Full wwPDB EM Validation Report

Feb 28, 2023 – 02:36 PM JST

PDB ID	:	7YFN
EMDB ID	:	EMD-33794
Title	:	Core module of the NuA4 complex in S. cerevisiae
Authors	:	Ji, L.T.; Zhao, L.X.; Xu, K.; Gao, H.H.; Zhou, Y.; Kornberg, R.D.; Zhang, H.Q.
Deposited on	:	2022-07-08
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

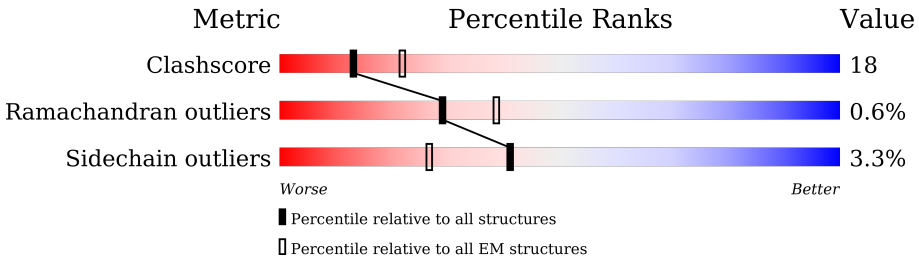
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	372	8% 65% 35%
2	B	489	60% 22% 18%
3	D	982	28% 18% 54%
4	E	476	25% 17% 58%
5	T	3744	32% 12% 55%
6	F	832	8% 6% 85%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26397 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 Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	372	2904	1841	491	553	19	0	0

- Molecule 2 is a protein called ARP4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	402	3172	2024	518	619	11	0	0

- Molecule 3 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	454	3777	2392	683	691	11	0	0

- Molecule 4 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	201	1668	1069	276	319	4	0	0

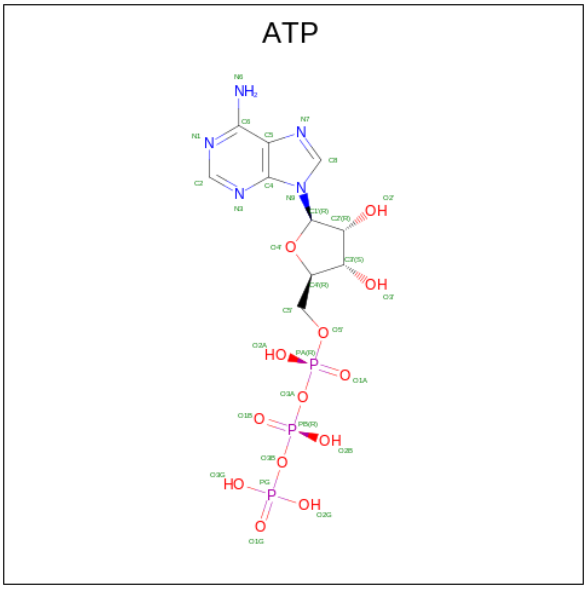
- Molecule 5 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	T	1688	13822	8905	2353	2512	52	0	0

- Molecule 6 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	124	1023	653	177	190	3	0	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



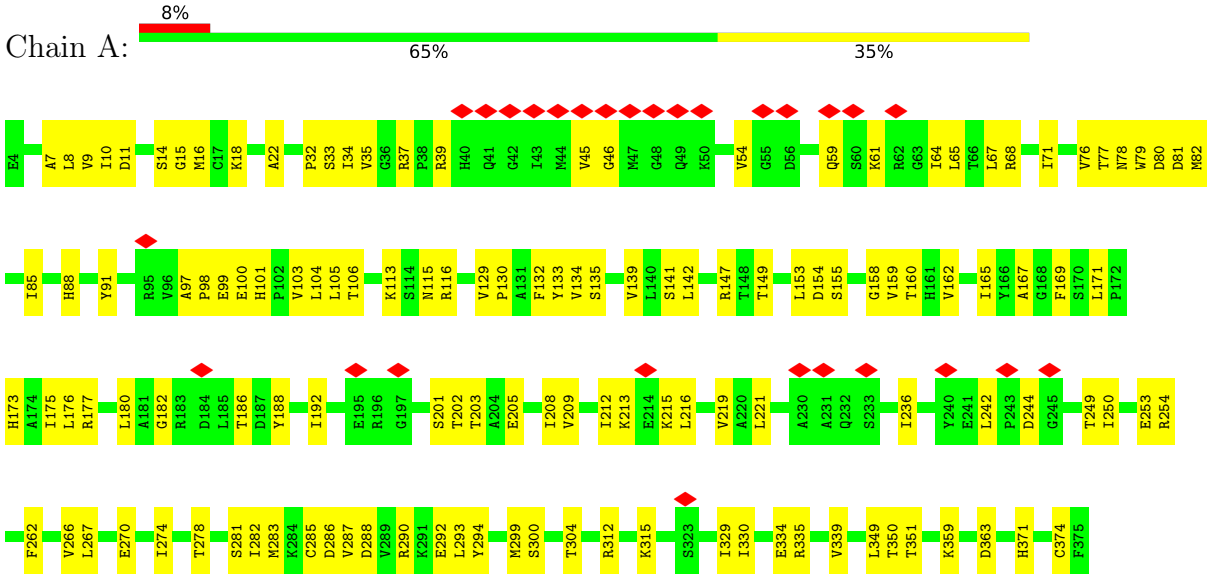
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	31	10	5	13	3	0

3 Residue-property plots (i)

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

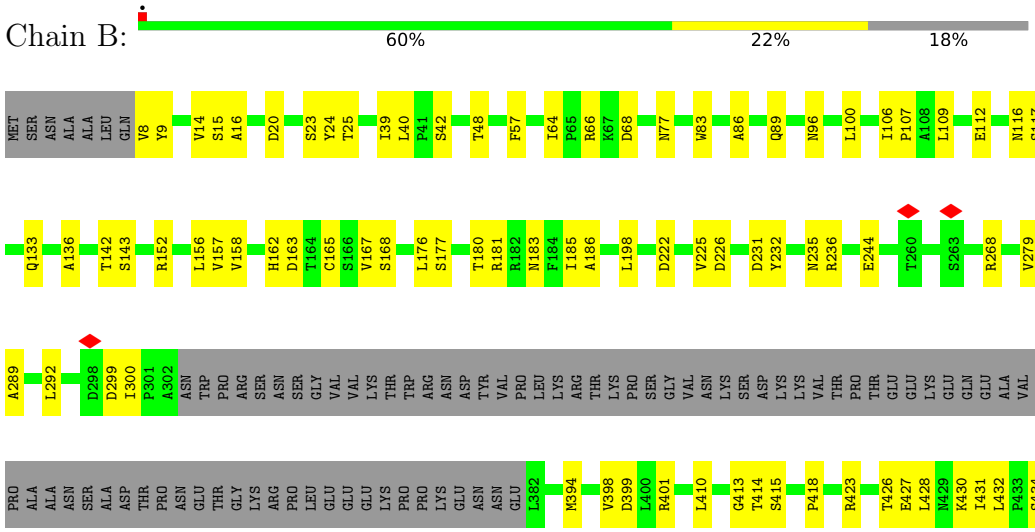
• Molecule 1: Actin

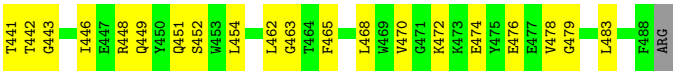
Chain A:



• Molecule 2: ARP4 isoform 1

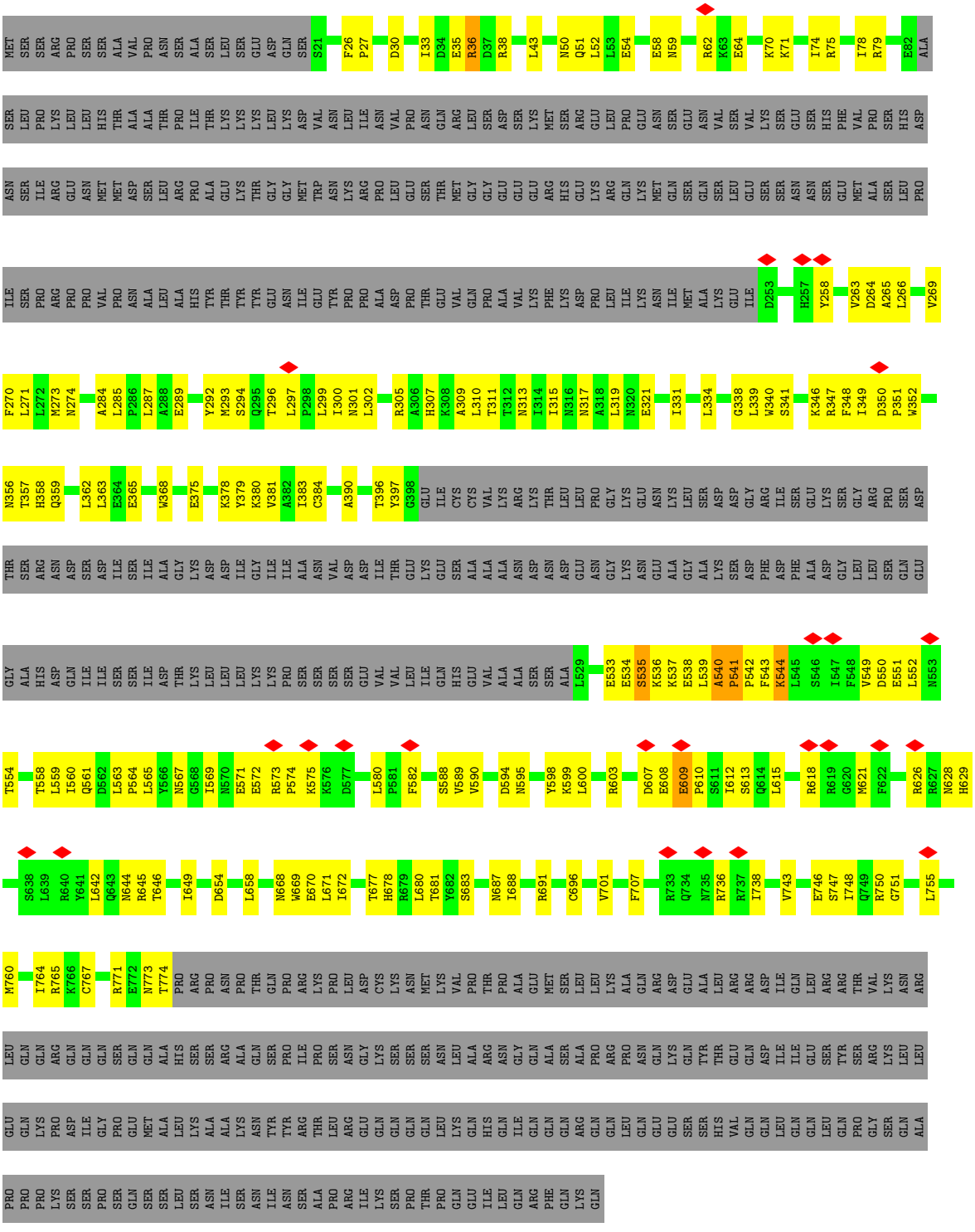
Chain B:





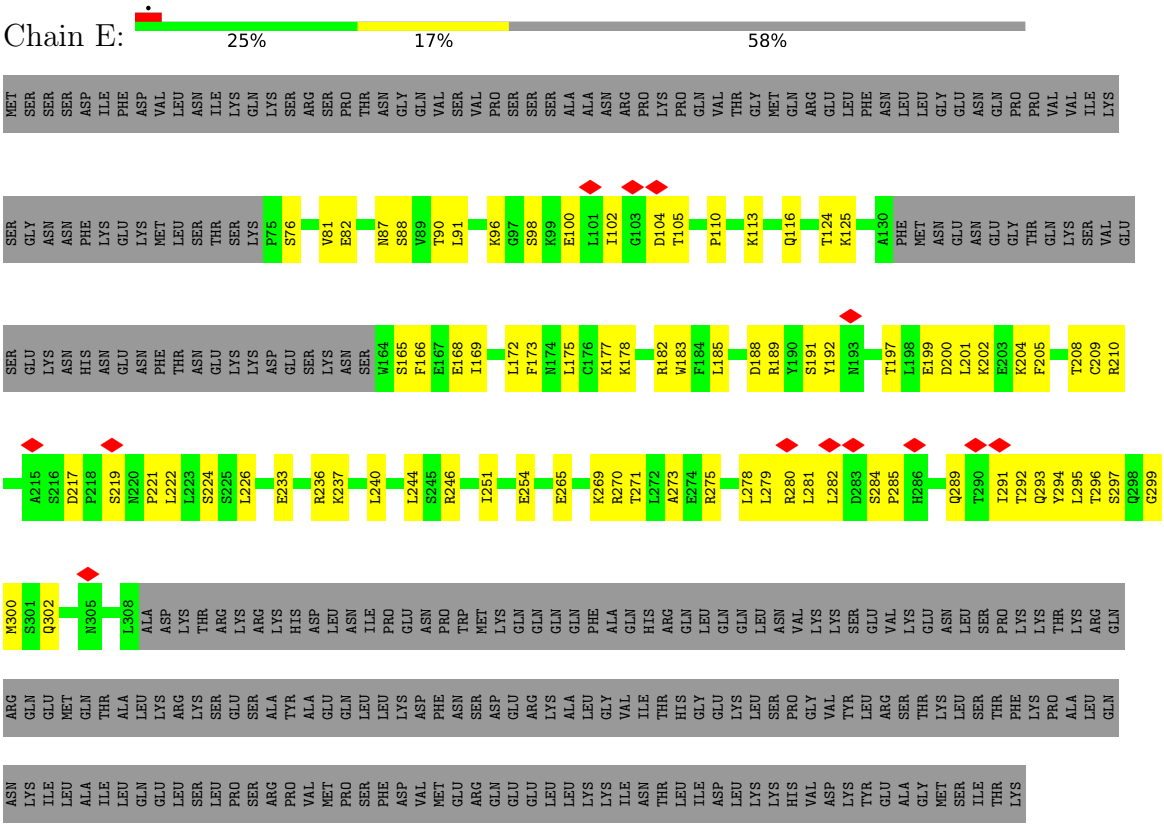
• Molecule 3: Chromatin modification-related protein EAF1

