:ADP:H2'	1.89	0.55
1:D:591:GLU:HA	1:D:594:ASN:HD22	1.72	0.55
1:A:664:TYR:CE2	1:A:666:ASN:HB3	2.41	0.55
1:B:1096:LYS:NZ	1:B:1172:GLU:HG3	2.22	0.55
1:C:370:LEU:HB2	1:C:397:ILE:HG22	1.89	0.55
1:D:969:GLU:OE2	1:D:969:GLU:N	2.35	0.55
1:B:791:ALA:HB1	1:B:794:LEU:HB2	1.89	0.55
2:H:231:PHE:O	2:H:235:LEU:HG	2.07	0.55
1:D:587:ARG:HH22	1:D:615:GLU:HG3	1.72	0.55
1:A:456:LEU:HD12	1:A:559:LEU:HD23	1.88	0.54
1:A:147:LYS:NZ	1:A:179:GLU:OE1	2.41	0.54
1:A:308:PHE:CG	1:A:367:PHE:HB2	2.42	0.54
1:B:811:ILE:HG21	1:B:814:ALA:HB2	1.89	0.54
2:H:167:GLU:OE2	2:H:207:LYS:NZ	2.39	0.54
1:A:242:ASP:O	1:A:246:MET:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLN:NE2	1:B:84:LYS:HB3	2.21	0.54
1:A:803:SER:O	1:A:827:SER:OG	2.23	0.54
1:A:266:MET:HE1	1:A:300:LEU:HD13	1.89	0.54
1:B:657:ARG:HE	1:B:679:VAL:HG21	1.72	0.54
1:A:225:HIS:CE1	1:A:227:HIS:HB3	2.42	0.54
1:B:990:PRO:HB2	1:B:993:VAL:HG13	1.90	0.54
1:C:1071:MET:HA	1:C:1158:ILE:O	2.06	0.54
2:E:86:ASN:OD1	2:E:87:ASP:N	2.40	0.54
1:D:698:LEU:HD12	1:D:701:LEU:HD22	1.89	0.54
1:D:831:LEU:HB3	1:D:835:ILE:HD12	1.89	0.54
1:A:963:TYR:HB2	1:A:980:LEU:HD11	1.90	0.54
1:C:147:LYS:NZ	1:C:179:GLU:OE1	2.39	0.54
1:A:600:SER:HA	1:A:628:HIS:HB3	1.88	0.54
1:B:453:ALA:HB2	1:B:463:LEU:HD12	1.89	0.54
1:C:968:LYS:HE3	1:C:992:TRP:CE3	2.42	0.54
2:F:295:SER:OG	2:F:298:GLN:OE1	2.25	0.54
1:D:332:GLN:HG2	1:D:381:ALA:HB2	1.90	0.54
1:B:930:SER:HA	1:B:953:TRP:HE1	1.73	0.54
2:F:108:ILE:HD12	2:F:166:LEU:HD21	1.89	0.54
1:D:606:ILE:HD11	1:D:630:PHE:CZ	2.43	0.54
1:A:877:VAL:O	1:A:878:GLU:HG3	2.07	0.54
1:A:969:GLU:OE1	1:A:969:GLU:N	2.41	0.54
1:B:272:LEU:HD12	1:B:414:TYR:HB2	1.90	0.54
1:B:1022:TYR:HB3	1:B:1024:TYR:CE1	2.43	0.54
1:C:631:GLN:O	1:C:657:ARG:HB3	2.07	0.54
1:C:943:ILE:HG13	1:C:944:LYS:N	2.22	0.54
2:F:231:PHE:HA	2:F:234:VAL:HG12	1.89	0.54
1:D:149:TYR:HB3	1:D:192:PHE:CE2	2.43	0.54
1:D:669:LEU:HD21	1:D:683:MET:HE1	1.89	0.54
1:B:332:GLN:HG2	1:B:381:ALA:HB2	1.89	0.54
1:C:872:ASN:N	1:C:895:ARG:O	2.40	0.54
1:A:527:LEU:HA	1:A:657:ARG:HH11	1.73	0.53
1:D:811:ILE:HG21	1:D:814:ALA:HB2	1.89	0.53
1:B:707:SER:HB2	1:B:730:ARG:HB3	1.89	0.53
1:C:364:LYS:HA	1:D:82:ILE:HG23	1.90	0.53
1:C:456:LEU:HD12	1:C:559:LEU:HD23	1.89	0.53
1:C:660:HIS:NE2	1:C:680:GLU:OE1	2.37	0.53
1:A:738:LEU:HB3	1:A:742:ILE:HD11	1.90	0.53
1:B:587:ARG:HH22	1:B:615:GLU:HG3	1.74	0.53
1:C:959:PHE:HD2	1:C:977:ILE:HA	1.73	0.53
1:B:917:LEU:HD13	1:B:923:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1096:LYS:NZ	1:D:1133:GLU:OE1	2.41	0.53
1:A:295:THR:HG21	3:A:1301:ADP:H2'	1.89	0.53
1:B:669:LEU:HD12	1:B:692:TRP:HE1	1.73	0.53
1:B:1095:LEU:HD21	1:B:1192:ILE:HD11	1.90	0.53
2:E:298:GLN:HA	2:E:301:GLU:HG3	1.90	0.53
2:H:125:THR:OG1	1:D:869:TYR:OH	2.25	0.53
1:C:223:GLY:O	1:D:123:ARG:NH2	2.39	0.53
1:D:1096:LYS:HE3	1:D:1171:THR:HG22	1.90	0.53
1:C:776:LEU:HB2	1:C:799:LEU:HD23	1.91	0.53
1:D:286:TRP:CZ3	1:D:545:SER:HB3	2.44	0.53
1:D:760:VAL:HG12	1:D:761:GLU:HG3	1.90	0.53
1:D:1120:ASP:O	1:D:1122:LYS:HG3	2.08	0.53
1:A:286:TRP:CZ3	1:A:545:SER:HB3	2.44	0.53
1:A:370:LEU:HB2	1:A:397:ILE:HG22	1.89	0.52
1:A:959:PHE:HD2	1:A:977:ILE:HA	1.73	0.52
2:H:231:PHE:HA	2:H:234:VAL:HG12	1.90	0.52
1:A:312:ALA:HB2	1:A:343:MET:HA	1.91	0.52
1:A:1044:ARG:NH1	1:A:1148:CYS:SG	2.82	0.52
2:E:101:LEU:HB3	2:E:108:ILE:HD11	1.90	0.52
1:A:182:PRO:HD3	1:A:225:HIS:CD2	2.44	0.52
1:D:984:LYS:HZ1	1:D:1005:ASN:HB3	1.73	0.52
1:B:606:ILE:HD11	1:B:630:PHE:CZ	2.45	0.52
1:D:368:LEU:HB3	1:D:395:ILE:HG22	1.90	0.52
1:A:1027:ASN:HA	1:A:1049:LYS:HB2	1.91	0.52
1:B:588:ASP:OD1	1:B:589:ILE:HD12	2.10	0.52
1:C:930:SER:HA	1:C:953:TRP:CZ2	2.44	0.52
2:G:308:ARG:H	2:G:308:ARG:HD3	1.74	0.52
1:D:194:LYS:O	1:D:198:LYS:NZ	2.39	0.52
1:A:943:ILE:HG13	1:A:944:LYS:N	2.24	0.52
2:G:167:GLU:OE2	2:G:207:LYS:NZ	2.43	0.52
1:C:286:TRP:CZ3	1:C:545:SER:HB3	2.44	0.52
1:C:1142:THR:OG1	1:C:1143:PRO:HD3	2.10	0.52
1:A:1143:PRO:HG2	1:A:1163:LEU:HD23	1.90	0.52
1:C:308:PHE:CG	1:C:367:PHE:HB2	2.45	0.52
1:C:690:LYS:HG3	1:C:690:LYS:O	2.08	0.52
1:C:733:SER:HA	1:C:757:SER:H	1.75	0.52
2:H:73:LEU:HD21	2:H:101:LEU:HD22	1.90	0.52
1:D:272:LEU:HD12	1:D:414:TYR:HB2	1.91	0.52
1:D:692:TRP:CZ3	1:D:698:LEU:HD21	2.44	0.52
1:A:692:TRP:CH2	1:A:698:LEU:HD21	2.44	0.52
1:B:587:ARG:HH21	1:B:617:LEU:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:981:GLN:HE21	1:D:1005:ASN:HD21	1.58	0.52
1:A:669:LEU:HD21	1:A:683:MET:HE1	1.90	0.52
1:D:526:GLY:O	1:D:657:ARG:NH1	2.43	0.52
1:B:286:TRP:CZ3	1:B:545:SER:HB3	2.45	0.51
1:C:1073:PRO:HA	1:C:1157:HIS:ND1	2.25	0.51
2:H:85:LEU:HD23	2:H:85:LEU:H	1.75	0.51
2:G:254:TRP:HA	2:G:257:GLN:NE2	2.26	0.51
1:D:1073:PRO:HA	1:D:1157:HIS:ND1	2.26	0.51
1:A:775:ASN:OD1	1:A:798:SER:OG	2.25	0.51
1:B:904:PRO:HB2	1:B:907:ILE:HD12	1.91	0.51
2:H:108:ILE:HD12	2:H:166:LEU:HD21	1.92	0.51
1:A:1142:THR:OG1	1:A:1143:PRO:HD3	2.09	0.51
1:B:984:LYS:NZ	1:B:1006:ASN:HB2	2.25	0.51
1:C:547:ILE:HD11	1:C:554:ILE:HB	1.91	0.51
2:H:305:GLU:HA	2:H:308:ARG:NH1	2.26	0.51
2:F:305:GLU:HA	2:F:308:ARG:NH1	2.25	0.51
1:A:309:GLN:HE21	1:B:84:LYS:HB3	1.73	0.51
1:A:796:GLU:HG2	1:A:818:TRP:HE3	1.75	0.51
1:B:1093:ILE:HB	1:B:1175:PHE:HB2	1.92	0.51
1:D:346:HIS:HB3	1:D:349:ILE:HD11	1.91	0.51
1:D:994:LYS:HE2	1:D:996:MET:HE3	1.92	0.51
1:B:1044:ARG:NH1	1:B:1148:CYS:SG	2.84	0.51
1:C:656:ILE:HD12	1:C:673:PHE:HE1	1.75	0.51
1:C:690:LYS:HE3	1:C:714:GLU:OE1	2.11	0.51
1:C:281:ARG:HH21	1:C:412:HIS:CE1	2.28	0.51
1:C:578:THR:HB	1:C:601:ARG:NH1	2.26	0.51
1:C:866:GLU:HA	1:C:889:LEU:HA	1.93	0.51
1:A:1081:PHE:HA	1:A:1193:LEU:HB2	1.93	0.51
1:B:1128:ILE:HG12	1:B:1177:PHE:HD1	1.76	0.51
1:C:629:ASP:HB3	1:C:654:PRO:HD2	1.93	0.51
1:C:877:VAL:O	1:C:878:GLU:HG3	2.11	0.51
2:F:85:LEU:H	2:F:85:LEU:HD23	1.76	0.51
1:D:681:LEU:HD11	1:D:683:MET:HE3	1.93	0.51
1:C:1025:ALA:O	1:C:1048:PRO:HD2	2.11	0.51
1:A:230:ARG:HA	1:D:98:LYS:HE2	1.93	0.50
1:A:1107:LYS:HD2	1:A:1162:GLU:HG2	1.94	0.50
1:B:166:ARG:HD2	1:B:173:VAL:HG21	1.93	0.50
1:C:577:TYR:HE2	1:D:589:ILE:HG12	1.76	0.50
1:D:660:HIS:CD2	1:D:682:ASP:HB3	2.47	0.50
1:C:308:PHE:CD2	1:C:367:PHE:HB2	2.45	0.50
1:D:527:LEU:O	1:D:657:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1004:LEU:HB3	1:D:1007:CYS:SG	2.51	0.50
1:A:351:ILE:HD11	1:A:356:VAL:HB	1.93	0.50
1:A:1095:LEU:HD11	1:A:1173:LEU:HD12	1.94	0.50
1:B:1105:THR:HG22	1:B:1164:GLU:HG2	1.92	0.50
1:C:266:MET:HE1	1:C:300:LEU:HD13	1.92	0.50
2:E:231:PHE:HA	2:E:234:VAL:HG12	1.94	0.50
1:A:866:GLU:HA	1:A:889:LEU:HA	1.92	0.50
1:B:217:ASP:O	1:B:220:THR:OG1	2.27	0.50
1:C:1096:LYS:HD2	1:C:1171:THR:HG22	1.94	0.50
1:A:877:VAL:HG12	1:A:899:LYS:O	2.12	0.50
2:E:85:LEU:HD23	2:E:85:LEU:H	1.76	0.50
2:E:232:SER:O	2:E:236:HIS:ND1	2.45	0.50
1:D:640:HIS:O	1:D:640:HIS:ND1	2.44	0.50
1:D:984:LYS:NZ	1:D:1005:ASN:HB3	2.27	0.50
1:B:619:ILE:HD11	1:B:645:ARG:HB3	1.94	0.50
1:B:1092:LYS:HZ1	1:B:1176:GLU:CD	2.19	0.50
1:C:772:GLU:HG3	1:C:795:GLN:HG2	1.92	0.50
1:D:295:THR:HG21	3:D:1301:ADP:H2'	1.94	0.50
1:D:425:PHE:HD1	1:D:450:MET:SD	2.34	0.50
1:A:943:ILE:HG13	1:A:944:LYS:H	1.76	0.50
1:A:989:VAL:HG12	1:A:1014:PRO:HG3	1.94	0.50
1:B:266:MET:HE3	1:B:299:PHE:CD2	2.47	0.49
1:D:949:SER:O	1:D:952:SER:OG	2.20	0.49
1:C:1128:ILE:HG21	1:C:1163:LEU:HD21	1.94	0.49
2:H:296:LEU:HA	2:H:299:ILE:HD12	1.94	0.49
1:A:1139:VAL:HB	1:A:1167:GLU:CD	2.37	0.49
1:B:872:ASN:N	1:B:895:ARG:O	2.37	0.49
1:A:1112:LEU:HB3	1:A:1117:MET:HE1	1.94	0.49
1:B:259:LEU:HD13	1:B:262:MET:SD	2.52	0.49
1:B:1134:GLN:HG2	1:B:1135:ASN:N	2.26	0.49
2:G:188:ILE:HD12	2:G:205:LEU:HD13	1.94	0.49
1:D:1108:ALA:HA	1:D:1192:ILE:HG22	1.93	0.49
1:B:323:ARG:HB2	1:B:324:PRO:HD3	1.94	0.49
1:D:273:LEU:HA	1:D:283:ILE:HD11	1.95	0.49
1:D:490:ILE:HG21	1:D:559:LEU:HD23	1.95	0.49
1:D:877:VAL:O	1:D:878:GLU:HG3	2.11	0.49
1:D:1105:THR:HG22	1:D:1164:GLU:HG2	1.93	0.49
1:B:232:GLU:HG3	1:C:99:THR:HA	1.94	0.49
1:B:530:LYS:HE3	1:B:657:ARG:NH2	2.28	0.49
1:B:585:GLY:HA3	1:B:589:ILE:HD13	1.94	0.49
1:C:1095:LEU:HD21	1:C:1192:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:108:ILE:HD12	2:G:166:LEU:HD21	1.94	0.49
1:D:979:GLU:HG2	1:D:1001:ALA:HB3	1.94	0.49
1:C:407:ALA:HA	1:D:469:GLY:HA3	1.94	0.49
1:C:606:ILE:HD11	1:C:630:PHE:CZ	2.47	0.49
1:C:930:SER:HA	1:C:953:TRP:HZ2	1.78	0.49
1:C:1155:THR:HG1	1:C:1156:GLU:CD	2.15	0.49
2:H:125:THR:HG1	1:D:869:TYR:HH	1.60	0.49
2:G:85:LEU:HD23	2:G:85:LEU:H	1.77	0.49
1:D:1092:LYS:HZ1	1:D:1176:GLU:CD	2.19	0.49
1:A:894:MET:HB2	1:A:917:LEU:HD23	1.93	0.49
1:B:1127:ASP:OD1	1:B:1128:ILE:N	2.45	0.49
1:C:225:HIS:CE1	1:C:227:HIS:HB3	2.47	0.49
1:A:794:LEU:HD21	1:A:797:LEU:HB2	1.95	0.49
1:B:105:LEU:O	1:B:109:ARG:HG2	2.13	0.49
1:B:987:GLN:OE1	1:B:1009:ASN:ND2	2.46	0.49
1:C:365:LYS:HD3	1:C:392:GLY:O	2.13	0.49
1:D:318:LYS:HD3	1:D:374:ASP:HB2	1.94	0.49
1:D:323:ARG:HB2	1:D:324:PRO:HD3	1.94	0.49
1:A:729:LEU:HB3	1:A:732:CYS:SG	2.53	0.49
1:B:172:ILE:HD13	1:B:246:MET:HE1	1.95	0.49
1:C:961:ILE:HG22	1:C:977:ILE:HD11	1.93	0.49
1:D:791:ALA:HB1	1:D:794:LEU:HB2	1.95	0.49
1:D:1110:ILE:HG23	1:D:1187:ILE:HG23	1.95	0.49
1:A:162:ILE:HG22	1:A:163:MET:HE2	1.93	0.48
1:B:291:ILE:HA	1:B:457:PRO:HD2	1.95	0.48
1:B:293:LYS:N	3:B:1301:ADP:O3B	2.46	0.48
1:B:1026:ASP:O	1:B:1048:PRO:HB2	2.13	0.48
1:C:222:ALA:HB2	1:D:127:ILE:HG13	1.95	0.48
2:E:254:TRP:HA	2:E:257:GLN:NE2	2.27	0.48
1:D:1094:LYS:HG2	1:D:1174:VAL:HG22	1.94	0.48
1:A:841:LEU:HD21	1:A:844:LEU:HD13	1.95	0.48
1:B:163:MET:HA	1:B:166:ARG:HG2	1.94	0.48
1:B:358:GLN:O	1:B:362:ARG:HG3	2.12	0.48
2:E:230:TYR:CD2	2:E:255:MET:HE3	2.49	0.48
2:H:122:LEU:HD13	1:D:937:ARG:HD2	1.95	0.48
1:A:1016:LEU:H	1:A:1036:CYS:HB3	1.78	0.48
1:B:664:TYR:CE2	1:B:666:ASN:HB3	2.49	0.48
1:B:796:GLU:HG2	1:B:818:TRP:HE3	1.78	0.48
1:B:800:THR:OG1	1:B:801:ASN:N	2.45	0.48
1:B:1058:ARG:HG3	1:B:1072:LEU:HD11	1.95	0.48
1:C:274:ARG:HB2	1:C:281:ARG:HH12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:753:LEU:HB3	1:C:756:CYS:SG	2.54	0.48
1:D:1154:LEU:HB2	1:D:1157:HIS:CD2	2.47	0.48
1:A:982:LEU:HB3	1:A:986:ILE:HD12	1.95	0.48
1:B:1045:LEU:HB3	1:B:1047:PHE:HE1	1.78	0.48
1:B:1134:GLN:NE2	1:B:1169:THR:OG1	2.47	0.48
1:D:358:GLN:O	1:D:362:ARG:HG3	2.13	0.48
1:D:800:THR:OG1	1:D:801:ASN:N	2.45	0.48
1:A:775:ASN:C	1:A:776:LEU:HD12	2.39	0.48
1:B:1109:CYS:SG	1:B:1158:ILE:HG23	2.54	0.48
1:C:274:ARG:HH21	1:C:277:LEU:HD11	1.78	0.48
2:G:181:SER:HB3	2:G:218:ALA:HB2	1.95	0.48
1:D:1106:PHE:CE1	1:D:1194:GLN:HG2	2.48	0.48
1:A:690:LYS:HD2	1:A:690:LYS:O	2.14	0.48
1:C:93:GLY:HA2	1:C:97:ARG:HB2	1.96	0.48
1:C:282:MET:HG2	1:C:395:ILE:HD11	1.96	0.48
1:C:470:LYS:HB3	1:C:474:GLU:HB3	1.96	0.48
1:C:657:ARG:HE	1:C:679:VAL:HG21	1.76	0.48
1:A:308:PHE:CD2	1:A:367:PHE:HB2	2.49	0.48
1:A:1110:ILE:HG23	1:A:1187:ILE:HG23	1.96	0.48
1:B:1044:ARG:HB3	1:B:1046:TYR:CE1	2.49	0.48
1:D:293:LYS:N	3:D:1301:ADP:O3B	2.47	0.48
1:D:611:TYR:CB	1:D:638:LYS:HD3	2.43	0.48
1:D:959:PHE:CD2	1:D:977:ILE:HA	2.48	0.48
1:A:1155:THR:OG1	1:A:1156:GLU:N	2.46	0.47
1:C:909:LEU:H	1:C:931:THR:HG22	1.79	0.47
2:E:256:PHE:HB3	2:E:310:TYR:HE2	1.78	0.47
2:F:256:PHE:HE1	2:F:306:TYR:HB2	1.79	0.47
1:D:340:LEU:HB3	1:D:349:ILE:HD12	1.96	0.47
1:D:872:ASN:N	1:D:895:ARG:O	2.38	0.47
1:D:1133:GLU:HB2	1:D:1172:GLU:HB3	1.96	0.47
1:C:730:ARG:HD2	1:C:754:HIS:HB3	1.96	0.47
1:C:1030:SER:HB2	1:C:1032:GLU:OE2	2.13	0.47
2:E:104:ARG:HG2	2:E:106:ASP:OD1	2.14	0.47
1:C:584:VAL:HG22	1:C:607:ASN:HB3	1.95	0.47
1:C:775:ASN:OD1	1:C:798:SER:OG	2.31	0.47
1:A:831:LEU:HB2	1:A:856:PRO:HD3	1.96	0.47
1:B:909:LEU:H	1:B:931:THR:HG22	1.79	0.47
1:A:291:ILE:HA	1:A:457:PRO:HD2	1.97	0.47
1:A:800:THR:OG1	1:A:801:ASN:N	2.45	0.47
1:A:1134:GLN:OE1	1:A:1172:GLU:HG3	2.15	0.47
1:B:370:LEU:HB2	1:B:397:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1026:ASP:HA	1:C:1048:PRO:HG2	1.97	0.47
1:A:961:ILE:HG22	1:A:977:ILE:HD11	1.95	0.47