Chain D:



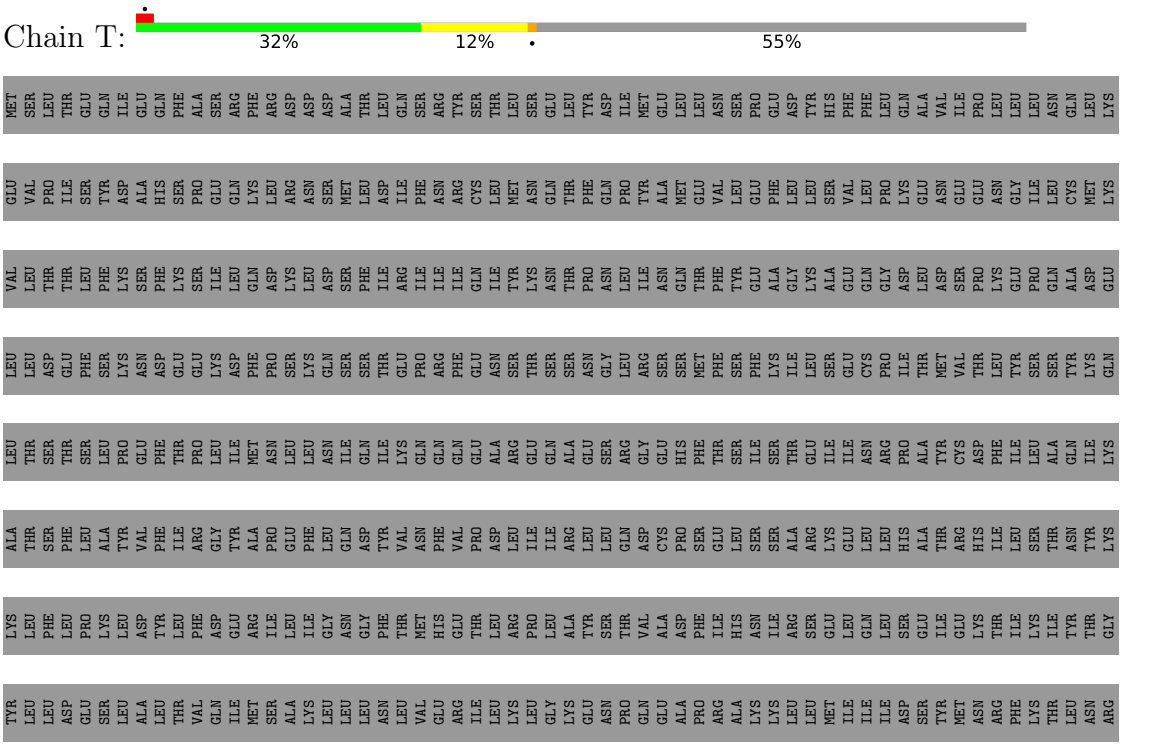
• Molecule 4: SWR1-complex protein 4

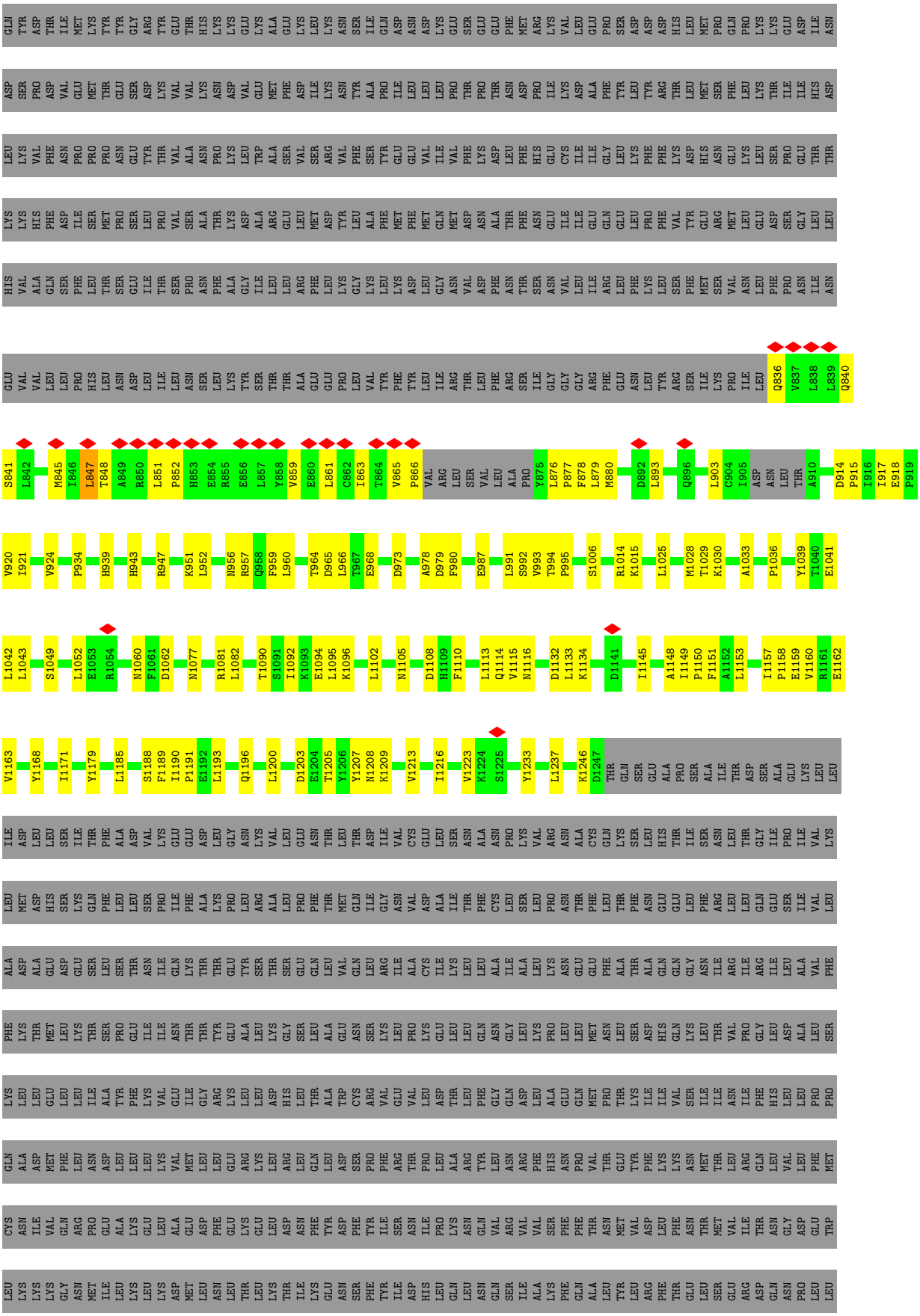
Chain E:

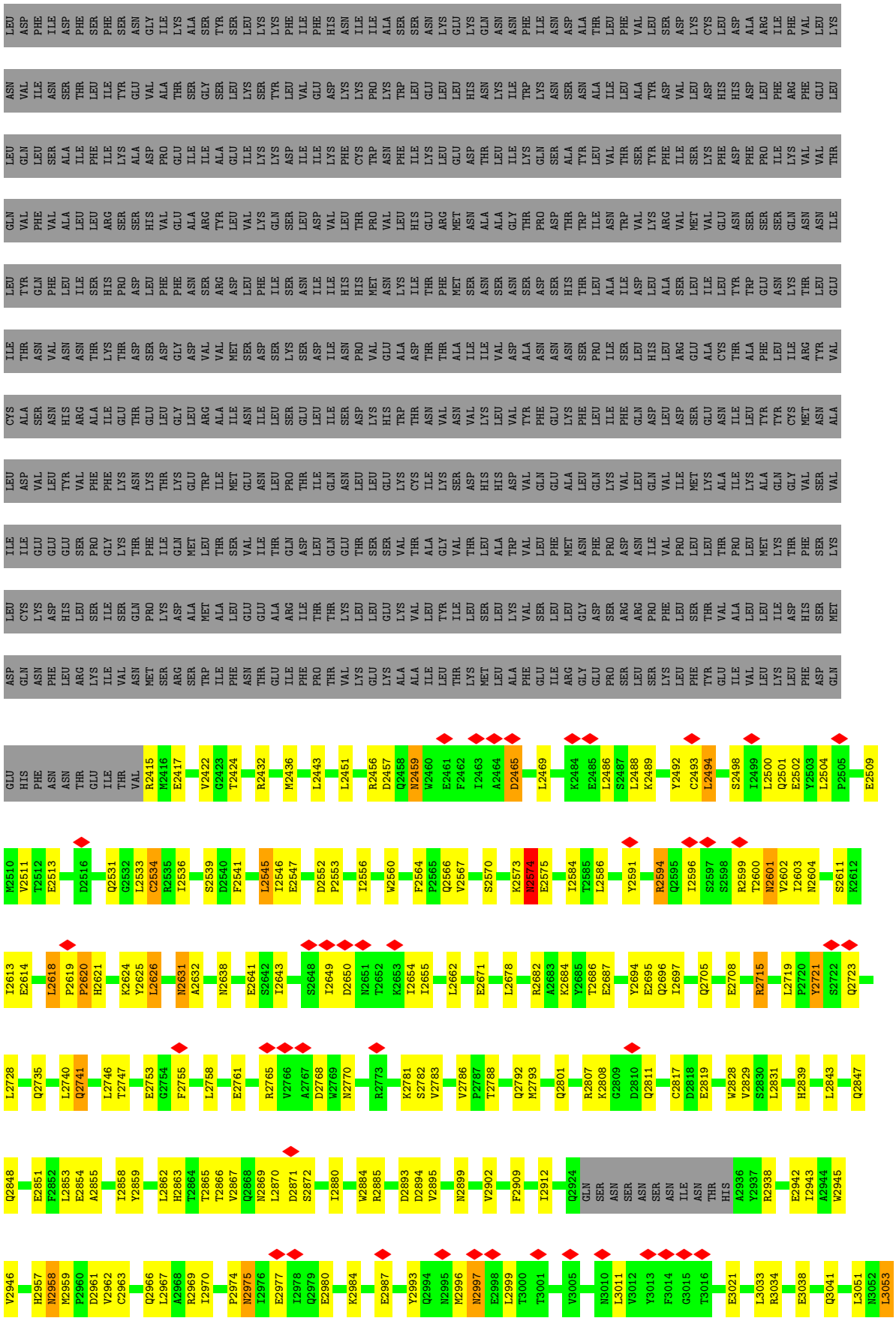


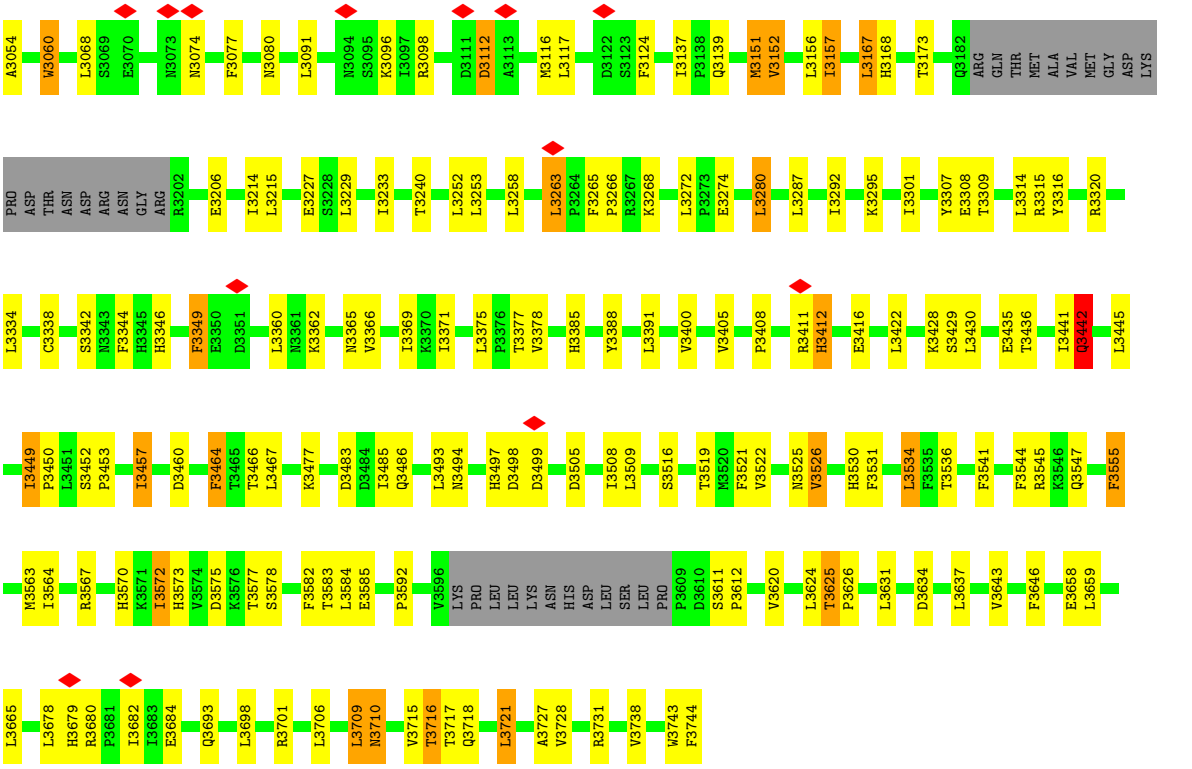
• Molecule 5: Transcription-associated protein 1