1:B:1134:GLN:OE1	1:B:1172:GLU:HB2	2.14	0.47
1:C:577:TYR:CE2	1:D:589:ILE:HG12	2.49	0.47
1:D:278:ASP:HA	1:D:392:GLY:HA2	1.95	0.47
1:D:656:ILE:HD12	1:D:673:PHE:HE1	1.78	0.47
1:D:894:MET:HE1	1:D:900:LEU:HD22	1.96	0.47
1:A:1006:ASN:O	1:A:1007:CYS:C	2.58	0.47
1:B:439:HIS:HB2	1:B:442:PHE:CD2	2.50	0.47
1:C:410:ILE:HG22	1:C:412:HIS:H	1.78	0.47
1:C:899:LYS:HG2	1:C:922:ARG:HH12	1.80	0.47
1:D:291:ILE:HA	1:D:457:PRO:HD2	1.97	0.47
1:D:904:PRO:HB2	1:D:907:ILE:HD12	1.95	0.47
1:A:269:LEU:HD23	1:A:300:LEU:HD22	1.95	0.47
1:B:877:VAL:O	1:B:878:GLU:HB2	2.15	0.47
1:B:1118:SER:HB3	1:B:1121:LEU:HG	1.96	0.47
1:C:127:ILE:HG22	1:C:154:TRP:CD1	2.50	0.47
2:G:271:ARG:HA	2:G:274:ALA:HB3	1.96	0.47
1:D:989:VAL:O	1:D:990:PRO:C	2.58	0.47
1:A:281:ARG:HH21	1:A:412:HIS:CE1	2.33	0.47
1:B:186:LYS:HE3	1:B:187:LYS:NZ	2.30	0.47
1:B:1106:PHE:CE1	1:B:1194:GLN:HG2	2.50	0.47
1:C:829:ILE:HG22	1:C:830:GLU:HG3	1.97	0.47
1:D:439:HIS:HB2	1:D:442:PHE:CD2	2.50	0.47
1:D:596:ASP:HB2	1:D:622:LYS:NZ	2.29	0.47
1:A:650:ILE:O	1:A:653:SER:OG	2.23	0.47
1:B:1096:LYS:HZ2	1:B:1172:GLU:HG3	1.80	0.47
1:C:1140:GLN:HE21	1:C:1167:GLU:HG3	1.79	0.47
1:A:347:LYS:HD2	1:A:347:LYS:O	2.15	0.46
1:A:879:LEU:HD12	1:A:879:LEU:HA	1.82	0.46
1:B:273:LEU:HA	1:B:283:ILE:HD11	1.98	0.46
1:B:656:ILE:HD12	1:B:673:PHE:HE1	1.80	0.46
2:H:256:PHE:HE1	2:H:306:TYR:HB2	1.80	0.46
2:F:256:PHE:CE1	2:F:306:TYR:HB2	2.50	0.46
1:D:294:THR:HG23	1:D:371:ASP:OD2	2.15	0.46
1:A:365:LYS:HD3	1:A:392:GLY:O	2.15	0.46
1:B:950:ILE:HG23	1:B:953:TRP:CE3	2.50	0.46
1:B:1054:ASN:HB3	1:B:1056:GLU:CD	2.40	0.46
1:C:598:ILE:HD12	1:C:626:ARG:CZ	2.46	0.46
1:A:574:HIS:HA	1:A:578:THR:O	2.15	0.46
1:B:422:ASP:OD2	1:B:426:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:LEU:HB3	1:B:1007:CYS:SG	2.55	0.46
1:C:574:HIS:HA	1:C:578:THR:O	2.15	0.46
1:C:963:TYR:HB2	1:C:980:LEU:HD11	1.97	0.46
1:C:997:SER:OG	1:C:998:ARG:N	2.46	0.46
1:C:1022:TYR:HB3	1:C:1024:TYR:CE2	2.50	0.46
1:C:1060:LEU:O	1:C:1064:THR:OG1	2.22	0.46
2:H:104:ARG:HG2	2:H:106:ASP:OD1	2.16	0.46
1:A:1096:LYS:HE3	1:A:1096:LYS:HA	1.98	0.46
1:B:760:VAL:HG12	1:B:761:GLU:HG3	1.97	0.46
1:B:1050:CYS:O	1:B:1073:PRO:HG2	2.14	0.46
1:B:337:ASN:HD21	1:B:350:MET:HA	1.80	0.46
1:B:743:GLU:HA	1:B:765:PHE:O	2.15	0.46
1:B:1134:GLN:HG2	1:B:1135:ASN:H	1.81	0.46
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.81	0.46
1:C:937:ARG:HH21	2:G:122:LEU:HD12	1.80	0.46
1:A:515:LEU:HD23	1:A:607:ASN:HB2	1.98	0.46
1:B:859:ILE:HD13	1:B:862:MET:HE1	1.98	0.46
1:C:507:TYR:CE1	1:C:573:ILE:HA	2.51	0.46
1:C:1081:PHE:HA	1:C:1193:LEU:HB2	1.98	0.46
1:C:1109:CYS:SG	1:C:1158:ILE:HG23	2.56	0.46
1:C:1154:LEU:HB2	1:C:1157:HIS:CD2	2.47	0.46
2:E:220:PHE:CD1	2:E:255:MET:HE1	2.51	0.46
2:H:256:PHE:CE1	2:H:306:TYR:HB2	2.50	0.46
2:F:262:LYS:HB3	2:F:264:PHE:CE1	2.51	0.46
1:A:946:VAL:HG11	1:A:973:ALA:HB2	1.98	0.46
1:C:310:LEU:HD11	1:C:343:MET:O	2.16	0.46
1:C:1127:ASP:OD1	1:C:1128:ILE:N	2.48	0.46
2:E:262:LYS:HB3	2:E:264:PHE:CE1	2.51	0.46
1:D:726:GLU:HB2	1:D:750:ILE:HB	1.97	0.46
1:A:223:GLY:O	1:B:123:ARG:NH2	2.46	0.46
1:B:778:ASN:OD1	1:B:801:ASN:ND2	2.49	0.46
1:B:959:PHE:CD2	1:B:977:ILE:HA	2.46	0.46
1:B:1142:THR:OG1	1:B:1143:PRO:HD3	2.16	0.46
1:C:968:LYS:HE3	1:C:992:TRP:CD2	2.51	0.46
1:C:1050:CYS:O	1:C:1073:PRO:HG2	2.15	0.46
1:B:706:LEU:HB2	1:B:729:LEU:HD23	1.98	0.46
1:B:877:VAL:HG22	1:B:899:LYS:HB3	1.97	0.46
1:C:692:TRP:HH2	1:C:698:LEU:HD21	1.81	0.46
1:D:898:SER:HA	1:D:921:SER:H	1.80	0.46
1:D:1128:ILE:HG12	1:D:1177:PHE:HD1	1.81	0.46
1:A:598:ILE:HB	1:A:626:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ASN:OD1	1:A:1009:ASN:N	2.48	0.46
1:B:295:THR:HG21	3:B:1301:ADP:H2'	1.98	0.46
1:B:756:CYS:HB3	1:B:759:LEU:HG	1.98	0.46
1:C:224:TYR:OH	1:C:242:ASP:OD2	2.26	0.46
1:C:841:LEU:HD21	1:C:844:LEU:HD13	1.97	0.46
1:C:976:ILE:O	1:C:976:ILE:HG22	2.16	0.46
2:F:70:VAL:O	2:F:74:ILE:HG12	2.16	0.46
2:G:88:GLU:HA	2:G:91:MET:HB3	1.98	0.46
1:A:93:GLY:HA2	1:A:97:ARG:HB2	1.97	0.45
1:A:996:MET:CG	1:A:999:LEU:HD21	2.47	0.45
1:C:291:ILE:HA	1:C:457:PRO:HD2	1.97	0.45
1:C:455:GLU:H	1:C:557:HIS:HE2	1.64	0.45
1:C:982:LEU:HB3	1:C:986:ILE:HD12	1.98	0.45
1:C:1121:LEU:HD12	1:C:1121:LEU:HA	1.81	0.45
1:D:664:TYR:CE2	1:D:666:ASN:HB3	2.50	0.45
1:A:1141:CYS:SG	1:A:1163:LEU:HD22	2.56	0.45
1:B:601:ARG:NH2	1:B:627:ILE:O	2.49	0.45
2:F:253:LYS:HD2	2:F:310:TYR:OH	2.17	0.45
2:G:253:LYS:HA	2:G:256:PHE:HD2	1.82	0.45
1:D:667:ILE:HG22	1:D:668:CYS:SG	2.57	0.45
1:D:841:LEU:HD21	1:D:844:LEU:HD13	1.98	0.45
1:A:627:ILE:HG22	1:A:627:ILE:O	2.17	0.45
1:A:843:HIS:HE1	1:A:869:TYR:CE2	2.34	0.45
1:A:1105:THR:HG22	1:A:1164:GLU:HG3	1.98	0.45
1:B:726:GLU:HB2	1:B:750:ILE:HB	1.97	0.45
1:A:134:ALA:O	1:A:138:SER:OG	2.35	0.45
1:A:660:HIS:NE2	1:A:680:GLU:OE1	2.44	0.45
1:A:999:LEU:O	1:A:1020:LEU:HD13	2.16	0.45
1:B:281:ARG:HD2	1:B:412:HIS:NE2	2.31	0.45
1:B:471:SER:N	1:B:474:GLU:OE1	2.39	0.45
1:B:616:GLU:OE1	1:B:643:HIS:HA	2.17	0.45
1:C:1093:ILE:HB	1:C:1175:PHE:HB2	1.98	0.45
1:C:1110:ILE:HD13	1:C:1161:PHE:CE2	2.52	0.45
1:B:949:SER:O	1:B:952:SER:OG	2.23	0.45
1:C:982:LEU:HB2	1:C:1004:LEU:HD13	1.98	0.45
2:H:262:LYS:HB3	2:H:264:PHE:CE1	2.51	0.45
2:F:252:LYS:HE2	2:F:256:PHE:HE2	1.82	0.45
1:D:565:ARG:O	1:D:568:SER:OG	2.33	0.45
1:D:738:LEU:HD11	1:D:753:LEU:HD21	1.99	0.45
1:A:1058:ARG:NH2	1:A:1073:PRO:O	2.50	0.45
1:C:343:MET:HA	1:C:343:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:252:LYS:HE2	2:H:256:PHE:HE2	1.82	0.45
2:G:220:PHE:CD1	2:G:255:MET:HE1	2.50	0.45
2:G:262:LYS:HB3	2:G:264:PHE:CE1	2.52	0.45
1:A:274:ARG:C	1:A:394:ARG:HH12	2.24	0.45
1:A:914:THR:HG21	2:E:116:PHE:HE2	1.82	0.45
1:B:269:LEU:HD21	1:B:300:LEU:HD22	1.99	0.45
1:B:667:ILE:HG22	1:B:668:CYS:SG	2.56	0.45
1:B:841:LEU:HD21	1:B:844:LEU:HD13	1.98	0.45
1:B:866:GLU:HA	1:B:889:LEU:HA	1.98	0.45
1:B:1128:ILE:HG12	1:B:1177:PHE:CD1	2.51	0.45
1:C:692:TRP:CH2	1:C:698:LEU:HD21	2.51	0.45
2:F:104:ARG:HG2	2:F:106:ASP:OD1	2.16	0.45
1:D:981:GLN:HE21	1:D:1005:ASN:ND2	2.14	0.45
1:B:606:ILE:HD11	1:B:630:PHE:CE2	2.52	0.45
1:C:1107:LYS:HD2	1:C:1162:GLU:HG2	1.98	0.45
2:H:156:LEU:HD11	1:D:752:ASP:OD2	2.17	0.45
2:F:231:PHE:O	2:F:235:LEU:HG	2.17	0.45
2:G:240:LYS:HA	2:G:240:LYS:HD3	1.74	0.45
1:A:439:HIS:CG	1:A:443:ASP:HB2	2.52	0.45
1:B:346:HIS:HB3	1:B:349:ILE:HD11	1.98	0.45
1:D:778:ASN:OD1	1:D:801:ASN:ND2	2.50	0.45
1:D:997:SER:OG	1:D:998:ARG:N	2.50	0.45
1:D:1055:GLN:O	1:D:1059:ASP:N	2.37	0.45
1:B:796:GLU:HG2	1:B:818:TRP:CE3	2.52	0.44
2:E:271:ARG:HH12	2:E:275:ALA:HA	1.82	0.44
1:D:165:CYS:SG	1:D:169:LEU:HD12	2.57	0.44
1:A:549:ILE:HG12	1:A:554:ILE:HG22	1.99	0.44
1:A:984:LYS:HD3	1:A:1006:ASN:HB2	1.98	0.44
1:B:84:LYS:HE2	1:B:134:ALA:HA	1.98	0.44
1:B:216:GLU:O	1:B:220:THR:HG23	2.17	0.44
1:B:776:LEU:O	1:B:799:LEU:HA	2.17	0.44
1:C:614:VAL:HG21	1:C:643:HIS:HE1	1.82	0.44
2:H:91:MET:SD	2:H:142:GLY:HA2	2.56	0.44
2:H:299:ILE:O	2:H:303:VAL:HG23	2.17	0.44
2:G:141:ARG:HG2	2:G:187:SER:HA	1.99	0.44
1:D:266:MET:HE3	1:D:299:PHE:HD2	1.83	0.44
1:A:292:GLY:N	3:A:1301:ADP:O2A	2.51	0.44
1:A:370:LEU:O	1:A:397:ILE:HA	2.17	0.44
1:A:631:GLN:O	1:A:657:ARG:HB2	2.18	0.44
1:A:976:ILE:HG22	1:A:976:ILE:O	2.16	0.44
2:G:174:TRP:CD1	2:G:179:TYR:HE2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:VAL:HG22	1:A:1010:LEU:HD11	2.00	0.44
1:B:274:ARG:HB2	1:B:281:ARG:NH2	2.32	0.44
1:C:294:THR:OG1	3:C:1301:ADP:O1A	2.36	0.44
1:D:201:LYS:HD3	1:D:201:LYS:HA	1.85	0.44
1:A:1001:ALA:HB2	1:A:1022:TYR:HD2	1.83	0.44
1:B:163:MET:O	1:B:166:ARG:HG2	2.17	0.44
1:C:707:SER:CB	1:C:730:ARG:HB3	2.47	0.44
2:E:304:GLU:O	2:E:308:ARG:NH1	2.49	0.44
1:D:246:MET:HE2	1:D:246:MET:HB2	1.82	0.44
1:A:752:ASP:OD2	2:E:156:LEU:HD11	2.17	0.44
1:C:473:PRO:HB2	1:C:477:ARG:NH2	2.29	0.44
1:C:559:LEU:HD12	1:C:559:LEU:HA	1.87	0.44
1:D:281:ARG:HD2	1:D:412:HIS:NE2	2.32	0.44
1:D:508:LEU:HB2	1:D:532:LEU:HD11	1.98	0.44
1:D:584:VAL:HG13	1:D:607:ASN:HB3	1.99	0.44
1:A:294:THR:OG1	3:A:1301:ADP:O1A	2.36	0.44
1:C:1102:THR:HG22	1:C:1103:THR:N	2.33	0.44
2:E:190:THR:OG1	2:E:195:ASP:OD2	2.33	0.44
1:D:866:GLU:HA	1:D:889:LEU:HA	1.99	0.44
1:A:667:ILE:HG22	1:A:668:CYS:SG	2.57	0.44
1:A:829:ILE:HG22	1:A:830:GLU:HG3	1.99	0.44
1:A:1166:GLU:N	1:A:1166:GLU:OE1	2.51	0.44
1:B:660:HIS:CD2	1:B:682:ASP:HB3	2.53	0.44
1:C:332:GLN:HG3	1:C:381:ALA:CB	2.46	0.44
1:C:353:HIS:CD2	1:C:355:GLY:H	2.36	0.44
1:C:600:SER:HB3	1:C:626:ARG:HH21	1.83	0.44
1:C:938:LEU:O	1:C:961:ILE:HA	2.18	0.44
2:F:205:LEU:O	2:F:209:VAL:HG12	2.18	0.44
1:A:151:SER:HB3	1:A:195:ALA:HB1	2.00	0.43
1:B:178:TYR:HA	1:B:226:SER:HB2	1.99	0.43
1:B:601:ARG:HH21	1:B:628:HIS:HA	1.81	0.43
1:C:778:ASN:CG	1:C:801:ASN:HD22	2.26	0.43
2:E:296:LEU:HA	2:E:299:ILE:HD12	1.98	0.43
2:E:299:ILE:O	2:E:303:VAL:HG23	2.18	0.43
2:E:308:ARG:H	2:E:308:ARG:HD3	1.82	0.43
2:G:304:GLU:O	2:G:308:ARG:NH1	2.51	0.43
1:D:603:PHE:HB3	1:D:630:PHE:HE1	1.82	0.43
1:A:407:ALA:HA	1:B:469:GLY:HA3	1.99	0.43
1:A:1060:LEU:O	1:A:1064:THR:OG1	2.22	0.43
1:A:1090:SER:N	1:A:1176:GLU:OE2	2.50	0.43
1:C:660:HIS:ND1	1:C:682:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:300:GLU:O	2:G:304:GLU:N	2.37	0.43
1:D:268:MET:HE3	1:D:268:MET:HB3	1.76	0.43
1:D:435:GLN:HG3	1:D:437:GLN:O	2.18	0.43
1:D:689:GLN:HG2	1:D:711:TYR:O	2.18	0.43
1:A:666:ASN:OD1	1:A:667:ILE:N	2.46	0.43
1:C:759:LEU:HD23	1:C:759:LEU:HA	1.83	0.43
1:C:1110:ILE:HG23	1:C:1187:ILE:HG23	2.00	0.43
1:D:269:LEU:HD23	1:D:300:LEU:HD22	2.00	0.43
1:B:108:PHE:HE1	1:B:240:ALA:HA	1.84	0.43
1:B:1110:ILE:HG23	1:B:1187:ILE:HG23	1.99	0.43
1:C:151:SER:HA	1:C:199:THR:OG1	2.19	0.43
1:C:182:PRO:HD3	1:C:225:HIS:CD2	2.53	0.43
1:C:238:LYS:NZ	1:C:242:ASP:OD2	2.50	0.43
1:C:1013:LEU:HD23	1:C:1013:LEU:HA	1.86	0.43
1:C:1168:VAL:HG12	1:C:1168:VAL:O	2.17	0.43
1:A:370:LEU:HD22	1:A:382:LEU:HD13	1.99	0.43
1:A:938:LEU:O	1:A:961:ILE:HA	2.18	0.43
1:A:1017:PRO:O	1:A:1020:LEU:HD23	2.18	0.43
1:A:1073:PRO:HA	1:A:1157:HIS:ND1	2.33	0.43
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.88	0.43
2:F:299:ILE:O	2:F:303:VAL:HG23	2.18	0.43
1:D:105:LEU:O	1:D:109:ARG:HG2	2.18	0.43
1:D:1133:GLU:H	1:D:1172:GLU:HB3	1.83	0.43
1:C:536:GLN:HE21	1:C:540:ILE:HD11	1.82	0.43
1:C:627:ILE:HG22	1:C:627:ILE:O	2.19	0.43
1:C:894:MET:HB3	1:C:917:LEU:HD23	1.99	0.43
1:C:1140:GLN:HE22	1:C:1166:GLU:N	2.15	0.43
2:E:205:LEU:HD23	2:E:215:ALA:HB1	2.00	0.43
2:G:273:LEU:HD23	2:G:299:ILE:HG23	1.99	0.43
1:D:259:LEU:HD13	1:D:262:MET:SD	2.58	0.43
1:A:255:ASP:OD2	1:D:329:TYR:OH	2.27	0.43
1:A:336:GLN:HE21	1:A:357:ALA:HB2	1.83	0.43
1:A:828:LEU:HD23	1:A:828:LEU:HA	1.86	0.43
1:A:1103:THR:HB	1:A:1166:GLU:HG3	1.99	0.43
1:A:1109:CYS:SG	1:A:1158:ILE:HG23	2.58	0.43
1:C:221:ILE:O	4:D:1302:ATP:N6	2.45	0.43
1:C:904:PRO:HB2	1:C:907:ILE:CD1	2.48	0.43
1:D:410:ILE:HG22	1:D:412:HIS:H	1.82	0.43
1:A:879:LEU:HG	1:A:883:ILE:HD11	2.01	0.43
1:B:828:LEU:HD23	1:B:828:LEU:HA	1.90	0.43
1:A:1110:ILE:HD13	1:A:1161:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:HD3	1:B:203:LYS:HA	1.84	0.43
1:B:669:LEU:HD21	1:B:683:MET:HE1	2.01	0.43
1:B:817:LEU:HD23	1:B:817:LEU:HA	1.87	0.43
1:C:370:LEU:HD22	1:C:382:LEU:HD13	2.00	0.43
1:C:515:LEU:HD23	1:C:607:ASN:HB2	2.00	0.43
2:G:231:PHE:O	2:G:235:LEU:HD23	2.19	0.43
1:D:669:LEU:HD12	1:D:692:TRP:HE1	1.84	0.43
1:D:1102:THR:HG22	1:D:1103:THR:N	2.34	0.43
1:D:1166:GLU:OE1	1:D:1166:GLU:N	2.52	0.43
1:A:410:ILE:HG22	1:A:412:HIS:H	1.83	0.43
1:B:368:LEU:O	1:B:395:ILE:HA	2.18	0.43
1:C:87:VAL:HG13	1:C:140:ILE:HG23	2.01	0.43
1:C:273:LEU:O	1:C:394:ARG:NH1	2.52	0.43
2:H:205:LEU:O	2:H:209:VAL:HG12	2.19	0.43
2:H:240:LYS:HA	2:H:240:LYS:HD3	1.74	0.43
1:D:191:GLU:C	1:D:193:GLY:H	2.26	0.43
1:A:783:VAL:HA	1:A:804:ARG:O	2.19	0.42
1:A:1076:GLN:N	1:A:1076:GLN:OE1	2.52	0.42
1:B:1190:CYS:SG	1:B:1191:GLY:N	2.92	0.42
1:C:120:ASN:O	1:C:123:ARG:HG3	2.19	0.42