Chain T:



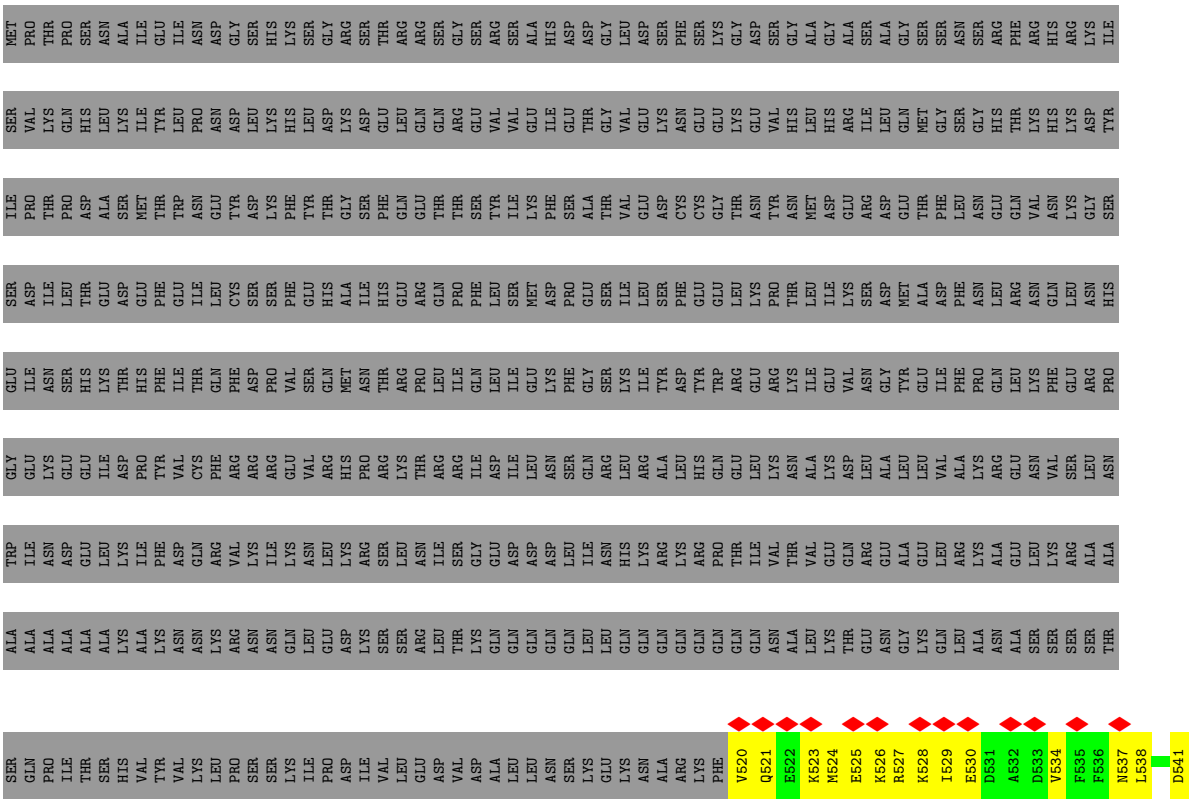


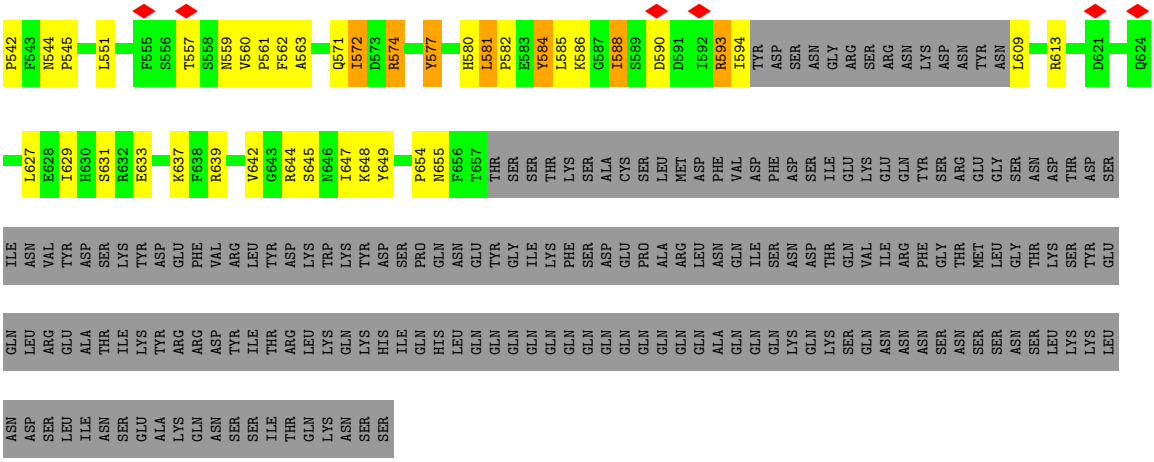




• Molecule 6: Enhancer of polycomb-like protein 1

Chain F:




P542 F543 N544 P545 L551 F555 S556 T557 S558 N559 V560 P561 F562 A563 Q571 I572 D573 R574 Y577 H580 L581 P582 E583 Y584 L585 K586 G587 I588 S589 D590 D591 I592 R593 I594 TYR ASP SER ASN GLY ARG SER ARG ASN LYS ASP ASN TYR ASN L609 R613 D621 Q624
L627 E628 I629 H630 S631 R632 E633 K637 F638 R639 V642 G643 R644 S645 N646 I647 K648 Y649 P654 N655 F656 T657 THR SER SER THR LYS SER ALA CYS SER LEU MET ASP PHE VAL ASP PHE ASP SER ILE GLU LYS GLU GLN TYR SER ARG GLU GLY SER ASN ASP THR ASP SER
ILE ASN VAL TYR ASP SER LYS TYR ASP GLU PHE VAL ARG LEU TYR ASP LYS TRP LYS TYR ASP SER PRO GLN ASN GLU TYR GLY ILE LYS PHE SER ASP GLU PRO ALA ARG LEU ASN GLN ILE SER ASN ASP THR GLN VAL ILE ARG PHE GLY THR MET LEU GLY THR LYS SER TYR GLU
GLN LEU ARG GLU ALA THR ILE LYS TYR ARG ARG ASP TYR ILE THR ARG LEU LYS GLN LYS HIS ILE GLN HIS LEU GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN ALA GLN GLN GLN ILE GLN LYS GLN LYS SER GLN ASN ASN SER ASN SER ASN SER LEU LYS LYS LEU
ASN ASP SER LEU ILE ASN SER GLU ALA LYS GLN ASN SER SER ILE THR GLN LYS ASN SER SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197044	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.233	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0396	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	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

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	0.28	0/2968	0.45	0/4017
2	B	0.30	0/3241	0.45	0/4398
3	D	0.29	0/3859	0.48	0/5212
4	E	0.29	0/1707	0.44	0/2300
5	T	0.55	2/14149 (0.0%)	0.72	7/19199 (0.0%)
6	F	0.40	0/1046	0.60	0/1405
All	All	0.45	2/26970 (0.0%)	0.61	7/36531 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	3
5	T	0	4
6	F	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	2620	PRO	N-CA	11.64	1.67	1.47
5	T	2619	PRO	C-N	6.06	1.45	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	2620	PRO	CA-N-CD	-13.99	91.91	111.50
5	T	2957	HIS	C-N-CA	5.81	136.22	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	2631	ASN	CB-CA-C	5.69	121.77	110.40
5	T	2958	ASN	CB-CA-C	5.44	121.27	110.40
5	T	2740	LEU	C-N-CA	5.30	134.95	121.70
5	T	2573	LYS	C-N-CA	5.03	134.27	121.70
5	T	3592	PRO	N-CA-CB	5.03	109.33	103.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	535	SER	Peptide
3	D	540	ALA	Peptide
3	D	609	GLU	Peptide
6	F	541	ASP	Peptide
5	T	2697	ILE	Mainchain
5	T	3112	ASP	Peptide
5	T	3442	GLN	Mainchain
5	T	847	LEU	Peptide

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	2904	0	2874	99	0
2	B	3172	0	3125	81	0
3	D	3777	0	3763	250	0
4	E	1668	0	1630	88	0
5	T	13822	0	13785	472	0
6	F	1023	0	998	109	0
7	B	31	0	12	1	0
All	All	26397	0	26187	964	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 18.