1:C:600:SER:HA	1:C:628:HIS:HB3	2.01	0.42
1:C:1030:SER:O	1:C:1031:LEU:HD22	2.19	0.42
2:E:167:GLU:OE2	2:E:207:LYS:NZ	2.52	0.42
1:A:660:HIS:ND1	1:A:682:ASP:OD2	2.52	0.42
1:A:1006:ASN:O	1:A:1028:CYS:HA	2.19	0.42
1:A:1029:LYS:HA	1:A:1029:LYS:HD3	1.80	0.42
1:B:271:GLN:O	1:B:274:ARG:HG3	2.19	0.42
1:B:410:ILE:HG22	1:B:412:HIS:H	1.85	0.42
1:C:442:PHE:HD2	1:C:444:GLU:H	1.66	0.42
1:C:950:ILE:HG23	1:C:953:TRP:CE3	2.54	0.42
1:D:828:LEU:HD23	1:D:828:LEU:HA	1.89	0.42
1:A:598:ILE:HD12	1:A:626:ARG:NH1	2.35	0.42
1:B:1140:GLN:NE2	1:B:1166:GLU:HB2	2.34	0.42
2:G:91:MET:HE2	2:G:91:MET:HB2	1.81	0.42
1:D:619:ILE:O	1:D:645:ARG:NH1	2.53	0.42
1:D:660:HIS:HE2	1:D:680:GLU:CD	2.24	0.42
1:D:796:GLU:HG2	1:D:818:TRP:HE3	1.84	0.42
1:A:997:SER:OG	1:A:998:ARG:N	2.50	0.42
1:B:318:LYS:HD3	1:B:374:ASP:HB2	2.02	0.42
1:B:376:LEU:CD2	1:C:468:ARG:HD3	2.49	0.42
1:B:514:CYS:O	1:B:607:ASN:ND2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:LYS:HE2	1:B:992:TRP:NE1	2.34	0.42
1:B:1017:PRO:O	1:B:1020:LEU:HD23	2.19	0.42
1:C:182:PRO:HD3	1:C:225:HIS:NE2	2.34	0.42
1:C:586:GLU:HG2	1:C:609:ASP:HB3	2.01	0.42
1:C:738:LEU:HB3	1:C:742:ILE:HD11	2.02	0.42
1:C:831:LEU:HB2	1:C:856:PRO:HD3	2.00	0.42
2:F:240:LYS:HD3	2:F:240:LYS:HA	1.74	0.42
2:G:192:HIS:HB2	2:G:195:ASP:OD2	2.19	0.42
1:D:929:ILE:HG22	1:D:931:THR:HG23	2.01	0.42
1:A:346:HIS:ND1	1:A:346:HIS:O	2.53	0.42
1:A:929:ILE:O	1:A:929:ILE:HG13	2.20	0.42
1:B:562:GLN:O	1:B:566:GLU:HG2	2.20	0.42
1:C:439:HIS:CG	1:C:443:ASP:HB2	2.55	0.42
1:C:697:GLN:C	1:C:698:LEU:HD12	2.45	0.42
1:C:877:VAL:HG22	1:C:899:LYS:O	2.19	0.42
2:E:166:LEU:HD23	2:E:166:LEU:HA	1.88	0.42
1:D:729:LEU:HB3	1:D:732:CYS:SG	2.59	0.42
1:D:778:ASN:CG	1:D:801:ASN:HD22	2.27	0.42
1:D:940:GLY:H	1:D:962:SER:HB3	1.85	0.42
1:D:950:ILE:HG23	1:D:953:TRP:CE3	2.55	0.42
1:D:1128:ILE:HG12	1:D:1177:PHE:CD1	2.55	0.42
1:D:1168:VAL:HG12	1:D:1168:VAL:O	2.20	0.42
1:A:1095:LEU:HD21	1:A:1192:ILE:HD11	2.00	0.42
1:B:163:MET:CE	1:B:217:ASP:HB3	2.50	0.42
1:B:191:GLU:C	1:B:193:GLY:H	2.26	0.42
1:B:376:LEU:HD21	1:C:468:ARG:HD3	2.02	0.42
1:B:775:ASN:OD1	1:B:777:GLU:HG3	2.19	0.42
1:B:1058:ARG:HG2	1:B:1062:MET:CE	2.49	0.42
1:C:205:LYS:HD2	1:C:205:LYS:HA	1.76	0.42
1:C:791:ALA:HB3	1:C:811:ILE:HG23	2.01	0.42
1:C:879:LEU:HA	1:C:879:LEU:HD12	1.79	0.42
1:C:931:THR:OG1	1:C:933:ILE:HG13	2.18	0.42
1:C:1083:HIS:ND1	1:C:1095:LEU:HD22	2.35	0.42
1:C:1162:GLU:C	1:C:1163:LEU:HD12	2.45	0.42
2:E:298:GLN:O	2:E:301:GLU:HG3	2.20	0.42
1:D:280:VAL:HB	1:D:386:THR:HB	2.01	0.42
1:D:622:LYS:HA	1:D:625:GLU:HG2	2.02	0.42
1:D:1044:ARG:HB3	1:D:1046:TYR:CE1	2.54	0.42
1:A:185:ILE:O	1:A:188:GLN:NE2	2.53	0.42
1:A:640:HIS:HA	1:A:665:GLN:CD	2.45	0.42
1:A:656:ILE:HD11	1:A:673:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:913:HIS:NE2	2:F:117:GLU:HG2	2.35	0.42
1:C:134:ALA:O	1:C:138:SER:OG	2.35	0.42
1:C:512:ILE:HG22	1:C:556:MET:HE2	2.01	0.42
1:C:776:LEU:HB3	1:C:779:CYS:SG	2.60	0.42
1:C:909:LEU:H	1:C:931:THR:CG2	2.32	0.42
1:C:1016:LEU:HD23	1:C:1038:PHE:CD2	2.55	0.42
1:D:930:SER:HA	1:D:953:TRP:HE1	1.85	0.42
1:D:1104:LEU:HB2	1:D:1165:VAL:HG23	2.02	0.42
1:D:1139:VAL:HG23	1:D:1167:GLU:CD	2.45	0.42
1:A:738:LEU:HD23	1:A:738:LEU:HA	1.84	0.42
1:B:149:TYR:HB3	1:B:192:PHE:CE2	2.54	0.42
1:C:648:GLY:O	1:C:652:GLN:HG2	2.19	0.42
1:C:1044:ARG:HB3	1:C:1046:TYR:CZ	2.55	0.42
2:E:253:LYS:HA	2:E:256:PHE:HD2	1.84	0.42
2:H:117:GLU:HG2	1:D:913:HIS:NE2	2.35	0.42
1:D:1156:GLU:O	1:D:1157:HIS:ND1	2.52	0.42
1:B:435:GLN:HG3	1:B:437:GLN:O	2.19	0.42
1:B:603:PHE:HB3	1:B:630:PHE:HE1	1.84	0.42
1:B:701:LEU:HD21	1:B:704:MET:HE3	2.01	0.42
1:B:1108:ALA:O	1:B:1160:THR:HA	2.20	0.42
1:B:1154:LEU:HB2	1:B:1157:HIS:CD2	2.47	0.42
1:C:739:PRO:O	1:C:742:ILE:HG13	2.20	0.42
1:D:1140:GLN:NE2	1:D:1166:GLU:HB2	2.35	0.42
1:A:205:LYS:HD2	1:A:205:LYS:HA	1.81	0.42
1:A:256:PHE:HB2	1:A:259:LEU:HG	2.02	0.42
1:A:1134:GLN:OE1	1:A:1134:GLN:N	2.53	0.42
1:A:1140:GLN:NE2	1:A:1166:GLU:H	2.18	0.42
1:A:1181:ASN:OD1	2:E:140:ASP:HB2	2.19	0.42
1:B:689:GLN:HG2	1:B:711:TYR:O	2.19	0.42
1:C:216:GLU:O	1:C:220:THR:HG23	2.19	0.42
1:C:698:LEU:HD23	1:C:701:LEU:CD2	2.50	0.42
1:C:813:ASN:O	1:C:837:THR:HG22	2.20	0.42
1:C:1125:SER:HB2	1:C:1147:GLN:HG2	2.02	0.42
2:G:305:GLU:HA	2:G:308:ARG:HH12	1.84	0.42
1:D:1090:SER:N	1:D:1176:GLU:OE2	2.53	0.42
1:A:950:ILE:HG23	1:A:953:TRP:CE3	2.55	0.41
1:A:1048:PRO:O	1:A:1157:HIS:CE1	2.71	0.41
1:A:1128:ILE:HG12	1:A:1177:PHE:HD1	1.84	0.41
1:B:399:THR:OG1	1:B:400:GLU:N	2.53	0.41
1:B:914:THR:HG21	2:F:116:PHE:HE2	1.85	0.41
1:B:1139:VAL:HG23	1:B:1167:GLU:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:GLY:N	3:C:1301:ADP:O2A	2.52	0.41
1:C:879:LEU:HG	1:C:883:ILE:HD11	2.01	0.41
1:C:998:ARG:O	1:C:999:LEU:HD22	2.19	0.41
1:C:1057:ALA:O	1:C:1061:ILE:HG13	2.20	0.41
2:F:192:HIS:HB2	2:F:195:ASP:OD2	2.20	0.41
1:A:350:MET:HE3	1:A:351:ILE:N	2.16	0.41
1:A:536:GLN:HE21	1:A:540:ILE:HD11	1.84	0.41
1:B:505:ASP:CG	1:C:481:ARG:HH22	2.26	0.41
1:B:703:TRP:HD1	1:B:726:GLU:HG2	1.84	0.41
1:B:778:ASN:CG	1:B:801:ASN:HD22	2.27	0.41
1:B:813:ASN:HB3	1:B:815:THR:HG23	2.02	0.41
1:C:269:LEU:HD23	1:C:300:LEU:HD22	2.01	0.41
2:E:106:ASP:OD1	2:E:106:ASP:N	2.51	0.41
1:D:1062:MET:O	1:D:1107:LYS:HE2	2.19	0.41
1:A:98:LYS:HG3	1:D:230:ARG:O	2.20	0.41
1:A:909:LEU:H	1:A:931:THR:CG2	2.28	0.41
1:A:938:LEU:O	1:A:961:ILE:HD12	2.20	0.41
1:A:1139:VAL:HB	1:A:1167:GLU:OE2	2.20	0.41
1:C:799:LEU:O	1:C:822:LEU:HA	2.20	0.41
1:C:1128:ILE:HG12	1:C:1177:PHE:HD1	1.85	0.41
1:C:1140:GLN:H	1:C:1140:GLN:HG3	1.67	0.41
1:C:1166:GLU:N	1:C:1166:GLU:OE1	2.53	0.41
2:H:253:LYS:HD2	2:H:310:TYR:OH	2.20	0.41
1:D:269:LEU:HD13	1:D:414:TYR:CD2	2.55	0.41
1:A:634:ARG:HA	1:A:660:HIS:HB2	2.03	0.41
1:A:707:SER:CB	1:A:730:ARG:HB3	2.48	0.41
1:A:885:ASN:O	1:A:887:ARG:NH1	2.53	0.41
1:A:1094:LYS:HG2	1:A:1174:VAL:HG23	2.03	0.41
1:B:859:ILE:O	1:B:862:MET:HE3	2.19	0.41
1:B:996:MET:HE2	1:B:996:MET:HB3	1.85	0.41
1:C:979:GLU:HG2	1:C:1001:ALA:HB3	2.03	0.41
2:E:181:SER:HB3	2:E:218:ALA:HB2	2.02	0.41
1:D:269:LEU:HD12	1:D:269:LEU:HA	1.91	0.41
1:D:551:ASP:OD1	1:D:551:ASP:N	2.53	0.41
1:A:1127:ASP:OD1	1:A:1128:ILE:N	2.53	0.41
1:B:149:TYR:HB3	1:B:192:PHE:HE2	1.85	0.41
1:B:246:MET:HB2	1:B:246:MET:HE2	1.85	0.41
1:B:278:ASP:HA	1:B:392:GLY:HA2	2.02	0.41
1:B:286:TRP:HZ3	1:B:545:SER:HB3	1.85	0.41
1:B:586:GLU:OE2	1:B:612:LYS:HG2	2.21	0.41
1:C:596:ASP:O	1:C:598:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:127:ASP:HB3	2:G:169:ALA:HB2	2.02	0.41
1:D:135:ILE:HG21	1:D:161:GLU:HG3	2.03	0.41
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.84	0.41
1:B:767:ASN:HA	1:B:790:ASN:OD1	2.20	0.41
1:B:994:LYS:HE2	1:B:994:LYS:HB3	1.87	0.41
1:C:996:MET:HG3	1:C:999:LEU:CD2	2.43	0.41
1:D:225:HIS:HB3	1:D:227:HIS:CE1	2.55	0.41
1:D:594:ASN:OD1	1:D:619:ILE:HA	2.21	0.41
1:A:544:LYS:O	1:A:545:SER:OG	2.35	0.41
1:B:667:ILE:O	1:B:688:LEU:HA	2.21	0.41
1:C:379:LEU:HA	1:C:379:LEU:HD23	1.84	0.41
1:C:531:PHE:HD2	1:C:575:HIS:CD2	2.39	0.41
1:C:579:LYS:O	1:C:601:ARG:NH1	2.53	0.41
1:C:893:LEU:HD22	2:G:124:ASP:O	2.21	0.41
1:C:1111:MET:HE2	1:C:1111:MET:HB3	1.92	0.41
2:H:216:ASN:HA	2:H:219:ILE:HG22	2.03	0.41
2:F:174:TRP:CD1	2:F:179:TYR:HE2	2.39	0.41
2:F:216:ASN:HA	2:F:219:ILE:HG22	2.03	0.41
1:D:925:SER:O	1:D:943:ILE:HG12	2.21	0.41
1:A:251:LYS:HE2	1:A:254:ARG:HD2	2.03	0.41
1:A:280:VAL:HG11	1:A:386:THR:O	2.21	0.41
1:A:722:THR:O	1:A:747:SER:OG	2.26	0.41
1:A:801:ASN:O	1:A:802:CYS:C	2.64	0.41
1:A:996:MET:HG3	1:A:999:LEU:CD2	2.50	0.41
1:A:1140:GLN:NE2	1:A:1166:GLU:HB2	2.36	0.41
1:B:191:GLU:O	1:B:192:PHE:HB3	2.21	0.41
1:B:929:ILE:O	1:B:929:ILE:HG13	2.21	0.41
1:B:1050:CYS:H	1:B:1073:PRO:HG2	1.86	0.41
1:C:203:LYS:HE2	1:C:211:TRP:HH2	1.85	0.41
1:C:422:ASP:O	1:C:426:GLN:HG3	2.21	0.41
1:C:507:TYR:OH	1:C:574:HIS:ND1	2.44	0.41
1:C:1140:GLN:NE2	1:C:1166:GLU:H	2.16	0.41
2:E:174:TRP:CD1	2:E:179:TYR:HE2	2.39	0.41
2:E:216:ASN:HA	2:E:219:ILE:HG22	2.02	0.41
2:H:295:SER:O	2:H:299:ILE:HG13	2.21	0.41
1:D:995:ARG:HE	1:D:995:ARG:HB2	1.49	0.41
1:D:1058:ARG:HG2	1:D:1062:MET:CE	2.51	0.41
1:A:394:ARG:HD3	1:A:394:ARG:HA	1.81	0.41
1:A:486:LEU:HD23	1:A:486:LEU:H	1.86	0.41
1:A:615:GLU:H	1:A:615:GLU:HG3	1.52	0.41
1:A:785:LEU:HD23	1:A:785:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:GLU:OE1	1:A:1032:GLU:N	2.49	0.41
1:A:1115:GLU:HB3	1:A:1116:GLU:H	1.71	0.41
1:B:99:THR:HA	1:C:232:GLU:HG3	2.03	0.41
1:B:353:HIS:HB2	1:C:256:PHE:CZ	2.56	0.41
1:B:1054:ASN:HB3	1:B:1056:GLU:OE1	2.21	0.41
1:C:179:GLU:N	1:C:226:SER:OG	2.48	0.41
1:C:733:SER:H	1:C:756:CYS:HA	1.86	0.41
2:E:295:SER:O	2:E:299:ILE:HG13	2.20	0.41
2:H:174:TRP:CD1	2:H:179:TYR:HE2	2.39	0.41
2:H:192:HIS:HB2	2:H:195:ASP:OD2	2.21	0.41
1:D:936:LEU:HD23	1:D:959:PHE:CE1	2.56	0.41
1:D:1127:ASP:OD1	1:D:1128:ILE:N	2.53	0.41
1:A:663:CYS:O	1:A:665:GLN:HG2	2.21	0.41
1:B:91:PHE:HB3	1:B:144:LEU:HB2	2.02	0.41
1:C:1096:LYS:NZ	1:C:1173:LEU:H	2.19	0.41
2:E:202:PHE:O	2:E:206:VAL:HG23	2.21	0.41
2:E:271:ARG:HA	2:E:274:ALA:HB3	2.03	0.41
1:D:591:GLU:HA	1:D:594:ASN:ND2	2.36	0.41
1:A:282:MET:HG2	1:A:395:ILE:HB	2.03	0.40
1:C:274:ARG:HB2	1:C:281:ARG:NH1	2.36	0.40
1:C:565:ARG:O	1:C:568:SER:OG	2.27	0.40
1:C:666:ASN:OD1	1:C:667:ILE:N	2.49	0.40
1:C:689:GLN:HG2	1:C:711:TYR:O	2.21	0.40
1:C:730:ARG:HD2	1:C:754:HIS:CB	2.51	0.40
2:E:192:HIS:HB2	2:E:195:ASP:OD2	2.20	0.40
2:H:116:PHE:HE2	1:D:914:THR:HG21	1.87	0.40
1:D:178:TYR:HA	1:D:226:SER:HB2	2.03	0.40
1:D:271:GLN:O	1:D:274:ARG:HG3	2.21	0.40
1:D:692:TRP:CH2	1:D:698:LEU:HD11	2.56	0.40
1:D:796:GLU:HG2	1:D:818:TRP:CE3	2.57	0.40
1:D:1121:LEU:HB3	1:D:1153:VAL:HB	2.03	0.40
1:C:938:LEU:O	1:C:961:ILE:HD12	2.20	0.40
1:C:1108:ALA:O	1:C:1160:THR:HA	2.21	0.40
1:A:280:VAL:HG13	1:A:393:SER:OG	2.21	0.40
1:A:574:HIS:NE2	1:A:579:LYS:HG2	2.37	0.40
1:B:135:ILE:HG21	1:B:161:GLU:HG3	2.03	0.40
1:C:1128:ILE:HG12	1:C:1177:PHE:CD1	2.56	0.40
1:C:1132:ASP:HB3	1:C:1172:GLU:HB3	2.03	0.40
2:F:305:GLU:HA	2:F:308:ARG:HH12	1.86	0.40
1:D:798:SER:HB3	1:D:819:LYS:HZ2	1.86	0.40
1:A:730:ARG:HD2	1:A:754:HIS:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:ILE:HG12	1:A:809:PRO:HB2	2.02	0.40
1:A:799:LEU:O	1:A:822:LEU:HA	2.22	0.40
1:A:979:GLU:HG2	1:A:1001:ALA:HB3	2.04	0.40
1:B:1094:LYS:HD3	1:B:1174:VAL:HG22	2.03	0.40
1:C:332:GLN:HG2	1:C:354:LEU:HD11	2.04	0.40
1:C:801:ASN:O	1:C:802:CYS:C	2.64	0.40
1:C:843:HIS:HE1	1:C:869:TYR:CE2	2.38	0.40
1:C:991:PRO:HD2	1:C:992:TRP:CZ3	2.56	0.40
1:C:1061:ILE:CG2	1:C:1072:LEU:HD21	2.51	0.40
2:E:88:GLU:HA	2:E:91:MET:HB3	2.04	0.40
1:D:91:PHE:HB3	1:D:144:LEU:HB2	2.02	0.40
1:D:183:THR:HA	1:D:186:LYS:HE2	2.04	0.40
1:B:662:LYS:HG3	1:B:684:SER:HB2	2.03	0.40
1:B:864:ASN:HA	1:B:888:LYS:HD2	2.02	0.40
1:B:1013:LEU:HA	1:B:1014:PRO:HD3	1.95	0.40
1:C:331:ALA:HA	1:C:334:GLN:HG2	2.03	0.40
1:C:726:GLU:HB2	1:C:750:ILE:HB	2.03	0.40
2:E:277:GLN:NE2	2:E:294:LEU:HB2	2.37	0.40
2:F:73:LEU:HD21	2:F:101:LEU:HD23	2.03	0.40
1:D:379:LEU:HD23	1:D:379:LEU:HA	1.93	0.40
1:D:776:LEU:HB3	1:D:779:CYS:SG	2.62	0.40
1:D:1007:CYS:HB3	1:D:1010:LEU:HB2	2.03	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	1104/1221 (90%)	997 (90%)	104 (9%)	3 (0%)	36	68
1	B	1108/1221 (91%)	997 (90%)	108 (10%)	3 (0%)	36	68
1	C	1104/1221 (90%)	995 (90%)	106 (10%)	3 (0%)	36	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1108/1221 (91%)	992 (90%)	113 (10%)	3 (0%)	36	68
2	E	234/311 (75%)	229 (98%)	5 (2%)	0	100	100
2	F	234/311 (75%)	229 (98%)	5 (2%)	0	100	100
2	G	234/311 (75%)	228 (97%)	6 (3%)	0	100	100
2	H	234/311 (75%)	229 (98%)	5 (2%)	0	100	100
All	All	5360/6128 (88%)	4896 (91%)	452 (8%)	12 (0%)	44	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1041	PRO
1	A	1099	PRO
1	A	1101	PRO
1	B	1041	PRO
1	B	1099	PRO
1	B	1101	PRO
1	C	1041	PRO
1	C	1099	PRO
1	C	1101	PRO
1	D	1041	PRO
1	D	1099	PRO
1	D	1101	PRO

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	1001/1114 (90%)	993 (99%)	8 (1%)	73	85
1	B	1004/1114 (90%)	998 (99%)	6 (1%)	78	87
1	C	1000/1114 (90%)	985 (98%)	15 (2%)	57	79
1	D	1004/1114 (90%)	991 (99%)	13 (1%)	61	80
2	E	198/265 (75%)	197 (100%)	1 (0%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	198/265 (75%)	196 (99%)	2 (1%)	68	83
2	G	198/265 (75%)	197 (100%)	1 (0%)	81	88
2	H	198/265 (75%)	196 (99%)	2 (1%)	68	83
All	All	4801/5516 (87%)	4753 (99%)	48 (1%)	65	83

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	LEU
1	A	614	VAL
1	A	615	GLU
1	A	622	LYS
1	A	638	LYS
1	A	1030	SER
1	A	1036	CYS
1	A	1121	LEU
1	B	736	VAL
1	B	754	HIS
1	B	1030	SER
1	B	1036	CYS
1	B	1116	GLU
1	B	1179	SER
1	C	553	ASN
1	C	614	VAL
1	C	638	LYS
1	C	1004	LEU
1	C	1007	CYS
1	C	1009	ASN
1	C	1016	LEU
1	C	1020	LEU
1	C	1023	LEU
1	C	1028	CYS
1	C	1029	LYS
1	C	1035	ASP
1	C	1116	GLU
1	C	1117	MET
1	C	1185	CYS
2	E	140	ASP
2	H	79[A]	ARG
2	H	79[B]	ARG
2	F	79[A]	ARG