All (964) 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)
3:D:269:VAL:CG2	6:F:588:ILE:HG21	1.23	1.67
6:F:582:PRO:CG	6:F:584:TYR:CE1	1.75	1.62
6:F:582:PRO:HG2	6:F:584:TYR:CE1	1.00	1.53
3:D:269:VAL:CG2	6:F:588:ILE:CG2	1.79	1.40
3:D:269:VAL:HG23	6:F:588:ILE:CG2	0.92	1.40
6:F:582:PRO:HG2	6:F:584:TYR:CD1	1.58	1.35
3:D:621:MET:HG2	5:T:2417:GLU:OE2	1.18	1.35
6:F:582:PRO:CG	6:F:584:TYR:HE1	1.21	1.31
5:T:2765:ARG:HD3	5:T:2969:ARG:NH1	1.52	1.24
5:T:2604:ASN:OD1	5:T:2632:ALA:HB2	1.35	1.23
5:T:2696:GLN:NE2	5:T:3643:VAL:HG21	1.57	1.19
5:T:3315:ARG:NE	5:T:3483:ASP:OD2	1.75	1.19
3:D:687:ASN:ND2	5:T:2755:PHE:CE2	2.12	1.17
3:D:269:VAL:CG2	6:F:588:ILE:HG23	1.71	1.11
6:F:593:ARG:HB3	6:F:593:ARG:HH21	1.13	1.10
3:D:565:LEU:CG	6:F:585:LEU:HD13	1.85	1.05
3:D:621:MET:CG	5:T:2417:GLU:OE2	2.05	1.03
5:T:3315:ARG:CD	5:T:3483:ASP:OD2	2.06	1.03
6:F:581:LEU:HD11	6:F:613:ARG:HG2	1.04	1.02
6:F:582:PRO:CB	6:F:584:TYR:HE1	1.71	1.02
3:D:687:ASN:CG	5:T:2755:PHE:CE2	2.34	1.01
3:D:35:GLU:OE1	5:T:3731:ARG:NH2	1.93	1.01
3:D:269:VAL:HG23	6:F:588:ILE:HG23	1.23	0.99
5:T:3315:ARG:CZ	5:T:3483:ASP:OD2	2.10	0.99
6:F:582:PRO:HG3	6:F:584:TYR:CE1	1.93	0.99
3:D:565:LEU:HG	6:F:585:LEU:HD13	1.44	0.99
3:D:687:ASN:ND2	5:T:2755:PHE:HE2	1.58	0.97
4:E:282:LEU:HD22	5:T:2686:THR:CG2	1.94	0.96
3:D:269:VAL:CB	6:F:588:ILE:HG21	1.97	0.95
5:T:2765:ARG:HD3	5:T:2969:ARG:HH11	1.07	0.95
3:D:565:LEU:HD21	6:F:585:LEU:CD1	1.96	0.95
3:D:565:LEU:HD21	6:F:585:LEU:HD12	1.47	0.95
3:D:535:SER:O	3:D:536:LYS:HG2	1.67	0.95
5:T:2599:ARG:HA	5:T:2631:ASN:HD22	1.32	0.92
6:F:593:ARG:HB3	6:F:593:ARG:NH2	1.85	0.92
5:T:2741:GLN:OE1	5:T:2899:ASN:ND2	2.03	0.92
3:D:51:GLN:NE2	3:D:54:GLU:OE2	2.02	0.91
3:D:302:LEU:HD21	4:E:279:LEU:HB3	1.51	0.91
5:T:1006:SER:O	5:T:1014:ARG:NH1	2.04	0.91
1:A:221:LEU:O	1:A:315:LYS:NZ	2.03	0.91
2:B:20:ASP:OD2	2:B:452:SER:OG	1.89	0.91
5:T:2604:ASN:OD1	5:T:2632:ALA:CB	2.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:588:ILE:HD12	6:F:593:ARG:HD3	1.51	0.90
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.05	0.89
3:D:269:VAL:HG23	6:F:588:ILE:CB	2.02	0.89
3:D:687:ASN:CB	5:T:2755:PHE:CE2	2.55	0.89
6:F:581:LEU:CD1	6:F:613:ARG:HG2	2.00	0.89
5:T:2599:ARG:HA	5:T:2631:ASN:ND2	1.86	0.89
5:T:1033:ALA:HB2	5:T:2534:CYS:SG	2.13	0.88
5:T:2885:ARG:NH1	5:T:2945:TRP:CD1	2.42	0.88
5:T:3385:HIS:NE2	5:T:3570:HIS:CE1	2.43	0.87
3:D:269:VAL:CB	6:F:588:ILE:CG2	2.50	0.87
3:D:341:SER:OG	4:E:254:GLU:OE2	1.92	0.87
5:T:3315:ARG:HD3	5:T:3483:ASP:OD2	1.71	0.87
5:T:3534:LEU:HD12	5:T:3534:LEU:O	1.76	0.86
5:T:3266:PRO:HB3	5:T:3498:ASP:HB3	1.58	0.86
5:T:2604:ASN:CG	5:T:2632:ALA:HB2	1.95	0.86
3:D:294:SER:OG	3:D:321:GLU:OE2	1.93	0.85
3:D:563:LEU:HG	3:D:564:PRO:HD3	1.57	0.85
5:T:1246:LYS:HB3	5:T:3346:HIS:NE2	1.91	0.85
4:E:110:PRO:O	4:E:113:LYS:NZ	2.09	0.85
3:D:269:VAL:HA	6:F:588:ILE:HG22	1.59	0.85
3:D:629:HIS:CE1	5:T:2591:TYR:HB3	2.12	0.85
3:D:270:PHE:N	6:F:588:ILE:HG23	1.90	0.85
3:D:615:LEU:HG	5:T:2456:ARG:HH21	1.42	0.84
6:F:633:GLU:OE2	6:F:655:ASN:ND2	2.11	0.84
6:F:637:LYS:NZ	6:F:654:PRO:O	2.11	0.83
4:E:221:PRO:O	4:E:224:SER:OG	1.97	0.83
3:D:269:VAL:HG21	6:F:588:ILE:HD13	1.61	0.82
5:T:2999:LEU:O	5:T:2999:LEU:HD23	1.80	0.82
5:T:2859:TYR:O	5:T:2863:HIS:ND1	2.13	0.82
3:D:687:ASN:HB2	5:T:2755:PHE:CD2	2.16	0.81
5:T:2885:ARG:NH1	5:T:2945:TRP:CG	2.48	0.81
1:A:363:ASP:O	4:E:96:LYS:NZ	2.13	0.81
2:B:472:LYS:NZ	2:B:476:GLU:OE1	2.14	0.81
5:T:957:ARG:NH2	5:T:2893:ASP:OD2	2.13	0.81
6:F:586:LYS:HE2	6:F:588:ILE:HD11	1.63	0.80
5:T:917:ILE:HG23	5:T:921:ILE:HD11	1.61	0.80
3:D:35:GLU:CD	5:T:3731:ARG:NH2	2.33	0.80
1:A:304:THR:O	1:A:335:ARG:NH1	2.15	0.80
4:E:98:SER:OG	4:E:100:GLU:OE1	2.00	0.80
4:E:281:LEU:HD13	5:T:2684:LYS:C	2.03	0.79
3:D:629:HIS:ND1	5:T:2591:TYR:HB3	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:2869:ASN:O	5:T:2872:SER:OG	2.01	0.79
3:D:565:LEU:CD2	6:F:585:LEU:CD1	2.60	0.79
5:T:2765:ARG:CD	5:T:2969:ARG:HH11	1.92	0.79
5:T:3215:LEU:HD12	5:T:3215:LEU:O	1.83	0.79
3:D:379:TYR:CG	3:D:534:GLU:HG2	2.18	0.79
3:D:269:VAL:HG22	6:F:588:ILE:HG23	1.64	0.79
5:T:993:VAL:CG2	5:T:2541:PHE:CE2	2.66	0.79
5:T:3167:LEU:HD12	5:T:3167:LEU:O	1.84	0.78
6:F:537:ASN:O	6:F:538:LEU:HG	1.84	0.78
3:D:269:VAL:CA	6:F:588:ILE:CG2	2.61	0.77
3:D:565:LEU:CD1	6:F:585:LEU:HD13	2.14	0.77
5:T:1042:LEU:HD23	5:T:2501:GLN:CB	2.15	0.77
4:E:281:LEU:HD22	5:T:2684:LYS:O	1.83	0.77
4:E:233:GLU:OE2	4:E:236:ARG:NH2	2.18	0.76
5:T:1171:ILE:HD11	5:T:1189:PHE:CZ	2.19	0.76
3:D:565:LEU:CD2	6:F:585:LEU:HD12	2.16	0.76
3:D:35:GLU:CD	5:T:3731:ARG:CZ	2.53	0.76
3:D:549:VAL:HG23	3:D:550:ASP:H	1.50	0.76
5:T:964:THR:HA	5:T:3578:SER:OG	1.87	0.75
3:D:537:LYS:HG3	3:D:538:GLU:HG3	1.68	0.75
3:D:269:VAL:CG2	6:F:588:ILE:HD13	2.16	0.75
3:D:536:LYS:HB2	3:D:539:LEU:HG	1.68	0.75
5:T:1028:MET:O	5:T:2493:CYS:SG	2.45	0.75
1:A:169:PHE:HZ	3:D:381:VAL:HG22	1.51	0.74
1:A:334:GLU:OE1	1:A:334:GLU:N	2.19	0.74
5:T:2696:GLN:NE2	5:T:3643:VAL:CG2	2.46	0.74
5:T:3096:LYS:HE2	5:T:3096:LYS:HA	1.70	0.74
3:D:302:LEU:CD2	4:E:279:LEU:HB3	2.18	0.74
5:T:993:VAL:HG22	5:T:2541:PHE:CE2	2.23	0.73
5:T:2765:ARG:CD	5:T:2969:ARG:NH1	2.43	0.73
6:F:581:LEU:HD11	6:F:613:ARG:CG	2.01	0.73
3:D:540:ALA:O	3:D:542:PRO:HD3	1.88	0.73
5:T:2545:LEU:HD12	5:T:2545:LEU:O	1.89	0.72
5:T:2626:LEU:HG	5:T:2626:LEU:O	1.88	0.72
2:B:474:GLU:OE2	4:E:88:SER:OG	2.07	0.72
5:T:2586:LEU:O	5:T:2586:LEU:HD12	1.90	0.72
5:T:2894:ASP:OD1	5:T:2895:VAL:N	2.22	0.72
5:T:3151:MET:SD	5:T:3151:MET:N	2.56	0.72
5:T:3449:ILE:N	5:T:3449:ILE:HD12	2.05	0.72
1:A:35:VAL:HG21	1:A:81:ASP:HB3	1.72	0.72
3:D:550:ASP:O	3:D:552:LEU:HG	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:551:GLU:O	3:D:551:GLU:HG3	1.90	0.71
5:T:3429:SER:OG	5:T:3658:GLU:OE2	2.06	0.71
3:D:618:ARG:HG3	5:T:2457:ASP:OD2	1.90	0.71
3:D:607:ASP:O	3:D:609:GLU:HG2	1.91	0.71
1:A:177:ARG:NH2	2:B:96:ASN:O	2.23	0.70
1:A:192:ILE:HD12	1:A:253:GLU:HG3	1.73	0.70
4:E:217:ASP:OD1	4:E:219:SER:OG	2.08	0.70
5:T:3051:LEU:O	5:T:3051:LEU:HD23	1.92	0.70
3:D:567:ASN:ND2	3:D:598:TYR:OH	2.23	0.70
5:T:956:ASN:ND2	5:T:2843:LEU:HD13	2.06	0.70
5:T:978:ALA:HB2	5:T:2488:LEU:HD23	1.73	0.70
3:D:269:VAL:HA	6:F:588:ILE:CG2	2.21	0.70
3:D:536:LYS:HG3	3:D:539:LEU:HD21	1.73	0.70
3:D:565:LEU:HG	6:F:585:LEU:CD1	2.22	0.70
5:T:1216:ILE:HD11	5:T:1237:LEU:HG	1.74	0.69
5:T:3659:LEU:HD23	5:T:3659:LEU:O	1.92	0.69
3:D:378:LYS:NZ	3:D:536:LYS:O	2.20	0.69
3:D:565:LEU:CG	6:F:585:LEU:CD1	2.67	0.69
6:F:582:PRO:CG	6:F:584:TYR:CZ	2.68	0.69
5:T:1042:LEU:HD21	5:T:2501:GLN:O	1.93	0.69
5:T:993:VAL:HG22	5:T:2541:PHE:HE2	1.57	0.69
3:D:540:ALA:O	3:D:542:PRO:CD	2.40	0.69
5:T:3706:LEU:C	5:T:3706:LEU:HD12	2.13	0.69
2:B:64:ILE:O	2:B:66:ARG:NH1	2.26	0.69
3:D:670:GLU:N	3:D:670:GLU:OE1	2.26	0.69
5:T:993:VAL:HG23	5:T:2541:PHE:CE2	2.28	0.69
4:E:281:LEU:HD22	5:T:2684:LYS:CG	2.23	0.69
5:T:979:ASP:OD2	5:T:2489:LYS:HE3	1.92	0.69
5:T:1042:LEU:CD2	5:T:2501:GLN:CB	2.72	0.68
4:E:282:LEU:HD22	5:T:2686:THR:HG21	1.72	0.68
5:T:2758:LEU:O	5:T:2758:LEU:HD23	1.94	0.68
5:T:3422:LEU:C	5:T:3422:LEU:HD23	2.14	0.68
5:T:3274:GLU:N	5:T:3274:GLU:OE1	2.26	0.68
3:D:572:GLU:HB3	3:D:574:PRO:HD3	1.74	0.68
4:E:289:GLN:NE2	4:E:291:ILE:O	2.25	0.68
3:D:301:ASN:O	3:D:305:ARG:NH2	2.26	0.68
5:T:1203:ASP:O	5:T:1209:LYS:NZ	2.19	0.68
1:A:249:THR:O	1:A:250:ILE:HD13	1.95	0.67
4:E:269:LYS:O	4:E:270:ARG:NE	2.27	0.67
4:E:282:LEU:HD22	5:T:2686:THR:HG22	1.76	0.67
4:E:284:SER:OG	4:E:285:PRO:HD3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:2531:GLN:HA	5:T:2531:GLN:OE1	1.95	0.67
1:A:82:MET:HA	1:A:85:ILE:HD12	1.75	0.67
2:B:244:GLU:O	3:D:75:ARG:NH2	2.28	0.67