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Mol	Chain	Res	Type
2	F	79[B]	ARG
2	G	140	ASP
1	D	398	THR
1	D	638	LYS
1	D	988	GLU
1	D	990	PRO
1	D	992	TRP
1	D	994	LYS
1	D	1026	ASP
1	D	1027	ASN
1	D	1030	SER
1	D	1036	CYS
1	D	1116	GLU
1	D	1117	MET
1	D	1185	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	336	GLN
1	A	495	GLN
1	A	618	ASN
1	A	643	HIS
1	A	723	ASN
1	A	790	ASN
1	A	824	ASN
1	A	840	ASN
1	A	1006	ASN
1	A	1140	GLN
1	B	227	HIS
1	B	302	ASN
1	B	337	ASN
1	B	345	ASN
1	B	421	ASN
1	B	495	GLN
1	B	553	ASN
1	B	575	HIS
1	B	580	HIS
1	B	628	HIS
1	B	643	HIS
1	B	723	ASN

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Mol	Chain	Res	Type
1	B	801	ASN
1	B	813	ASN
1	C	431	ASN
1	C	435	GLN
1	C	495	GLN
1	C	553	ASN
1	C	723	ASN
1	C	767	ASN
1	C	795	GLN
1	C	801	ASN
1	C	813	ASN
1	C	960	GLN
1	C	981	GLN
1	C	1140	GLN
2	H	162	GLN
2	H	298	GLN
2	F	162	GLN
2	G	164	HIS
1	D	302	ASN
1	D	303	GLN
1	D	495	GLN
1	D	517	ASN
1	D	539	HIS
1	D	553	ASN
1	D	575	HIS
1	D	580	HIS
1	D	801	ASN
1	D	813	ASN
1	D	821	ASN
1	D	981	GLN
1	D	987	GLN
1	D	1006	ASN
1	D	1027	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	ADP	D	1301	-	28,29,29	1.36	5 (17%)	43,45,45	1.83	10 (23%)
3	ADP	C	1301	-	28,29,29	1.36	5 (17%)	43,45,45	1.83	8 (18%)
4	ATP	B	1302	-	32,33,33	1.38	5 (15%)	48,52,52	1.76	9 (18%)
3	ADP	A	1301	-	28,29,29	1.35	5 (17%)	43,45,45	1.84	8 (18%)
3	ADP	B	1301	-	28,29,29	1.35	5 (17%)	43,45,45	1.83	11 (25%)
4	ATP	D	1302	-	32,33,33	1.38	5 (15%)	48,52,52	1.76	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	1301	-	-	0/16/32/32	0/3/3/3
3	ADP	C	1301	-	-	4/16/32/32	0/3/3/3
4	ATP	B	1302	-	-	1/22/38/38	0/3/3/3
3	ADP	A	1301	-	-	4/16/32/32	0/3/3/3
3	ADP	B	1301	-	-	1/16/32/32	0/3/3/3
4	ATP	D	1302	-	-	1/22/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1302	ATP	C5-C4	4.51	1.47	1.39
4	D	1302	ATP	C5-C4	4.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1301	ADP	C5-C4	4.30	1.46	1.39
3	A	1301	ADP	C5-C4	4.29	1.46	1.39
3	B	1301	ADP	C5-C4	4.26	1.46	1.39
3	D	1301	ADP	C5-C4	4.25	1.46	1.39
3	C	1301	ADP	C5-N7	-2.66	1.34	1.39
4	D	1302	ATP	C5-C6	2.64	1.48	1.41
4	B	1302	ATP	C5-C6	2.59	1.48	1.41
3	D	1301	ADP	C5-N7	-2.59	1.34	1.39
3	A	1301	ADP	C5-N7	-2.59	1.34	1.39
3	B	1301	ADP	C5-N7	-2.51	1.34	1.39
3	C	1301	ADP	C5-C6	2.46	1.47	1.41
3	A	1301	ADP	C5-C6	2.45	1.47	1.41
3	D	1301	ADP	C5-C6	2.41	1.47	1.41
3	B	1301	ADP	C5-C6	2.40	1.47	1.41
4	B	1302	ATP	C5-N7	-2.40	1.34	1.39
4	D	1302	ATP	C5-N7	-2.35	1.34	1.39
4	D	1302	ATP	C8-N7	2.32	1.36	1.31
4	B	1302	ATP	C8-N7	2.26	1.36	1.31
3	A	1301	ADP	C4-N9	-2.21	1.33	1.37
3	D	1301	ADP	C8-N7	2.20	1.35	1.31
3	C	1301	ADP	C4-N9	-2.19	1.33	1.37
3	D	1301	ADP	C4-N9	-2.19	1.33	1.37
3	B	1301	ADP	C4-N9	-2.16	1.33	1.37
3	B	1301	ADP	C8-N7	2.15	1.35	1.31
3	C	1301	ADP	C8-N7	2.14	1.35	1.31
3	A	1301	ADP	C8-N7	2.13	1.35	1.31
4	B	1302	ATP	PB-O3B	2.09	1.61	1.59
4	D	1302	ATP	PB-O3B	2.03	1.61	1.59

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1302	ATP	C5-C4-N3	-5.98	118.48	126.72
4	B	1302	ATP	C5-C4-N3	-5.95	118.52	126.72
3	A	1301	ADP	C5-C4-N3	-5.80	118.74	126.72
3	C	1301	ADP	C5-C4-N3	-5.72	118.84	126.72
3	D	1301	ADP	C5-C4-N3	-5.70	118.86	126.72
3	B	1301	ADP	C5-C4-N3	-5.69	118.88	126.72
4	B	1302	ATP	N3-C4-N9	4.68	135.13	127.17
4	D	1302	ATP	N3-C4-N9	4.61	135.01	127.17
3	D	1301	ADP	N3-C4-N9	4.53	134.87	127.17
3	A	1301	ADP	N3-C4-N9	4.52	134.86	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1301	ADP	N3-C4-N9	4.51	134.84	127.17
3	C	1301	ADP	N3-C4-N9	4.46	134.76	127.17
4	B	1302	ATP	C2-N3-C4	3.71	120.90	111.83
4	D	1302	ATP	C2-N3-C4	3.71	120.89	111.83
3	A	1301	ADP	C2-N3-C4	3.62	120.68	111.83
3	B	1301	ADP	C2-N3-C4	3.61	120.66	111.83
3	D	1301	ADP	C2-N3-C4	3.61	120.66	111.83
3	C	1301	ADP	C2-N3-C4	3.60	120.62	111.83
4	D	1302	ATP	C4-C5-N7	-3.52	106.55	110.58
4	B	1302	ATP	C4-C5-N7	-3.43	106.66	110.58
3	C	1301	ADP	C4-C5-N7	-3.41	106.68	110.58
3	A	1301	ADP	C4-C5-N7	-3.41	106.69	110.58
3	B	1301	ADP	C4-C5-N7	-3.37	106.73	110.58
3	D	1301	ADP	C4-C5-N7	-3.33	106.78	110.58
3	B	1301	ADP	N3-C2-N1	-3.20	123.73	128.58
3	A	1301	ADP	N3-C2-N1	-3.16	123.80	128.58
3	D	1301	ADP	N3-C2-N1	-3.15	123.81	128.58
3	C	1301	ADP	N3-C2-N1	-3.12	123.85	128.58
4	B	1302	ATP	N3-C2-N1	-3.11	123.88	128.58
4	D	1302	ATP	N3-C2-N1	-3.09	123.91	128.58
3	D	1301	ADP	C4-N9-C8	2.80	108.68	105.74
3	B	1301	ADP	C4-N9-C8	2.78	108.65	105.74
3	A	1301	ADP	C4-N9-C8	2.58	108.45	105.74
3	C	1301	ADP	C4-N9-C8	2.56	108.42	105.74
4	B	1302	ATP	C4-N9-C8	2.54	108.40	105.74
4	D	1302	ATP	C5-N7-C8	2.53	107.43	103.45
4	B	1302	ATP	C5-N7-C8	2.52	107.41	103.45
3	B	1301	ADP	C5-N7-C8	2.47	107.33	103.45
4	D	1302	ATP	C4-N9-C8	2.46	108.32	105.74
3	D	1301	ADP	C5-N7-C8	2.46	107.32	103.45
3	C	1301	ADP	C5-N7-C8	2.45	107.30	103.45
3	A	1301	ADP	C5-N7-C8	2.41	107.24	103.45
4	D	1302	ATP	C3'-C2'-C1'	2.32	105.85	101.46
4	B	1302	ATP	C3'-C2'-C1'	2.30	105.81	101.46
3	A	1301	ADP	C3'-C2'-C1'	2.27	105.75	101.46
3	C	1301	ADP	C3'-C2'-C1'	2.27	105.75	101.46
3	B	1301	ADP	C2'-C1'-N9	-2.22	107.79	113.30
3	D	1301	ADP	C2'-C1'-N9	-2.12	108.03	113.30
3	D	1301	ADP	N9-C8-N7	-2.10	110.96	113.94
3	B	1301	ADP	C3'-C2'-C1'	2.10	105.43	101.46
3	B	1301	ADP	N9-C8-N7	-2.07	111.00	113.94
3	D	1301	ADP	C3'-C2'-C1'	2.03	105.31	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1302	ATP	C6-C5-N7	2.01	135.96	132.09
3	B	1301	ADP	C6-C5-N7	2.00	135.95	132.09
4	D	1302	ATP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	ADP	C5'-O5'-PA-O3A
3	C	1301	ADP	C5'-O5'-PA-O3A
4	B	1302	ATP	C5'-O5'-PA-O1A
4	D	1302	ATP	C5'-O5'-PA-O1A
3	A	1301	ADP	O4'-C4'-C5'-O5'
3	C	1301	ADP	O4'-C4'-C5'-O5'
3	C	1301	ADP	C3'-C4'-C5'-O5'
3	A	1301	ADP	C5'-O5'-PA-O1A
3	C	1301	ADP	C5'-O5'-PA-O1A
3	A	1301	ADP	C3'-C4'-C5'-O5'
3	B	1301	ADP	PA-O3A-PB-O2B

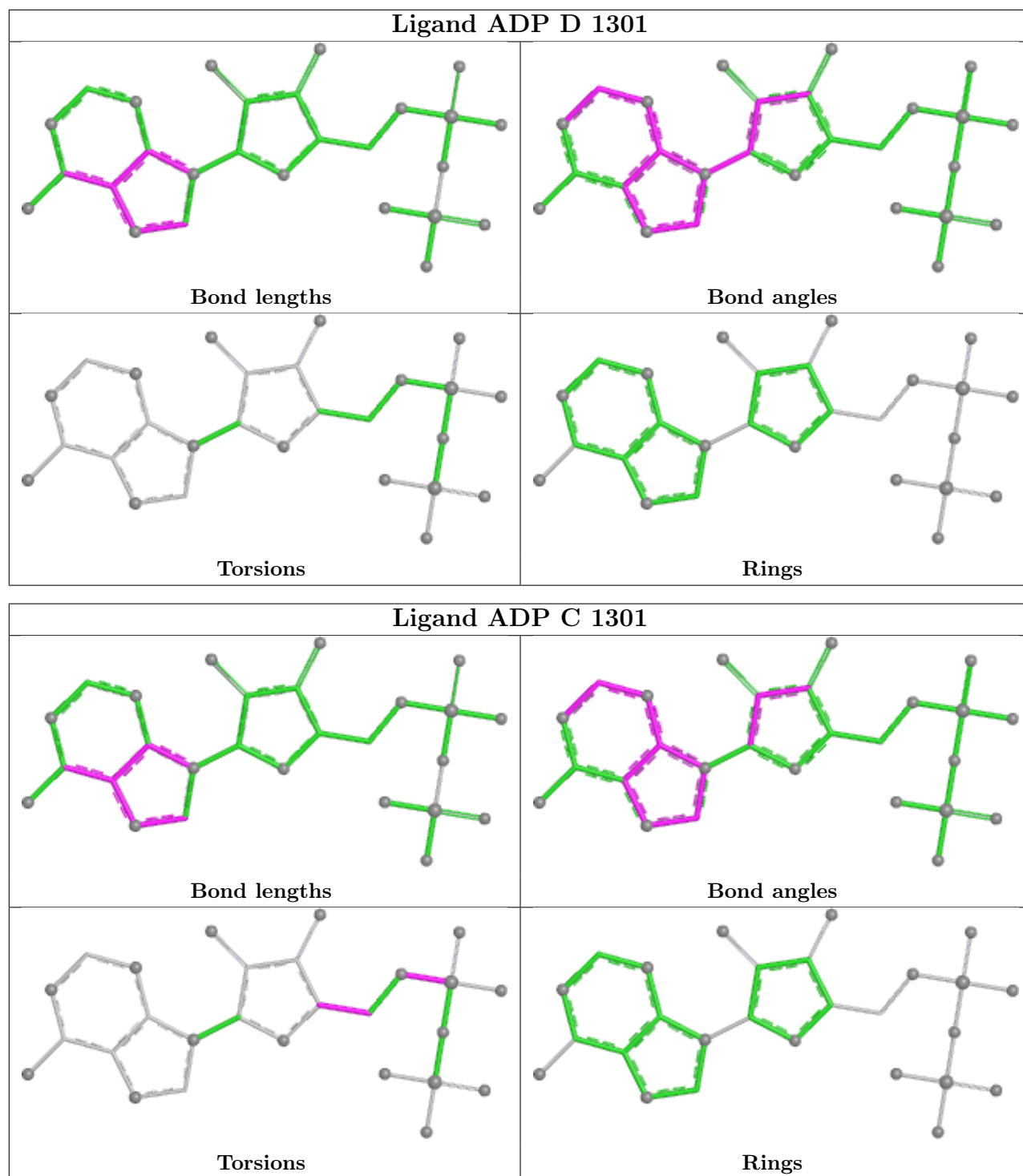
There are no ring outliers.

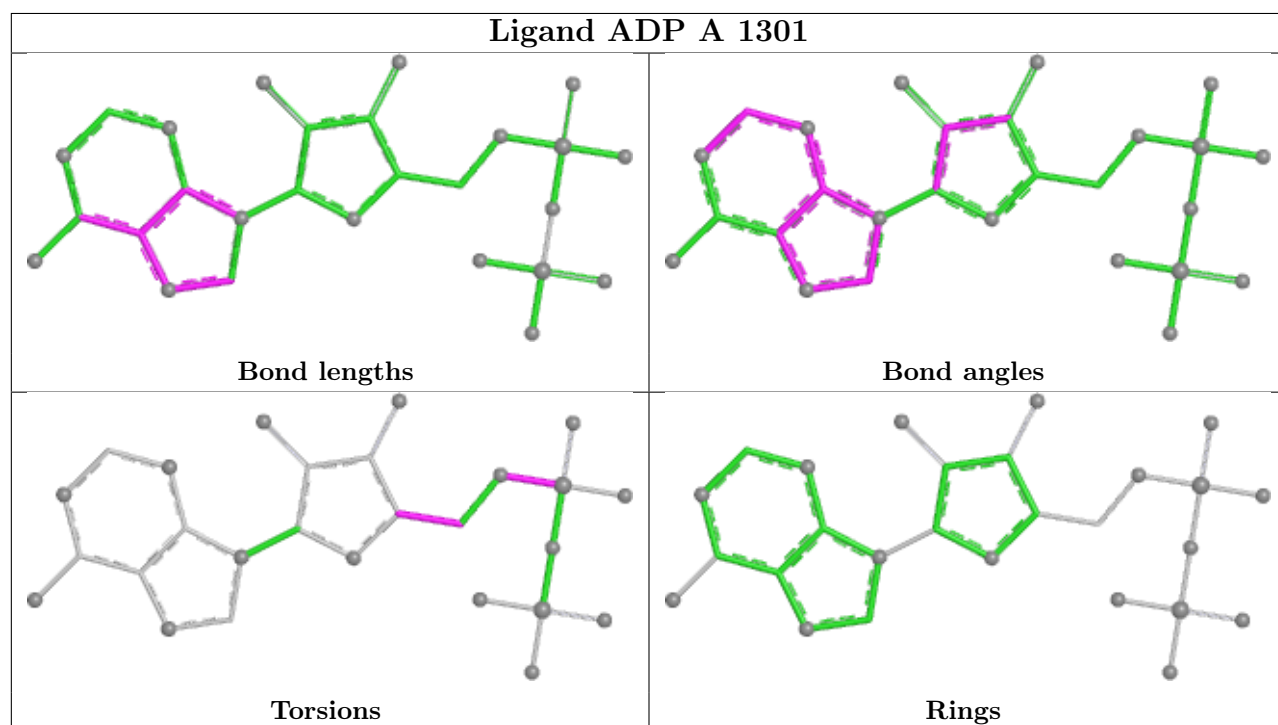
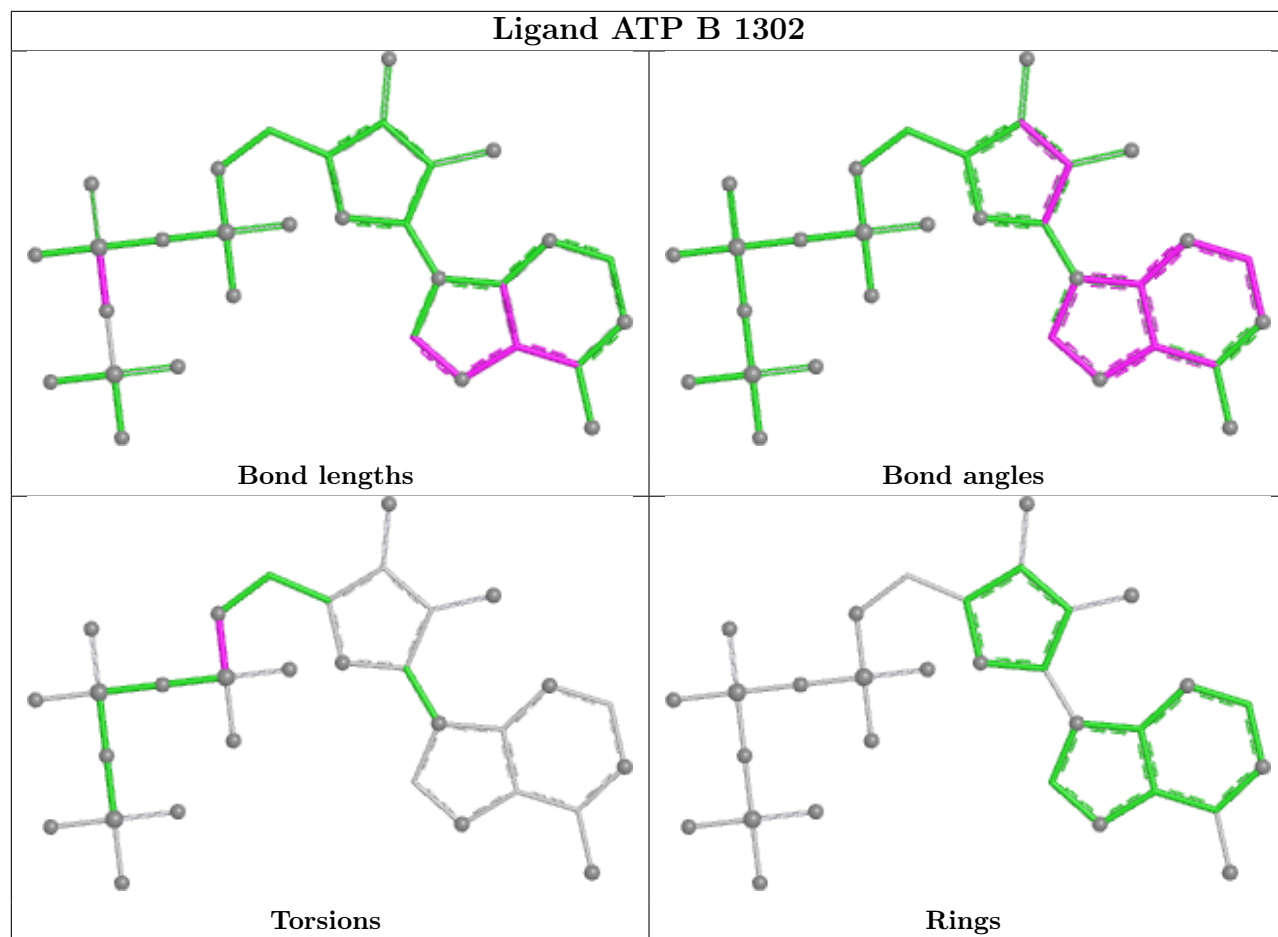
6 monomers are involved in 12 short contacts:

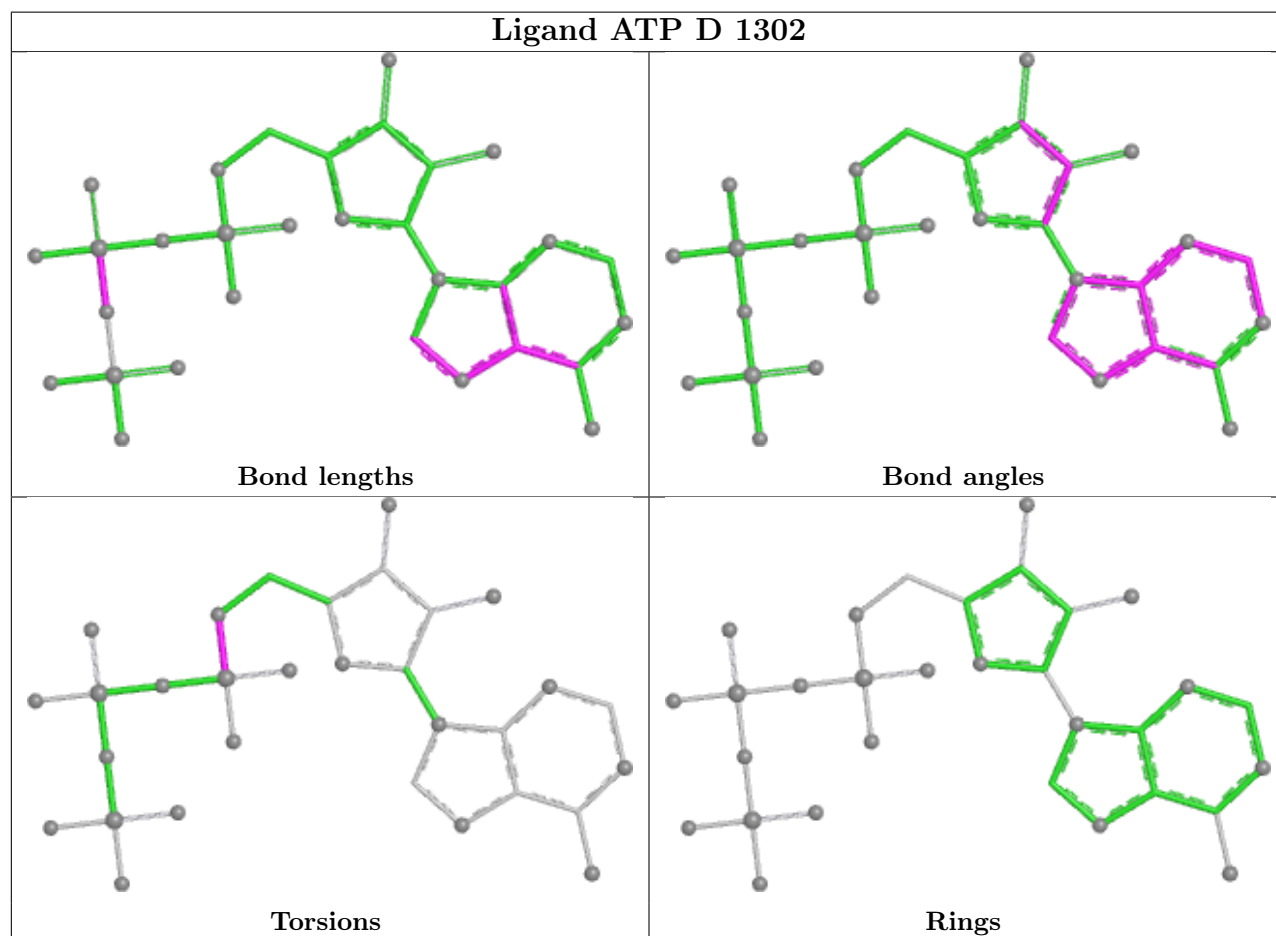
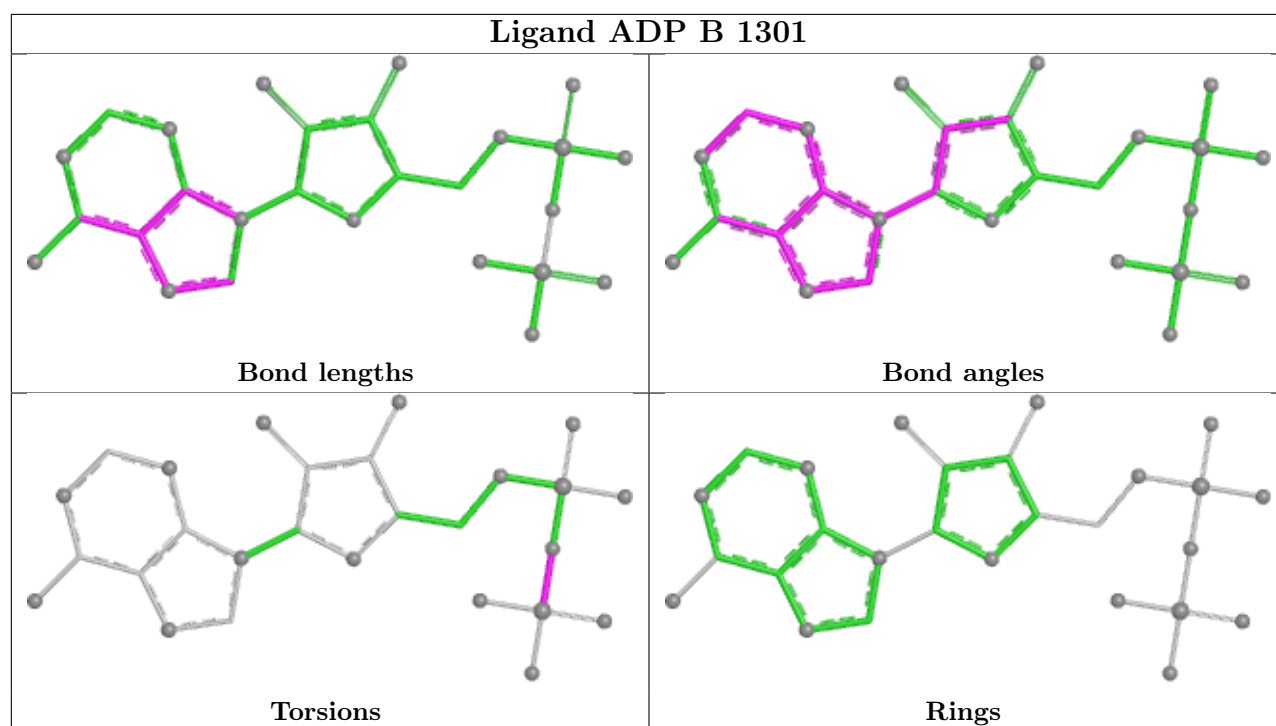
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1301	ADP	2	0
3	C	1301	ADP	3	0
4	B	1302	ATP	1	0
3	A	1301	ADP	3	0
3	B	1301	ADP	2	0
4	D	1302	ATP	1	0

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

equivalents in the CSD to analyse the geometry.







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

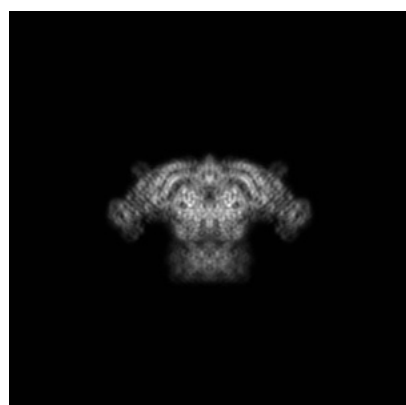
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30450. These allow visual inspection of the internal detail of the map and identification of artifacts.

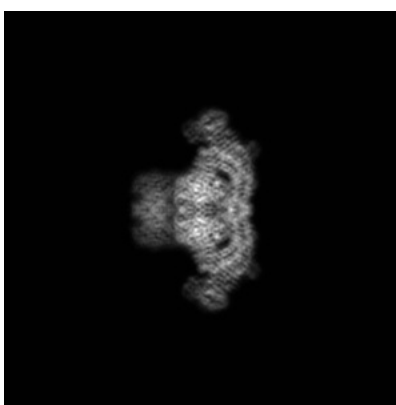
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

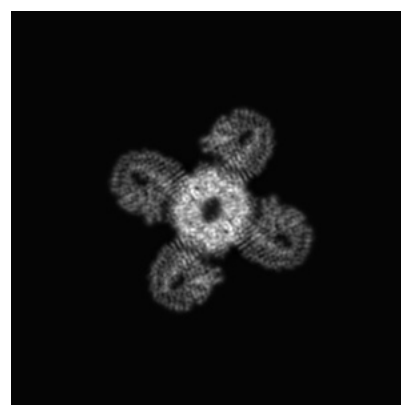
6.1.1 Primary map



X



Y



Z

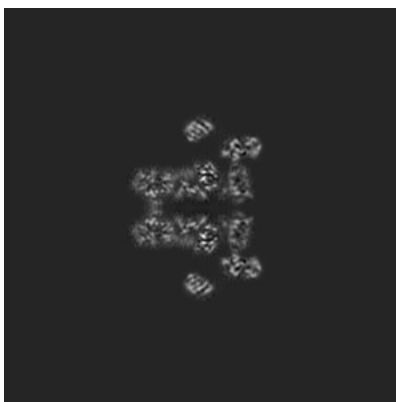
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

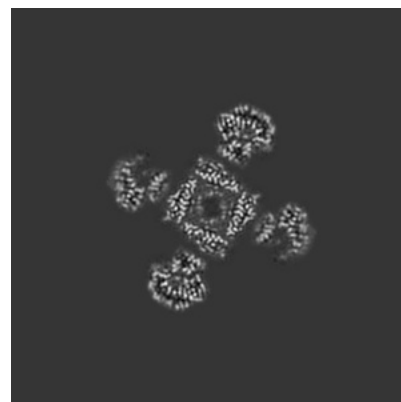
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

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

6.3 Largest variance slices [i](#)

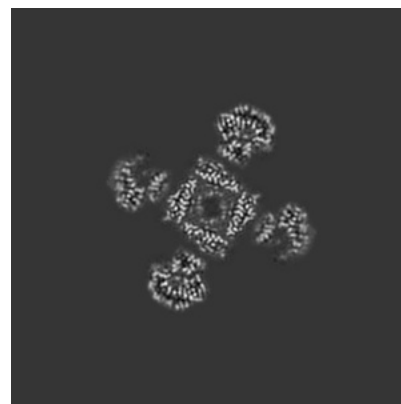
6.3.1 Primary map



X Index: 163



Y Index: 198

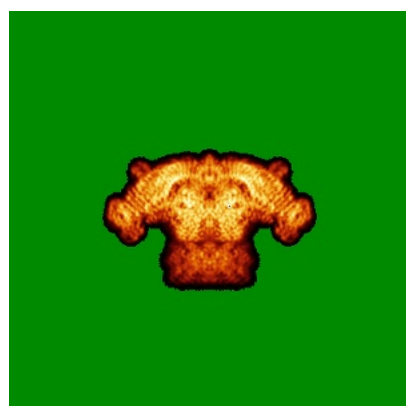


Z Index: 180

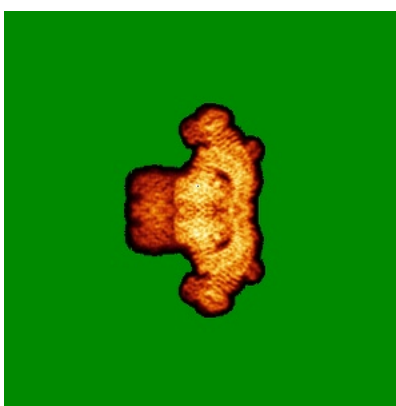
The images above show the largest variance slices of the map in three orthogonal directions.

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

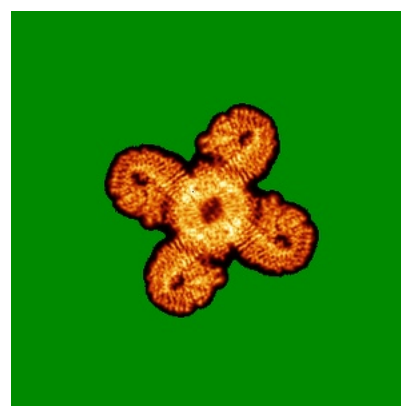
6.4.1 Primary map



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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

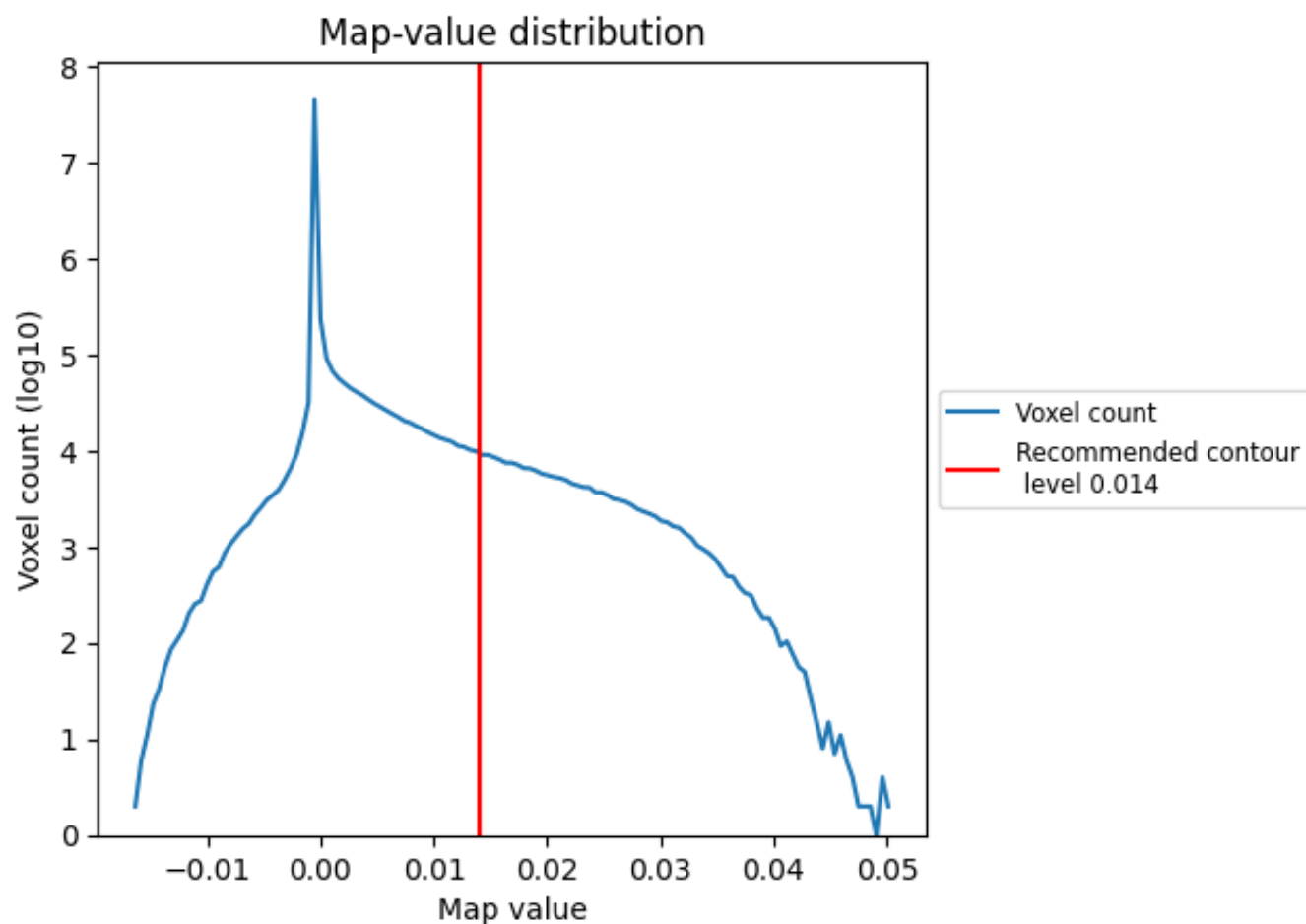
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

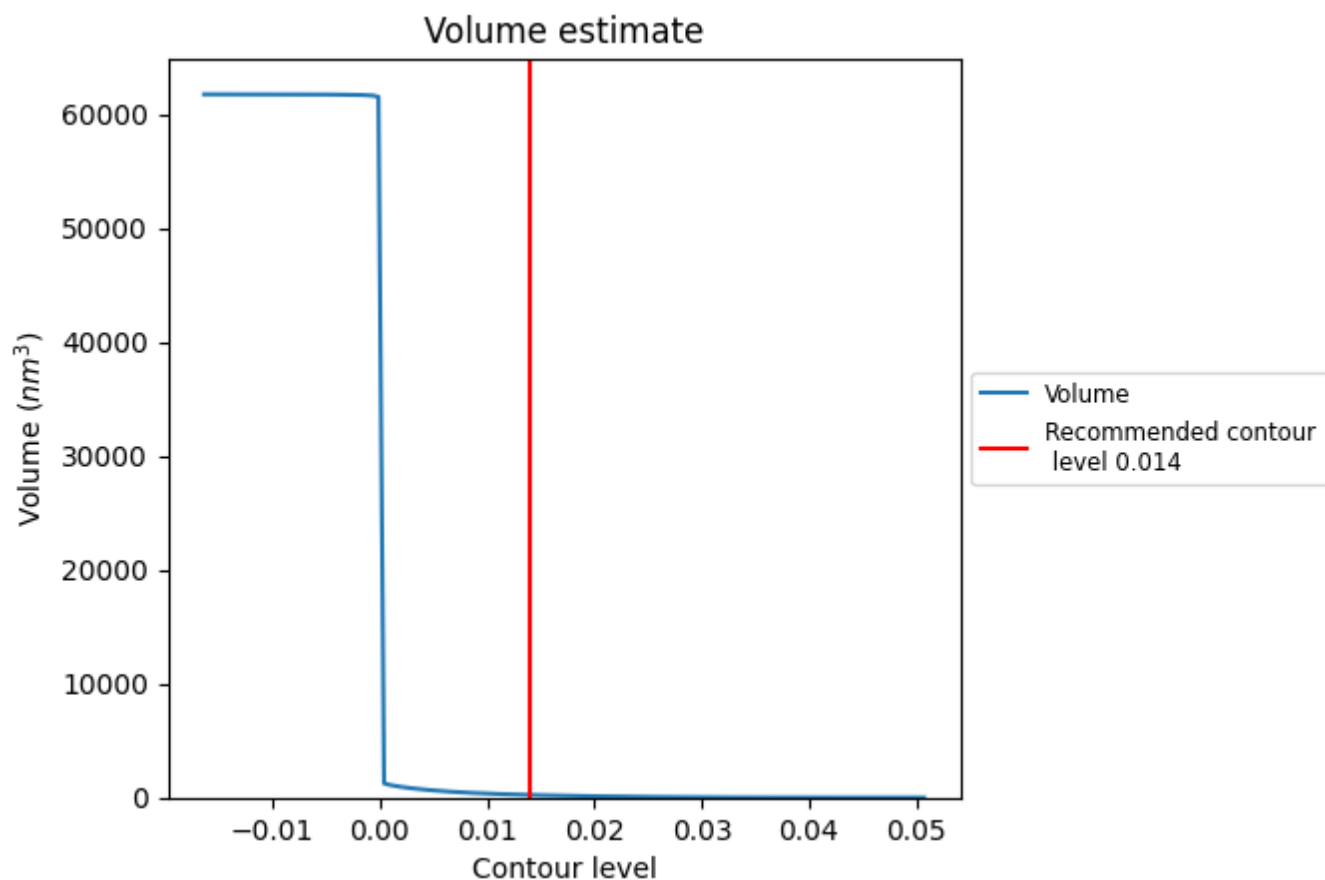
This section contains the results of statistical analysis of the map.