5:T:3467:LEU:CD1	5:T:3572:ILE:HD11	2.25	0.67
4:E:172:LEU:HD22	4:E:192:TYR:CE2	2.29	0.67
5:T:979:ASP:OD2	5:T:2489:LYS:CE	2.42	0.67
5:T:2851:GLU:OE1	5:T:2884:TRP:NE1	2.27	0.67
3:D:687:ASN:CB	5:T:2755:PHE:CZ	2.78	0.67
5:T:3509:LEU:HD12	5:T:3509:LEU:O	1.95	0.67
4:E:273:ALA:HB3	5:T:2649:ILE:HG21	1.76	0.66
2:B:463:GLY:N	3:D:365:GLU:OE2	2.29	0.66
3:D:293:MET:O	3:D:296:THR:OG1	2.13	0.66
3:D:644:ASN:OD1	5:T:2781:LYS:HE2	1.95	0.66
5:T:3229:LEU:C	5:T:3229:LEU:HD23	2.15	0.66
5:T:3428:LYS:HD2	5:T:3428:LYS:O	1.95	0.66
3:D:669:TRP:HA	3:D:672:ILE:HD12	1.77	0.66
3:D:565:LEU:HD11	6:F:585:LEU:HB3	1.76	0.66
6:F:590:ASP:HB3	6:F:593:ARG:HG3	1.77	0.66
5:T:3445:LEU:H	5:T:3445:LEU:HD23	1.60	0.66
5:T:3038:GLU:HA	5:T:3038:GLU:OE1	1.95	0.66
6:F:521:GLN:HA	6:F:524:MET:HE3	1.77	0.66
3:D:629:HIS:ND1	5:T:2591:TYR:CB	2.58	0.66
3:D:687:ASN:HB3	5:T:2755:PHE:CZ	2.31	0.66
1:A:216:LEU:O	1:A:254:ARG:NH2	2.29	0.66
5:T:2819:GLU:OE2	5:T:2819:GLU:HA	1.96	0.66
5:T:3430:LEU:C	5:T:3430:LEU:HD23	2.17	0.66
5:T:3449:ILE:HD12	5:T:3449:ILE:H	1.61	0.66
1:A:201:SER:N	1:A:205:GLU:OE2	2.29	0.65
3:D:565:LEU:HD11	6:F:585:LEU:HD13	1.77	0.65
3:D:569:ILE:HG22	3:D:571:GLU:OE2	1.96	0.65
5:T:3252:LEU:O	5:T:3252:LEU:HD23	1.96	0.65
5:T:3416:GLU:OE1	5:T:3585:GLU:HA	1.97	0.65
3:D:349:ILE:HD11	3:D:580:LEU:HD13	1.76	0.65
6:F:525:GLU:O	6:F:529:ILE:HG12	1.96	0.65
3:D:349:ILE:CD1	3:D:580:LEU:HD13	2.27	0.65
3:D:687:ASN:HB2	5:T:2755:PHE:CE2	2.29	0.65
1:A:91:TYR:OH	1:A:99:GLU:OE2	2.14	0.65
2:B:130:GLU:O	2:B:133:GLN:NE2	2.28	0.65
5:T:3391:LEU:HD12	5:T:3391:LEU:O	1.97	0.65
6:F:582:PRO:CB	6:F:584:TYR:CE1	2.59	0.65
4:E:282:LEU:C	4:E:285:PRO:HD2	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:973:ASP:OD2	5:T:3536:THR:HG21	1.97	0.65
5:T:3665:LEU:HD12	5:T:3665:LEU:O	1.96	0.65
5:T:3021:GLU:N	5:T:3021:GLU:OE1	2.28	0.64
5:T:3308:GLU:HA	5:T:3308:GLU:OE1	1.95	0.64
5:T:3659:LEU:HD23	5:T:3659:LEU:C	2.18	0.64
5:T:3698:LEU:C	5:T:3698:LEU:HD23	2.17	0.64
3:D:565:LEU:CD2	6:F:585:LEU:HD13	2.24	0.64
3:D:668:ASN:HB3	3:D:671:LEU:HD13	1.80	0.64
5:T:987:GLU:N	5:T:987:GLU:OE1	2.30	0.64
5:T:2684:LYS:O	5:T:2684:LYS:HG2	1.97	0.64
5:T:2792:GLN:NE2	5:T:2792:GLN:O	2.31	0.64
3:D:743:VAL:HG11	3:D:747:SER:HB2	1.78	0.64
6:F:629:ILE:HG22	6:F:631:SER:H	1.63	0.64
5:T:2513:GLU:OE1	5:T:2513:GLU:HA	1.97	0.64
3:D:681:THR:HG23	3:D:683:SER:HB3	1.78	0.64
2:B:158:VAL:HG22	2:B:167:VAL:HG22	1.80	0.64
5:T:952:LEU:HD23	5:T:952:LEU:H	1.62	0.64
5:T:861:LEU:O	5:T:865:VAL:HG23	1.98	0.64
1:A:212:ILE:HA	1:A:216:LEU:HD13	1.79	0.63
1:A:139:VAL:HG22	1:A:165:ILE:HD13	1.80	0.63
1:A:205:GLU:O	1:A:209:VAL:HG22	1.99	0.63
3:D:572:GLU:C	3:D:574:PRO:HD3	2.19	0.63
1:A:32:PRO:O	1:A:59:GLN:NE2	2.31	0.63
3:D:33:ILE:O	3:D:36:ARG:HD3	1.98	0.63
1:A:253:GLU:N	1:A:253:GLU:OE1	2.31	0.63
5:T:2959:MET:HG3	5:T:2959:MET:O	1.99	0.63
6:F:523:LYS:O	6:F:523:LYS:HD3	1.98	0.63
5:T:2728:LEU:HD12	5:T:2728:LEU:O	1.97	0.63
5:T:3631:LEU:C	5:T:3631:LEU:HD23	2.18	0.63
3:D:265:ALA:O	3:D:266:LEU:HG	1.97	0.63
4:E:282:LEU:O	4:E:285:PRO:HD2	1.99	0.63
5:T:2459:ASN:OD1	5:T:2459:ASN:N	2.28	0.63
6:F:574:ARG:O	6:F:574:ARG:HG2	1.97	0.63
5:T:3467:LEU:HD12	5:T:3572:ILE:HD11	1.81	0.62
5:T:2687:GLU:OE1	5:T:2687:GLU:N	2.32	0.62
5:T:3385:HIS:CD2	5:T:3570:HIS:CD2	2.87	0.62
3:D:378:LYS:HB3	3:D:539:LEU:HD12	1.81	0.62
3:D:544:LYS:HD2	3:D:544:LYS:O	2.00	0.62
4:E:273:ALA:HB3	5:T:2649:ILE:CG2	2.29	0.62
5:T:1102:LEU:CD1	5:T:2533:LEU:HD21	2.29	0.62
1:A:15:GLY:O	1:A:33:SER:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:O	1:A:68:ARG:NE	2.25	0.62
4:E:273:ALA:CB	5:T:2649:ILE:HG21	2.29	0.62
5:T:3385:HIS:NE2	5:T:3570:HIS:ND1	2.47	0.62
3:D:38:ARG:CG	5:T:3508:ILE:HG13	2.30	0.62
5:T:939:HIS:O	5:T:943:HIS:ND1	2.32	0.62
5:T:2723:GLN:OE1	5:T:2723:GLN:HA	2.00	0.62
5:T:2970:ILE:HG23	5:T:2970:ILE:O	2.00	0.62
3:D:687:ASN:ND2	5:T:2755:PHE:CZ	2.56	0.61
3:D:610:PRO:O	5:T:2574:ASN:OD1	2.17	0.61
3:D:626:ARG:HH12	3:D:628:ASN:HB2	1.65	0.61
5:T:3295:LYS:HD2	5:T:3295:LYS:O	2.00	0.61
4:E:278:LEU:CD2	4:E:279:LEU:HG	2.30	0.61
5:T:921:ILE:HA	5:T:924:VAL:HG12	1.80	0.61
5:T:1025:LEU:HB2	5:T:1082:LEU:HD23	1.81	0.61
2:B:152:ARG:CZ	2:B:440:LEU:HD11	2.30	0.61
4:E:172:LEU:HD22	4:E:192:TYR:CD2	2.35	0.61
5:T:3371:ILE:HG13	5:T:3371:ILE:O	2.01	0.61
6:F:582:PRO:HG3	6:F:584:TYR:CZ	2.34	0.61
3:D:760:MET:O	3:D:764:ILE:HD12	2.00	0.61
5:T:3206:GLU:OE1	5:T:3206:GLU:N	2.33	0.61
1:A:299:MET:O	1:A:300:SER:OG	2.15	0.60
2:B:462:LEU:HD11	2:B:465:PHE:HB3	1.83	0.60
5:T:2641:GLU:OE2	5:T:3545:ARG:NH2	2.33	0.60
4:E:166:PHE:HA	4:E:169:ILE:HD12	1.83	0.60
5:T:2509:GLU:OE1	5:T:2509:GLU:HA	2.01	0.60
1:A:282:ILE:HG21	1:A:294:TYR:CE1	2.36	0.60
3:D:536:LYS:HB2	3:D:539:LEU:CG	2.30	0.60
1:A:349:LEU:HD21	3:D:390:ALA:HB1	1.84	0.60
3:D:70:LYS:NZ	3:D:540:ALA:HB3	2.17	0.60
5:T:3452:SER:OG	5:T:3453:PRO:HD2	2.02	0.60
3:D:573:ARG:N	3:D:574:PRO:HD3	2.17	0.60
5:T:3534:LEU:HD12	5:T:3534:LEU:C	2.22	0.60
3:D:258:TYR:HB3	6:F:627:LEU:HD21	1.84	0.60
3:D:536:LYS:HA	3:D:536:LYS:HE2	1.84	0.60
5:T:3464:PHE:HB2	5:T:3575:ASP:HA	1.82	0.60
2:B:440:LEU:O	2:B:441:THR:OG1	2.19	0.60
4:E:246:ARG:NH1	4:E:254:GLU:OE1	2.29	0.60
5:T:3709:LEU:H	5:T:3709:LEU:HD23	1.67	0.60
2:B:398:VAL:HG12	2:B:398:VAL:O	2.02	0.59
3:D:270:PHE:O	6:F:588:ILE:HG12	2.02	0.59
3:D:565:LEU:HD23	3:D:565:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:2708:GLU:OE1	5:T:2708:GLU:HA	2.02	0.59
6:F:582:PRO:HB2	6:F:584:TYR:HE1	1.63	0.59
2:B:8:VAL:HG23	2:B:9:TYR:HD1	1.67	0.59
3:D:767:CYS:SG	3:D:771:ARG:NH2	2.75	0.59
2:B:394:MET:SD	2:B:401:ARG:NH1	2.76	0.59
3:D:558:THR:CB	3:D:561:GLN:HB2	2.32	0.59
5:T:1205:THR:O	5:T:1208:ASN:N	2.35	0.59
5:T:2552:ASP:OD1	5:T:2553:PRO:HD2	2.02	0.59
5:T:2867:VAL:HG12	5:T:2867:VAL:O	2.02	0.59
5:T:2942:GLU:OE1	5:T:2942:GLU:HA	2.02	0.59
6:F:551:LEU:O	6:F:551:LEU:HD12	2.03	0.59
4:E:282:LEU:CD2	5:T:2686:THR:CG2	2.76	0.59
5:T:2671:GLU:HA	5:T:2671:GLU:OE1	2.00	0.59
1:A:270:GLU:N	1:A:270:GLU:OE1	2.34	0.59
1:A:34:ILE:O	1:A:54:VAL:HG12	2.02	0.59
3:D:615:LEU:HG	5:T:2456:ARG:NH2	2.15	0.59
5:T:3157:ILE:HD12	5:T:3157:ILE:O	2.02	0.59
6:F:521:GLN:HA	6:F:524:MET:CE	2.33	0.59
6:F:572:ILE:O	6:F:572:ILE:HG23	2.02	0.59
1:A:71:ILE:HG23	1:A:71:ILE:O	2.03	0.59
3:D:309:ALA:HA	5:T:3721:LEU:HD12	1.85	0.59
5:T:3391:LEU:HD12	5:T:3391:LEU:C	2.23	0.59
5:T:3706:LEU:HD12	5:T:3706:LEU:O	2.02	0.59
5:T:3611:SER:OG	5:T:3612:PRO:HD2	2.02	0.58
5:T:2808:LYS:O	5:T:2808:LYS:HG2	2.02	0.58
3:D:746:GLU:OE1	3:D:746:GLU:N	2.36	0.58
4:E:293:GLN:OE1	4:E:302:GLN:NE2	2.36	0.58
5:T:1233:TYR:O	5:T:1237:LEU:HD13	2.03	0.58
5:T:2801:GLN:HA	5:T:2801:GLN:OE1	2.01	0.58
5:T:3252:LEU:HD23	5:T:3252:LEU:C	2.22	0.58
6:F:530:GLU:O	6:F:534:VAL:HG23	2.03	0.58
4:E:278:LEU:HD23	4:E:279:LEU:HG	1.84	0.58
3:D:334:LEU:O	3:D:338:GLY:HA3	2.04	0.58
3:D:738:ILE:O	3:D:738:ILE:HG22	2.04	0.58
5:T:1042:LEU:HD21	5:T:2501:GLN:C	2.23	0.58
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.84	0.58
5:T:2504:LEU:HD23	5:T:2504:LEU:O	2.03	0.58
5:T:2786:VAL:O	5:T:2786:VAL:HG13	2.03	0.58
3:D:565:LEU:HD21	6:F:585:LEU:HB2	1.84	0.58
5:T:2486:LEU:HD23	5:T:2536:ILE:HG22	1.86	0.58
5:T:2599:ARG:CA	5:T:2631:ASN:ND2	2.63	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:558:THR:O	3:D:560:ILE:HD12	2.04	0.58
5:T:1196:GLN:O	5:T:1200:LEU:HD23	2.04	0.58
1:A:105:LEU:HD23	1:A:106:THR:N	2.18	0.58
1:A:116:ARG:NH2	1:A:374:CYS:O	2.37	0.58
5:T:2584:ILE:HG12	5:T:2620:PRO:HG3	1.86	0.58
2:B:48:THR:N	2:B:68:ASP:OD2	2.37	0.57
2:B:157:VAL:HG22	2:B:168:SER:O	2.04	0.57
6:F:581:LEU:HD23	6:F:609:LEU:CB	2.34	0.57
1:A:7:ALA:HB3	1:A:22:ALA:HB3	1.86	0.57
6:F:581:LEU:HD22	6:F:581:LEU:H	1.69	0.57
2:B:112:GLU:OE1	2:B:116:ASN:ND2	2.37	0.57
3:D:558:THR:HB	3:D:561:GLN:HB2	1.87	0.57
5:T:3233:ILE:HD11	5:T:3405:VAL:HG11	1.86	0.57
3:D:71:LYS:HA	3:D:74:ILE:HG22	1.87	0.57
3:D:629:HIS:ND1	5:T:2591:TYR:HA	2.20	0.57
5:T:2614:GLU:OE1	5:T:2614:GLU:HA	2.05	0.57
3:D:307:HIS:CD2	4:E:282:LEU:HD21	2.40	0.57
3:D:379:TYR:CD1	3:D:534:GLU:HG2	2.40	0.57
3:D:558:THR:HB	3:D:561:GLN:CD	2.24	0.57
3:D:629:HIS:ND1	5:T:2591:TYR:CA	2.68	0.57
3:D:751:GLY:HA2	3:D:755:LEU:HD22	1.86	0.57
5:T:880:MET:HB3	5:T:920:VAL:HG11	1.87	0.57
5:T:1205:THR:HG22	5:T:1207:TYR:HB2	1.85	0.57
3:D:287:LEU:N	4:E:265:GLU:OE2	2.35	0.57
5:T:2611:SER:OG	5:T:2638:ASN:ND2	2.38	0.56
2:B:231:ASP:O	2:B:235:ASN:ND2	2.38	0.56
3:D:603:ARG:NE	6:F:631:SER:OG	2.38	0.56
4:E:289:GLN:HE22	4:E:295:LEU:HD11	1.70	0.56
5:T:3385:HIS:HD2	5:T:3570:HIS:CD2	2.24	0.56
3:D:270:PHE:H	6:F:588:ILE:HG23	1.69	0.56
3:D:331:ILE:HD11	3:D:340:TRP:CZ2	2.41	0.56
5:T:2603:ILE:HG12	5:T:2603:ILE:O	2.05	0.56
5:T:3117:LEU:HD12	5:T:3117:LEU:H	1.70	0.56
5:T:3377:THR:O	5:T:3377:THR:OG1	2.20	0.56
5:T:3464:PHE:CB	5:T:3575:ASP:HA	2.36	0.56
2:B:468:LEU:HD23	2:B:468:LEU:O	2.06	0.56
5:T:1223:VAL:HG12	5:T:1223:VAL:O	2.05	0.56
4:E:90:THR:O	4:E:91:LEU:HD23	2.06	0.56
5:T:956:ASN:HD21	5:T:2843:LEU:HD13	1.70	0.56
3:D:773:ASN:O	3:D:774:THR:OG1	2.23	0.56
5:T:3258:LEU:C	5:T:3258:LEU:HD23	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:VAL:HG22	2:B:401:ARG:NH2	2.21	0.56
2:B:177:SER:N	4:E:188:ASP:OD2	2.39	0.55
2:B:281:ASP:OD1	2:B:284:THR:HG22	2.06	0.55
3:D:309:ALA:HA	5:T:3721:LEU:CD1	2.35	0.55
3:D:375:GLU:OE2	3:D:534:GLU:O	2.24	0.55
5:T:2999:LEU:HD23	5:T:2999:LEU:C	2.26	0.55
1:A:9:VAL:HG13	1:A:9:VAL:O	2.06	0.55
2:B:399:ASP:N	2:B:399:ASP:OD1	2.39	0.55
4:E:289:GLN:HE22	4:E:295:LEU:HD21	1.71	0.55
1:A:149:THR:HG22	1:A:167:ALA:N	2.21	0.55
2:B:8:VAL:HG23	2:B:9:TYR:CD1	2.41	0.55
3:D:346:LYS:HA	6:F:538:LEU:HD21	1.88	0.55
3:D:540:ALA:C	3:D:542:PRO:HD3	2.27	0.55
3:D:38:ARG:HG2	5:T:3508:ILE:HG13	1.89	0.55
4:E:282:LEU:CD2	5:T:2686:THR:HG22	2.37	0.55
5:T:1039:TYR:O	5:T:1043:LEU:HD23	2.07	0.55
5:T:1246:LYS:HB3	5:T:3346:HIS:CD2	2.41	0.55
5:T:3167:LEU:HD12	5:T:3167:LEU:C	2.26	0.55
5:T:3253:LEU:HD12	5:T:3253:LEU:O	2.07	0.55
3:D:38:ARG:HG3	5:T:3508:ILE:HG13	1.89	0.55
3:D:549:VAL:HG23	3:D:550:ASP:N	2.22	0.55
5:T:2599:ARG:HG2	5:T:2599:ARG:O	2.05	0.55
2:B:23:SER:HG	7:B:501:ATP:PB	2.29	0.55
3:D:701:VAL:HG13	3:D:707:PHE:CD2	2.42	0.55
5:T:2662:LEU:HD23	5:T:2662:LEU:O	2.07	0.55
1:A:329:ILE:O	1:A:330:ILE:HD13	2.07	0.54
2:B:231:ASP:OD1	2:B:235:ASN:ND2	2.39	0.54
1:A:142:LEU:HD11	1:A:147:ARG:HB2	1.89	0.54
3:D:58:GLU:OE2	3:D:589:VAL:HG11	2.07	0.54
3:D:668:ASN:CB	3:D:671:LEU:HD13	2.38	0.54
5:T:3227:GLU:OE1	5:T:3227:GLU:HA	2.08	0.54
1:A:285:CYS:SG	1:A:286:ASP:N	2.79	0.54
1:A:212:ILE:HG23	1:A:216:LEU:HD22	1.89	0.54
1:A:283:MET:SD	1:A:290:ARG:NH1	2.80	0.54
4:E:173:PHE:HE2	4:E:208:THR:HG21	1.72	0.54
5:T:1090:THR:HG21	5:T:1163:VAL:HG11	1.88	0.54
5:T:2793:MET:CE	5:T:2848:GLN:HG2	2.38	0.54
5:T:2977:GLU:N	5:T:2977:GLU:OE1	2.39	0.54
5:T:3637:LEU:O	5:T:3637:LEU:HD12	2.08	0.54
2:B:441:THR:HG22	2:B:442:THR:N	2.23	0.54
3:D:263:VAL:HG22	3:D:264:ASP:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:3360:LEU:N	5:T:3360:LEU:HD12	2.22	0.54
5:T:968:GLU:N	5:T:968:GLU:OE1	2.41	0.53
2:B:136:ALA:HB1	2:B:470:VAL:O	2.08	0.53
5:T:2758:LEU:HD23	5:T:2758:LEU:C	2.29	0.53
5:T:3280:LEU:HD12	5:T:3301:ILE:HD13	1.89	0.53
5:T:3429:SER:CB	5:T:3658:GLU:OE2	2.56	0.53
3:D:747:SER:O	3:D:750:ARG:NH1	2.41	0.53
5:T:1110:PHE:HB3	5:T:1145:ILE:HD13	1.90	0.53
1:A:104:LEU:C	1:A:104:LEU:HD23	2.29	0.53
3:D:542:PRO:O	3:D:544:LYS:HG3	2.08	0.53
3:D:594:ASP:OD1	3:D:595:ASN:N	2.41	0.53
5:T:903:LEU:HD23	5:T:903:LEU:O	2.09	0.53
5:T:921:ILE:HG21	5:T:959:PHE:CG	2.43	0.53
5:T:1148:ALA:O	5:T:1151:PHE:N	2.40	0.53
5:T:1216:ILE:HD11	5:T:1237:LEU:CG	2.39	0.53
2:B:442:THR:OG1	2:B:451:GLN:NE2	2.41	0.53
5:T:1113:LEU:HD13	5:T:2494:LEU:CD1	2.39	0.53
5:T:1132:ASP:OD1	5:T:3316:TYR:OH	2.26	0.53
5:T:1171:ILE:HD11	5:T:1189:PHE:CE2	2.44	0.53
3:D:270:PHE:N	6:F:588:ILE:CG2	2.66	0.53
3:D:618:ARG:HG2	5:T:2457:ASP:OD1	2.09	0.52
1:A:176:LEU:HD12	1:A:281:SER:HB2	1.90	0.52
4:E:281:LEU:HD22	5:T:2684:LYS:HG3	1.90	0.52
2:B:430:LYS:NZ	3:D:52:LEU:HD11	2.24	0.52
3:D:258:TYR:HB3	6:F:627:LEU:CD2	2.39	0.52
5:T:947:ARG:O	5:T:951:LYS:HG2	2.10	0.52
5:T:3080:ASN:OD1	5:T:3080:ASN:N	2.41	0.52
1:A:160:THR:HG23	1:A:180:LEU:O	2.10	0.52
3:D:649:ILE:HD12	3:D:688:ILE:HG21	1.90	0.52
3:D:292:TYR:OH	6:F:523:LYS:HD2	2.09	0.52
3:D:572:GLU:OE1	3:D:574:PRO:HG3	2.09	0.52
1:A:236:ILE:HD11	1:A:254:ARG:NH1	2.25	0.52
3:D:33:ILE:CD1	3:D:300:ILE:HD11	2.40	0.52
1:A:14:SER:OG	1:A:158:GLY:N	2.42	0.52
3:D:70:LYS:O	3:D:74:ILE:HG22	2.09	0.52
6:F:577:TYR:O	6:F:580:HIS:O	2.27	0.52
3:D:349:ILE:HG23	3:D:349:ILE:O	2.10	0.52
5:T:966:LEU:HD23	5:T:3577:THR:O	2.10	0.52
5:T:1246:LYS:CB	5:T:3346:HIS:NE2	2.71	0.52
6:F:577:TYR:C	6:F:577:TYR:CD2	2.83	0.52
5:T:1102:LEU:HD13	5:T:2533:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:1149:ILE:HB	5:T:1150:PRO:HD3	1.92	0.52
5:T:2564:PHE:CD2	5:T:2613:ILE:HD11	2.45	0.51
5:T:2735:GLN:OE1	5:T:2735:GLN:HA	2.09	0.51
5:T:3173:THR:HG21	5:T:3450:PRO:HG2	1.92	0.51
6:F:544:ASN:N	6:F:545:PRO:CD	2.73	0.51
2:B:14:VAL:HG12	2:B:15:SER:N	2.25	0.51
2:B:268:ARG:O	2:B:279:VAL:HG13	2.11	0.51
3:D:396:THR:HG23	3:D:397:TYR:CD1	2.45	0.51
3:D:572:GLU:HG2	3:D:573:ARG:H	1.75	0.51
3:D:580:LEU:HD23	3:D:582:PHE:H	1.74	0.51
3:D:687:ASN:HB2	5:T:2755:PHE:CG	2.46	0.51
5:T:2694:TYR:HE1	5:T:3716:THR:HG1	1.59	0.51
5:T:2980:GLU:OE1	5:T:2980:GLU:N	2.34	0.51
1:A:165:ILE:HG23	1:A:169:PHE:O	2.11	0.51
1:A:182:GLY:O	1:A:186:THR:HG23	2.09	0.51
3:D:563:LEU:N	3:D:564:PRO:CD	2.74	0.51
3:D:677:THR:HG23	3:D:677:THR:O	2.10	0.51
1:A:16:MET:O	1:A:18:LYS:NZ	2.41	0.51
5:T:3718:GLN:OE1	5:T:3718:GLN:HA	2.09	0.51
1:A:141:SER:HB2	1:A:339:VAL:HG12	1.92	0.51
2:B:434:SER:HA	4:E:251:ILE:HD13	1.93	0.51
2:B:441:THR:HG22	2:B:442:THR:H	1.76	0.51
5:T:3068:LEU:C	5:T:3068:LEU:HD23	2.31	0.51
5:T:3493:LEU:C	5:T:3493:LEU:HD23	2.30	0.51
1:A:61:LYS:HG2	1:A:64:ILE:HD11	1.92	0.51
1:A:282:ILE:HG23	1:A:293:LEU:HD23	1.92	0.51
1:A:287:VAL:HG13	1:A:288:ASP:N	2.26	0.51
4:E:240:LEU:O	4:E:244:LEU:HD23	2.10	0.51
5:T:3378:VAL:O	5:T:3378:VAL:HG13	2.10	0.51
4:E:292:THR:HG23	4:E:292:THR:O	2.09	0.51
2:B:109:LEU:C	2:B:109:LEU:HD23	2.32	0.51
2:B:143:SER:HB3	2:B:157:VAL:HG21	1.93	0.51
5:T:2741:GLN:HG3	5:T:2962:VAL:HG23	1.91	0.51
5:T:3157:ILE:HD13	5:T:3214:ILE:HG21	1.92	0.51
5:T:3531:PHE:CE2	5:T:3544:PHE:HZ	2.29	0.51
5:T:964:THR:CA	5:T:3578:SER:OG	2.58	0.51
5:T:3625:THR:OG1	5:T:3626:PRO:HD2	2.10	0.51
1:A:79:TRP:HZ2	1:A:115:ASN:HD22	1.59	0.51
5:T:836:GLN:OE1	5:T:879:LEU:HD11	2.10	0.51
3:D:269:VAL:HG23	6:F:588:ILE:HG21	0.51	0.50
3:D:378:LYS:CB	3:D:539:LEU:HD12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:2432:ARG:HH21	5:T:2432:ARG:HG3	1.76	0.50
5:T:2694:TYR:HE1	5:T:3716:THR:OG1	1.94	0.50
3:D:350:ASP:N	3:D:351:PRO:HD3	2.26	0.50
5:T:3054:ALA:HB2	5:T:3091:LEU:HB3	1.93	0.50
6:F:581:LEU:HD22	6:F:581:LEU:N	2.26	0.50
2:B:176:LEU:O	2:B:180:THR:HG23	2.10	0.50
3:D:654:ASP:OD2	3:D:691:ARG:NH2	2.44	0.50
4:E:281:LEU:HD22	5:T:2684:LYS:HG2	1.92	0.50
5:T:3684:GLU:HA	5:T:3684:GLU:OE1	2.11	0.50
4:E:289:GLN:NE2	4:E:295:LEU:HD21	2.26	0.50
4:E:296:THR:HG22	4:E:297:SER:N	2.26	0.50
5:T:3531:PHE:CE2	5:T:3544:PHE:CZ	2.99	0.50
1:A:98:PRO:O	1:A:101:HIS:N	2.44	0.50
3:D:558:THR:HB	3:D:561:GLN:OE1	2.11	0.50
4:E:185:LEU:HD23	4:E:185:LEU:H	1.76	0.50