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.

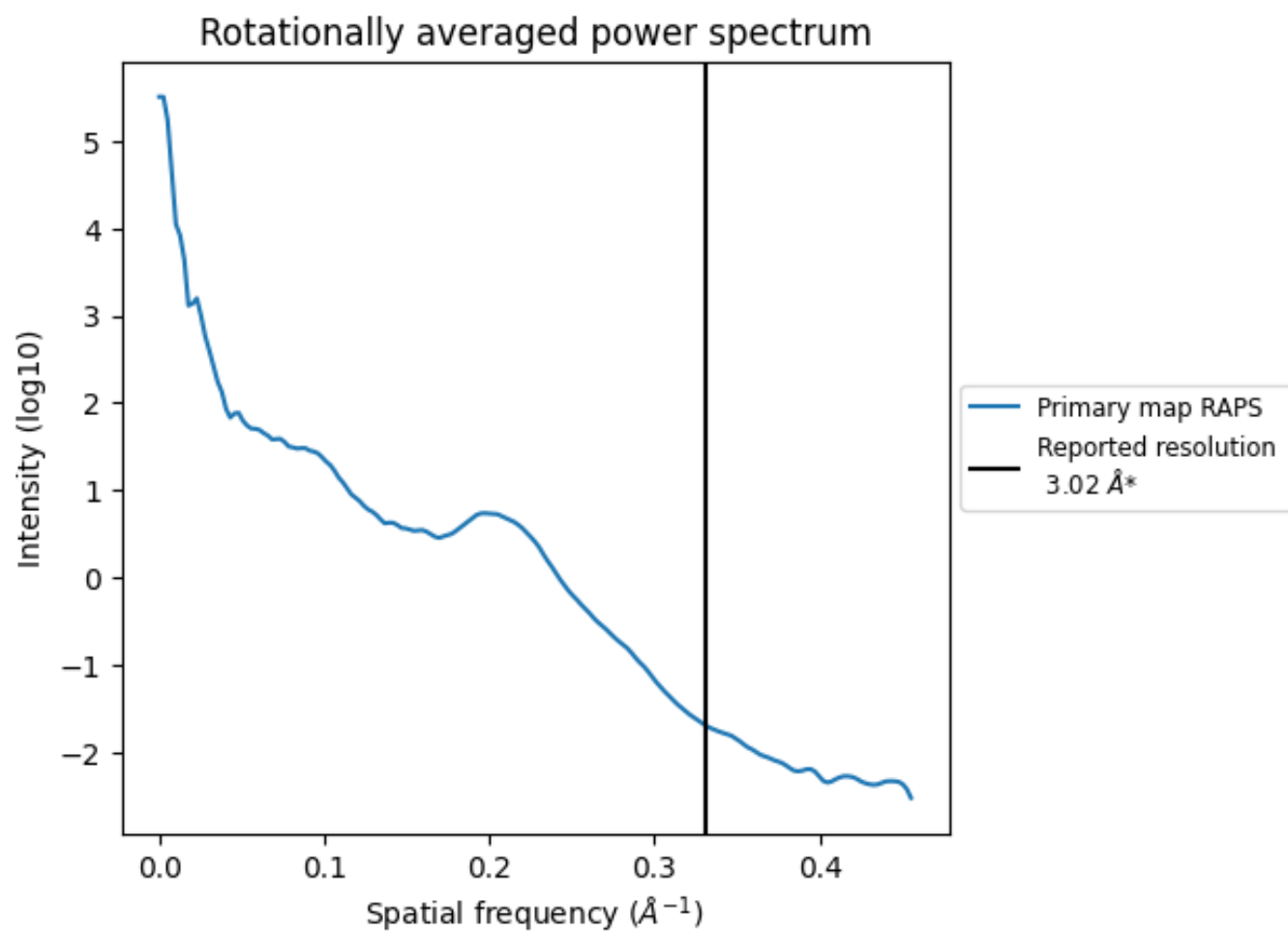
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm³; this corresponds to an approximate mass of 208 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 0.331 Å⁻¹

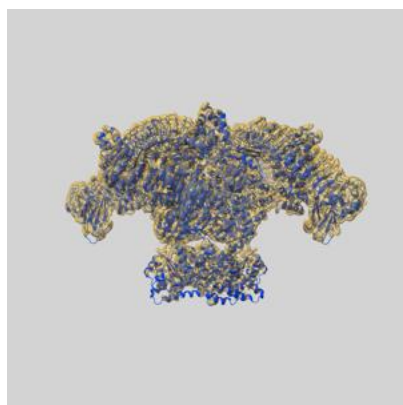
8 Fourier-Shell correlation

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

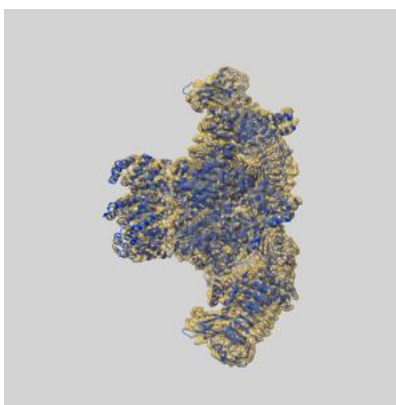
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30450 and PDB model 7CRC. Per-residue inclusion information can be found in section 3 on page 7.

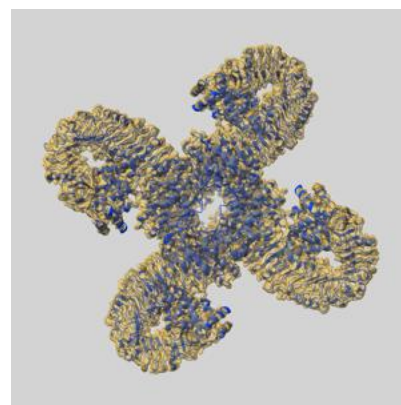
9.1 Map-model overlay [i](#)



X



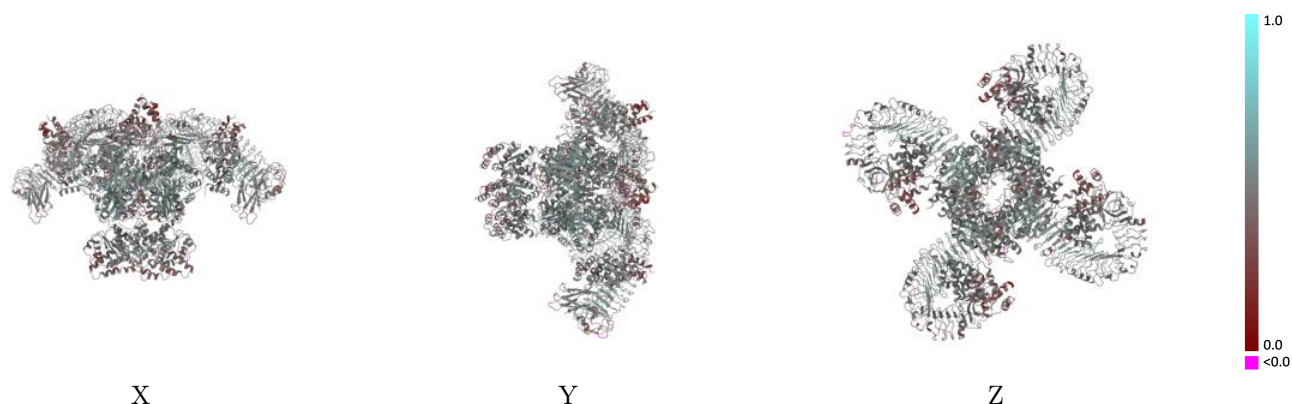
Y



Z

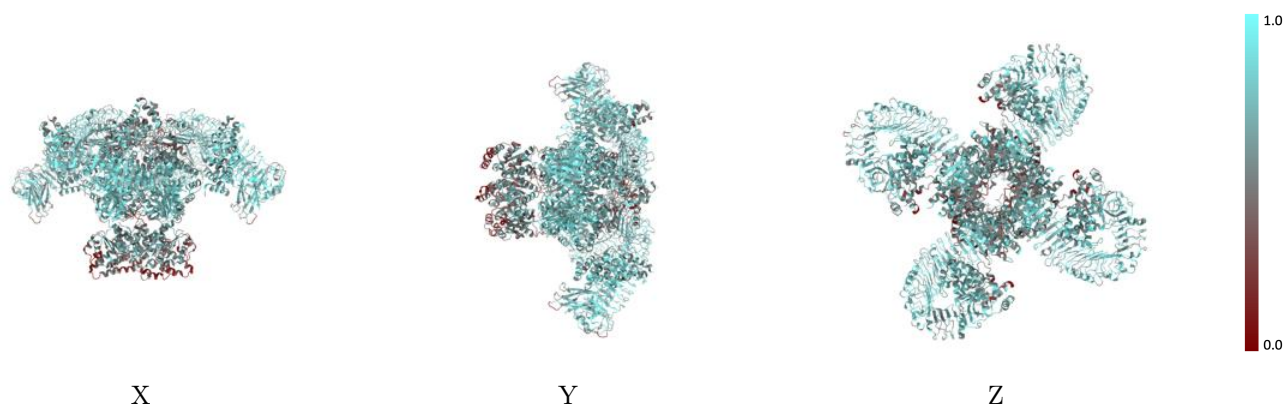
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



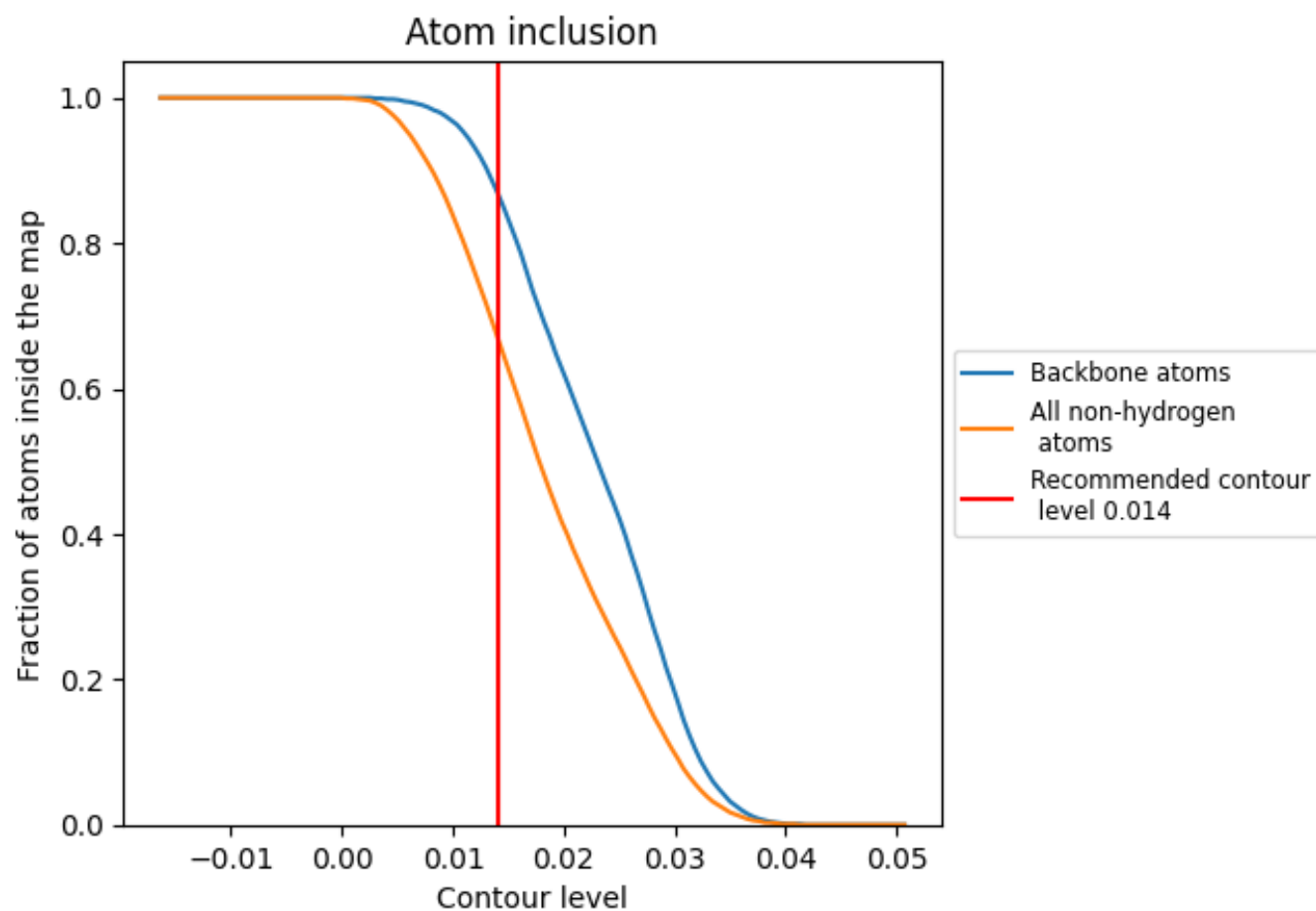
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 67% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6720	0.4690
A	0.6710	0.4680
B	0.6730	0.4810
C	0.6700	0.4680
D	0.6720	0.4810
E	0.6810	0.4420
F	0.6640	0.4380
G	0.6900	0.4440
H	0.6680	0.4390

1.0

0.0

<0.0