4:E:281:LEU:CD2	5:T:2684:LYS:HG3	2.41	0.50
4:E:281:LEU:HD23	4:E:281:LEU:N	2.27	0.50
5:T:1036:PRO:HD3	5:T:2498:SER:CB	2.42	0.50
5:T:3385:HIS:CD2	5:T:3570:HIS:CG	3.00	0.50
3:D:307:HIS:O	5:T:3721:LEU:HG	2.11	0.50
4:E:81:VAL:HG22	4:E:82:GLU:N	2.27	0.50
2:B:428:LEU:HA	2:B:431:ILE:HG22	1.92	0.50
5:T:3041:GLN:OE1	5:T:3041:GLN:HA	2.12	0.50
2:B:225:VAL:HG12	2:B:226:ASP:N	2.27	0.49
3:D:540:ALA:O	3:D:542:PRO:N	2.45	0.49
5:T:991:LEU:HD23	5:T:992:SER:O	2.12	0.49
2:B:446:ILE:O	2:B:449:GLN:N	2.33	0.49
5:T:3516:SER:OG	6:F:562:PHE:CG	2.63	0.49
5:T:3709:LEU:HD23	5:T:3709:LEU:N	2.27	0.49
6:F:560:VAL:HB	6:F:561:PRO:CD	2.43	0.49
1:A:80:ASP:OD1	1:A:81:ASP:N	2.45	0.49
3:D:30:ASP:O	3:D:33:ILE:HG22	2.13	0.49
3:D:618:ARG:CG	5:T:2457:ASP:OD2	2.58	0.49
4:E:87:ASN:OD1	4:E:88:SER:N	2.46	0.49
4:E:292:THR:HB	4:E:295:LEU:HD12	1.94	0.49
5:T:3116:MET:HE2	5:T:3116:MET:HA	1.94	0.49
2:B:86:ALA:O	2:B:89:GLN:HB3	2.12	0.49
1:A:159:VAL:HG22	1:A:160:THR:N	2.27	0.49
3:D:334:LEU:O	3:D:338:GLY:CA	2.60	0.49
4:E:271:THR:O	4:E:275:ARG:HG2	2.13	0.49
5:T:2486:LEU:HG	5:T:2486:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:2858:ILE:HD11	5:T:2880:ILE:HG21	1.94	0.49
2:B:418:PRO:HG3	3:D:75:ARG:NH1	2.27	0.49
3:D:590:VAL:HG12	3:D:590:VAL:O	2.13	0.49
3:D:645:ARG:O	3:D:736:ARG:NH2	2.42	0.49
5:T:1185:LEU:HD11	5:T:1223:VAL:HG11	1.94	0.49
3:D:284:ALA:O	3:D:285:LEU:HD23	2.13	0.49
6:F:525:GLU:OE1	6:F:525:GLU:HA	2.13	0.49
3:D:536:LYS:CG	3:D:539:LEU:HD21	2.43	0.49
5:T:2719:LEU:N	5:T:2719:LEU:HD22	2.27	0.49
5:T:3620:VAL:HG23	5:T:3727:ALA:HA	1.94	0.49
5:T:2987:GLU:HA	5:T:2987:GLU:OE1	2.11	0.48
2:B:478:VAL:HG23	2:B:483:LEU:HD11	1.94	0.48
3:D:59:ASN:OD1	3:D:62:ARG:N	2.45	0.48
3:D:533:GLU:HG3	3:D:554:THR:HG23	1.95	0.48
5:T:920:VAL:HG22	5:T:920:VAL:O	2.12	0.48
5:T:1157:ILE:O	5:T:1160:VAL:HG12	2.13	0.48
2:B:413:GLY:N	2:B:448:ARG:O	2.46	0.48
2:B:441:THR:HG21	2:B:448:ARG:NH2	2.29	0.48
3:D:296:THR:O	3:D:297:LEU:HD22	2.13	0.48
5:T:3547:GLN:HA	5:T:3547:GLN:OE1	2.13	0.48
2:B:83:TRP:HZ2	2:B:120:ASN:OD1	1.97	0.48
5:T:960:LEU:O	5:T:960:LEU:HD12	2.13	0.48
1:A:202:THR:HG22	1:A:203:THR:N	2.29	0.48
3:D:338:GLY:O	3:D:339:LEU:HD23	2.12	0.48
3:D:558:THR:O	3:D:559:LEU:HB2	2.14	0.48
5:T:1060:ASN:ND2	5:T:1133:LEU:O	2.41	0.48
1:A:103:VAL:HG12	1:A:129:VAL:HG11	1.95	0.48
1:A:299:MET:SD	1:A:300:SER:N	2.87	0.48
2:B:232:TYR:O	2:B:236:ARG:HG2	2.14	0.48
5:T:2696:GLN:HE21	5:T:3643:VAL:HG21	1.65	0.48
5:T:3315:ARG:CZ	5:T:3483:ASP:CG	2.80	0.48
5:T:3452:SER:OG	5:T:3453:PRO:CD	2.62	0.48
4:E:197:THR:HG23	4:E:199:GLU:HG3	1.94	0.48
5:T:3405:VAL:HG12	5:T:3457:ILE:HB	1.96	0.48
5:T:3522:VAL:CG2	5:T:3526:VAL:HG11	2.44	0.48
1:A:205:GLU:HA	1:A:208:ILE:HG22	1.96	0.48
2:B:156:LEU:HD11	2:B:167:VAL:HG13	1.96	0.48
5:T:3292:ILE:HG12	5:T:3292:ILE:O	2.13	0.48
1:A:100:GLU:N	1:A:100:GLU:OE1	2.46	0.48
2:B:289:ALA:O	2:B:292:LEU:N	2.43	0.48
2:B:410:LEU:CD2	2:B:415:SER:OG	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:1149:ILE:HG22	5:T:1153:LEU:HD11	1.96	0.48
4:E:209:CYS:SG	4:E:210:ARG:N	2.86	0.47
5:T:2996:MET:HA	5:T:2996:MET:HE2	1.95	0.47
5:T:3287:LEU:C	5:T:3287:LEU:HD12	2.34	0.47
1:A:39:ARG:NH2	1:A:65:LEU:O	2.46	0.47
4:E:165:SER:O	4:E:168:GLU:HG2	2.14	0.47
5:T:879:LEU:HD12	5:T:879:LEU:N	2.29	0.47
5:T:2865:THR:HG23	5:T:2865:THR:O	2.14	0.47
5:T:3486:GLN:HG2	5:T:3738:VAL:HG21	1.95	0.47
2:B:16:ALA:HB2	2:B:107:PRO:HG2	1.96	0.47
3:D:270:PHE:H	6:F:588:ILE:CG2	2.25	0.47
4:E:236:ARG:HD2	4:E:240:LEU:HD12	1.95	0.47
5:T:1015:LYS:NZ	5:T:1094:GLU:OE2	2.31	0.47
2:B:431:ILE:HG23	2:B:432:LEU:N	2.28	0.47
3:D:356:ASN:O	4:E:116:GLN:NE2	2.40	0.47
3:D:599:LYS:C	3:D:600:LEU:HD22	2.35	0.47
5:T:960:LEU:HD12	5:T:960:LEU:C	2.35	0.47
6:F:557:THR:HG22	6:F:557:THR:O	2.14	0.47
1:A:169:PHE:CZ	3:D:381:VAL:HG22	2.41	0.47
5:T:3157:ILE:CD1	5:T:3214:ILE:HG21	2.45	0.47
5:T:3555:PHE:CD1	5:T:3555:PHE:C	2.86	0.47
1:A:61:LYS:CG	1:A:64:ILE:HD11	2.44	0.47
1:A:97:ALA:HB1	1:A:99:GLU:OE1	2.14	0.47
1:A:134:VAL:HG22	1:A:135:SER:N	2.30	0.47
3:D:269:VAL:C	6:F:588:ILE:HG23	2.34	0.47
3:D:565:LEU:HD21	6:F:585:LEU:CB	2.45	0.47
5:T:2961:ASP:N	5:T:2961:ASP:OD1	2.47	0.47
5:T:2966:GLN:OE1	5:T:2966:GLN:HA	2.13	0.47
5:T:2996:MET:N	5:T:2996:MET:CE	2.78	0.47
5:T:3117:LEU:HD12	5:T:3117:LEU:N	2.30	0.47
6:F:581:LEU:N	6:F:581:LEU:HD13	2.30	0.47
2:B:116:ASN:OD1	2:B:117:SER:N	2.45	0.47
3:D:35:GLU:CG	5:T:3731:ARG:NH2	2.77	0.47
5:T:3272:LEU:N	5:T:3272:LEU:HD12	2.30	0.47
1:A:188:TYR:HE1	1:A:266:VAL:HG21	1.80	0.47
5:T:1096:LYS:NZ	5:T:1159:GLU:OE2	2.40	0.47
4:E:104:ASP:OD1	4:E:105:THR:N	2.48	0.47
4:E:281:LEU:O	4:E:284:SER:N	2.43	0.47
5:T:3314:LEU:HD23	5:T:3314:LEU:HA	1.82	0.47
5:T:2566:GLN:OE1	5:T:2566:GLN:HA	2.14	0.46
5:T:2601:ASN:OD1	5:T:2601:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:3522:VAL:O	5:T:3522:VAL:HG22	2.15	0.46
6:F:560:VAL:O	6:F:562:PHE:O	2.32	0.46
3:D:33:ILE:HD13	3:D:300:ILE:HD11	1.97	0.46
3:D:302:LEU:HD11	4:E:280:ARG:HA	1.98	0.46
5:T:1092:ILE:HG21	5:T:1095:LEU:HD12	1.97	0.46
5:T:1094:GLU:O	5:T:1095:LEU:HD23	2.16	0.46
5:T:2436:MET:HA	5:T:2436:MET:CE	2.43	0.46
5:T:2723:GLN:O	5:T:2723:GLN:HG3	2.16	0.46
1:A:350:THR:HG23	1:A:351:THR:N	2.29	0.46
2:B:198:LEU:HD21	2:B:280:PHE:CZ	2.51	0.46
3:D:50:ASN:OD1	3:D:51:GLN:N	2.49	0.46
3:D:764:ILE:HG21	4:E:294:TYR:HE2	1.79	0.46
4:E:175:LEU:HD13	4:E:192:TYR:CZ	2.50	0.46
5:T:1039:TYR:CE2	5:T:1043:LEU:HD21	2.50	0.46
6:F:590:ASP:HB3	6:F:593:ARG:CG	2.45	0.46
3:D:540:ALA:HB1	3:D:541:PRO:CD	2.45	0.46
1:A:10:ILE:HG22	1:A:11:ASP:N	2.30	0.46
3:D:618:ARG:HG2	5:T:2457:ASP:CG	2.35	0.46
3:D:678:HIS:O	3:D:678:HIS:ND1	2.47	0.46
5:T:918:GLU:HA	5:T:921:ILE:HD12	1.97	0.46
3:D:612:ILE:HG12	3:D:613:SER:N	2.31	0.46
5:T:994:THR:N	5:T:995:PRO:CD	2.79	0.46
5:T:2866:THR:HG22	5:T:2866:THR:O	2.16	0.46
5:T:3060:TRP:CD1	5:T:3060:TRP:C	2.89	0.46
5:T:3567:ARG:NE	5:T:3567:ARG:HA	2.31	0.46
6:F:644:ARG:C	6:F:645:SER:HG	2.18	0.46
5:T:1041:GLU:HB2	5:T:2511:VAL:O	2.15	0.46
5:T:1077:ASN:O	5:T:1081:ARG:HG2	2.15	0.46
5:T:2654:ILE:HG23	5:T:2655:ILE:HD12	1.98	0.46
2:B:180:THR:O	2:B:181:ARG:NH1	2.36	0.46
3:D:78:ILE:HG13	3:D:79:ARG:H	1.81	0.46
5:T:2705:GLN:NE2	5:T:2705:GLN:HA	2.31	0.46
6:F:523:LYS:NZ	6:F:527:ARG:HB2	2.31	0.46
6:F:647:ILE:HG21	6:F:649:TYR:HE1	1.80	0.46
3:D:368:TRP:CE3	3:D:571:GLU:HG2	2.51	0.46
4:E:294:TYR:CD1	4:E:299:GLY:HA2	2.50	0.46
5:T:876:LEU:O	5:T:876:LEU:HG	2.16	0.46
5:T:876:LEU:HA	5:T:879:LEU:HD13	1.98	0.46
5:T:1185:LEU:CD1	5:T:1223:VAL:HG11	2.46	0.46
5:T:1188:SER:OG	5:T:1189:PHE:N	2.47	0.46
5:T:2469:LEU:HB3	5:T:2556:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:3701:ARG:HB2	5:T:3701:ARG:NH1	2.31	0.46
3:D:748:ILE:HG13	3:D:748:ILE:O	2.16	0.45
4:E:124:THR:HG23	4:E:125:LYS:N	2.31	0.45
5:T:3522:VAL:HG23	5:T:3526:VAL:HG11	1.98	0.45
5:T:3634:ASP:N	5:T:3634:ASP:OD1	2.48	0.45
1:A:142:LEU:HD21	1:A:149:THR:O	2.16	0.45
3:D:646:THR:HG21	3:D:687:ASN:ND2	2.31	0.45
4:E:169:ILE:HD13	4:E:204:LYS:HE2	1.97	0.45
1:A:363:ASP:O	4:E:76:SER:OG	2.31	0.45
4:E:275:ARG:NE	4:E:275:ARG:HA	2.32	0.45
5:T:966:LEU:HB2	5:T:3577:THR:O	2.17	0.45
5:T:3659:LEU:C	5:T:3659:LEU:CD2	2.85	0.45
5:T:1114:GLN:HG3	5:T:1189:PHE:CD1	2.50	0.45
3:D:75:ARG:O	3:D:75:ARG:HD3	2.17	0.45
3:D:356:ASN:C	3:D:356:ASN:OD1	2.55	0.45
4:E:173:PHE:CZ	4:E:177:LYS:HE3	2.52	0.45
5:T:3411:ARG:HA	5:T:3411:ARG:NE	2.31	0.45
5:T:1105:ASN:O	5:T:1108:ASP:OD1	2.35	0.45
5:T:2793:MET:HE1	5:T:2848:GLN:HG2	1.98	0.45
5:T:2828:TRP:O	5:T:2831:LEU:N	2.50	0.45
6:F:582:PRO:HB2	6:F:584:TYR:CE1	2.45	0.45
3:D:362:LEU:HD23	3:D:362:LEU:O	2.17	0.45
3:D:575:LYS:O	3:D:575:LYS:HG2	2.17	0.45
3:D:658:LEU:HD11	3:D:696:CYS:SG	2.57	0.45
4:E:273:ALA:CB	5:T:2649:ILE:CG2	2.93	0.45
1:A:37:ARG:NH2	1:A:81:ASP:OD1	2.50	0.45
3:D:26:PHE:N	3:D:27:PRO:HD2	2.31	0.45
4:E:177:LYS:O	4:E:178:LYS:HE2	2.16	0.45
5:T:841:SER:O	5:T:845:MET:HG3	2.17	0.45
5:T:2546:ILE:HD13	5:T:2546:ILE:HA	1.85	0.45
5:T:3139:GLN:OE1	5:T:3139:GLN:HA	2.16	0.45
5:T:3388:TYR:CD1	5:T:3388:TYR:C	2.90	0.45
3:D:379:TYR:HB2	3:D:534:GLU:HG2	1.98	0.45
5:T:1168:TYR:O	5:T:1171:ILE:HG22	2.17	0.45
5:T:2492:TYR:O	5:T:2492:TYR:CD1	2.70	0.45
5:T:3307:TYR:O	5:T:3307:TYR:CD1	2.70	0.45
5:T:3582:PHE:O	5:T:3582:PHE:CD1	2.70	0.45
2:B:225:VAL:HG12	2:B:226:ASP:H	1.82	0.45
3:D:681:THR:O	3:D:681:THR:OG1	2.33	0.45
5:T:2591:TYR:HD1	5:T:2591:TYR:O	1.99	0.45
5:T:3464:PHE:O	5:T:3464:PHE:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:847:LEU:N	5:T:848:THR:HA	2.32	0.44
5:T:1145:ILE:HD11	5:T:1189:PHE:CE2	2.52	0.44
5:T:1213:VAL:O	5:T:1216:ILE:HG22	2.18	0.44
5:T:2807:ARG:HH21	5:T:2807:ARG:HG2	1.82	0.44
5:T:3344:PHE:C	5:T:3344:PHE:CD1	2.91	0.44
5:T:3555:PHE:CD1	5:T:3555:PHE:O	2.70	0.44
5:T:3646:PHE:CD1	5:T:3646:PHE:C	2.91	0.44
5:T:3744:PHE:CD1	5:T:3744:PHE:C	2.90	0.44
2:B:438:ARG:NH1	3:D:64:GLU:OE1	2.50	0.44
3:D:289:GLU:N	6:F:528:LYS:HZ1	2.14	0.44
4:E:282:LEU:CD2	5:T:2686:THR:HG21	2.46	0.44
5:T:2682:ARG:HH11	5:T:2682:ARG:HG2	1.82	0.44
5:T:2758:LEU:C	5:T:2758:LEU:CD2	2.86	0.44
1:A:149:THR:HG22	1:A:167:ALA:H	1.83	0.44
5:T:876:LEU:HD23	5:T:876:LEU:H	1.82	0.44
5:T:876:LEU:HD23	5:T:876:LEU:N	2.32	0.44
5:T:2591:TYR:O	5:T:2591:TYR:CD1	2.70	0.44
5:T:3252:LEU:C	5:T:3252:LEU:CD2	2.86	0.44
6:F:526:LYS:O	6:F:526:LYS:HD3	2.16	0.44
6:F:647:ILE:HG22	6:F:648:LYS:N	2.33	0.44
2:B:57:PHE:CD1	2:B:89:GLN:OE1	2.70	0.44
3:D:271:LEU:HD12	3:D:271:LEU:O	2.18	0.44
5:T:1042:LEU:HD21	5:T:2501:GLN:CB	2.45	0.44
5:T:2625:TYR:CD1	5:T:2625:TYR:O	2.70	0.44
5:T:3320:ARG:HD3	5:T:3320:ARG:HA	1.90	0.44
5:T:3646:PHE:HB2	5:T:3717:THR:HG22	1.99	0.44
3:D:560:ILE:O	3:D:560:ILE:HG22	2.17	0.44
3:D:266:LEU:O	3:D:266:LEU:HD12	2.17	0.44
5:T:1189:PHE:O	5:T:1193:LEU:HD13	2.18	0.44
5:T:3034:ARG:HA	5:T:3034:ARG:NE	2.32	0.44
5:T:3466:THR:HG22	5:T:3573:HIS:CE1	2.52	0.44
5:T:3646:PHE:CD1	5:T:3646:PHE:O	2.70	0.44
2:B:77:ASN:N	2:B:163:ASP:OD2	2.43	0.44
4:E:281:LEU:CD1	5:T:2684:LYS:HA	2.48	0.44
5:T:994:THR:HG23	5:T:994:THR:O	2.17	0.44
5:T:2513:GLU:O	5:T:2513:GLU:HG3	2.18	0.44
5:T:2662:LEU:HD22	5:T:2678:LEU:CD2	2.48	0.44
5:T:2741:GLN:HG3	5:T:2962:VAL:CG2	2.48	0.44
2:B:423:ARG:NE	2:B:427:GLU:OE1	2.42	0.44
3:D:357:THR:HG22	3:D:358:HIS:N	2.32	0.44
4:E:281:LEU:HD13	5:T:2684:LYS:CA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:840:GLN:OE1	5:T:878:PHE:HB3	2.18	0.44
5:T:3229:LEU:C	5:T:3229:LEU:CD2	2.85	0.44
1:A:35:VAL:HA	1:A:54:VAL:HG12	2.00	0.44
5:T:2624:LYS:HD3	5:T:2624:LYS:N	2.33	0.44
5:T:3405:VAL:O	5:T:3405:VAL:HG23	2.18	0.44
1:A:54:VAL:HG23	1:A:88:HIS:CD2	2.52	0.43
1:A:154:ASP:OD1	1:A:155:SER:N	2.51	0.43
2:B:299:ASP:H	2:B:300:ILE:HD12	1.82	0.43
5:T:1029:THR:O	5:T:1029:THR:HG22	2.18	0.43
5:T:3493:LEU:HD23	5:T:3493:LEU:O	2.17	0.43
1:A:149:THR:OG1	1:A:292:GLU:OE2	2.26	0.43
5:T:952:LEU:O	5:T:956:ASN:N	2.52	0.43
5:T:3033:LEU:N	5:T:3033:LEU:HD22	2.33	0.43
5:T:3693:GLN:HA	5:T:3693:GLN:NE2	2.33	0.43
3:D:569:ILE:HD11	6:F:639:ARG:HD2	2.00	0.43
5:T:2855:ALA:O	5:T:2859:TYR:CD2	2.71	0.43
5:T:2997:ASN:OD1	5:T:2997:ASN:N	2.52	0.43
5:T:3077:PHE:O	5:T:3077:PHE:CD1	2.71	0.43
4:E:202:LYS:HA	4:E:205:PHE:HB3	2.01	0.43
5:T:2655:ILE:HD12	5:T:2655:ILE:H	1.83	0.43
1:A:78:ASN:OD1	1:A:80:ASP:OD1	2.36	0.43
3:D:362:LEU:HD23	3:D:362:LEU:C	2.39	0.43
3:D:672:ILE:HG21	3:D:696:CYS:SG	2.59	0.43
5:T:1030:LYS:HA	5:T:2534:CYS:SG	2.58	0.43
5:T:3442:GLN:OE1	5:T:3442:GLN:HA	2.18	0.43
6:F:581:LEU:HD21	6:F:613:ARG:HE	1.83	0.43
6:F:582:PRO:CG	6:F:584:TYR:CD1	2.54	0.43
5:T:2870:LEU:O	5:T:2871:ASP:HB2	2.18	0.43
5:T:3091:LEU:O	5:T:3091:LEU:HD23	2.18	0.43
2:B:222:ASP:OD1	2:B:222:ASP:N	2.52	0.43
5:T:1115:VAL:HA	5:T:1179:TYR:OH	2.19	0.43
5:T:3091:LEU:HD23	5:T:3091:LEU:C	2.39	0.43
5:T:3679:HIS:CG	5:T:3679:HIS:O	2.70	0.43
1:A:77:THR:O	1:A:77:THR:HG22	2.18	0.43
3:D:359:GLN:O	3:D:363:LEU:HG	2.18	0.43
4:E:281:LEU:HB3	5:T:2684:LYS:O	2.19	0.43
5:T:1113:LEU:O	5:T:1116:ASN:HB3	2.19	0.43
5:T:2993:TYR:CD1	5:T:2993:TYR:C	2.92	0.43
5:T:3112:ASP:OD1	5:T:3112:ASP:N	2.52	0.43
1:A:45:VAL:HG22	1:A:46:GLY:N	2.34	0.43
1:A:78:ASN:ND2	1:A:81:ASP:CG	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD11	1:A:274:ILE:CG1	2.48	0.43
1:A:278:THR:HG22	1:A:282:ILE:CD1	2.49	0.43
3:D:271:LEU:HD12	3:D:271:LEU:C	2.39	0.43
3:D:375:GLU:HG3	3:D:534:GLU:OE1	2.19	0.43
5:T:866:PRO:HG3	5:T:879:LEU:HD21	2.01	0.43
5:T:2451:LEU:HD22	5:T:2567:VAL:HG12	2.00	0.43
5:T:2847:GLN:O	5:T:2851:GLU:HG2	2.19	0.43
1:A:162:VAL:CG1	1:A:176:LEU:HB2	2.49	0.43
1:A:262:PHE:HE2	1:A:312:ARG:HG2	1.84	0.43
3:D:273:MET:HG2	3:D:274:ASN:N	2.34	0.43
4:E:222:LEU:O	4:E:226:LEU:HD23	2.19	0.43
5:T:3531:PHE:CD2	5:T:3544:PHE:CE1	3.07	0.43
6:F:560:VAL:O	6:F:561:PRO:C	2.57	0.43
3:D:70:LYS:HZ2	3:D:540:ALA:HB3	1.82	0.42
3:D:75:ARG:O	3:D:78:ILE:HG23	2.19	0.42
5:T:1237:LEU:N	5:T:1237:LEU:HD12	2.34	0.42
5:T:3706:LEU:C	5:T:3706:LEU:CD1	2.85	0.42
1:A:132:PHE:CD1	1:A:133:TYR:N	2.88	0.42
5:T:1168:TYR:HA	5:T:1171:ILE:HG22	2.00	0.42
5:T:1190:ILE:HG22	5:T:1191:PRO:HD3	2.00	0.42
5:T:2465:ASP:OD1	5:T:2465:ASP:N	2.52	0.42
5:T:2839:HIS:O	5:T:2843:LEU:HG	2.19	0.42
5:T:3263:LEU:HD23	5:T:3263:LEU:HA	1.86	0.42
5:T:3721:LEU:HD13	5:T:3721:LEU:HA	1.81	0.42
1:A:215:LYS:C	1:A:216:LEU:HD12	2.39	0.42
3:D:70:LYS:HD3	3:D:540:ALA:HB3	2.01	0.42
3:D:315:ILE:O	3:D:319:LEU:HG	2.19	0.42
5:T:3400:VAL:O	5:T:3400:VAL:HG23	2.19	0.42
5:T:3682:ILE:HG22	5:T:3682:ILE:O	2.19	0.42
6:F:523:LYS:HD3	6:F:523:LYS:C	2.39	0.42
6:F:577:TYR:C	6:F:577:TYR:HD2	2.21	0.42
1:A:129:VAL:HG13	1:A:130:PRO:HD2	2.01	0.42
3:D:569:ILE:HG13	6:F:639:ARG:NH1	2.34	0.42
5:T:965:ASP:OD1	5:T:965:ASP:O	2.38	0.42
5:T:2432:ARG:HD2	5:T:2432:ARG:O	2.19	0.42
5:T:3530:HIS:ND1	5:T:3530:HIS:C	2.73	0.42
5:T:3665:LEU:HD12	5:T:3665:LEU:C	2.39	0.42
5:T:3710:ASN:OD1	5:T:3710:ASN:N	2.51	0.42
6:F:559:ASN:O	6:F:559:ASN:ND2	2.52	0.42
2:B:57:PHE:HD1	2:B:89:GLN:OE1	2.03	0.42
3:D:270:PHE:O	6:F:588:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:615:LEU:CD1	5:T:2456:ARG:NH2	2.83	0.42
3:D:642:LEU:HD12	3:D:642:LEU:O	2.19	0.42
5:T:2817:CYS:SG	5:T:2853:LEU:HD11	2.59	0.42
6:F:655:ASN:N	6:F:655:ASN:OD1	2.53	0.42
3:D:379:TYR:CB	3:D:534:GLU:HG2	2.48	0.42
3:D:687:ASN:CB	5:T:2755:PHE:CD2	2.86	0.42
5:T:2662:LEU:HD22	5:T:2678:LEU:HD23	2.02	0.42
5:T:3366:VAL:HG22	5:T:3366:VAL:O	2.20	0.42
5:T:3541:PHE:CD1	5:T:3541:PHE:C	2.93	0.42
1:A:76:VAL:HG11	1:A:79:TRP:CZ3	2.54	0.42
2:B:162:HIS:O	2:B:186:ALA:HB3	2.20	0.42
3:D:680:LEU:HD23	3:D:680:LEU:H	1.85	0.42
5:T:980:PHE:HE2	5:T:991:LEU:HD22	1.83	0.42
5:T:1014:ARG:HH21	5:T:1092:ILE:HD12	1.84	0.42
5:T:2469:LEU:HD23	5:T:2469:LEU:HA	1.82	0.42
5:T:2552:ASP:OD1	5:T:2553:PRO:CD	2.68	0.42
5:T:2865:THR:O	5:T:2865:THR:CG2	2.68	0.42
5:T:3334:LEU:C	5:T:3334:LEU:HD23	2.39	0.42
5:T:3412:HIS:ND1	5:T:3412:HIS:C	2.73	0.42
1:A:219:VAL:HG11	1:A:312:ARG:CB	2.50	0.42
2:B:430:LYS:HZ2	3:D:52:LEU:HD11	1.85	0.42
3:D:352:TRP:N	3:D:352:TRP:CD1	2.88	0.42
3:D:588:SER:OG	3:D:589:VAL:N	2.53	0.42
3:D:646:THR:HG21	3:D:687:ASN:OD1	2.19	0.42
3:D:738:ILE:O	3:D:738:ILE:CG2	2.67	0.42
4:E:200:ASP:OD1	4:E:201:LEU:N	2.53	0.42
5:T:876:LEU:N	5:T:877:PRO:CD	2.82	0.42
5:T:2967:LEU:HD11	5:T:2987:GLU:HG3	2.00	0.42
5:T:3096:LYS:HE2	5:T:3096:LYS:CA	2.43	0.42
5:T:3485:ILE:HG21	5:T:3743:TRP:CZ2	2.54	0.42
6:F:520:VAL:N	6:F:523:LYS:HB3	2.35	0.42
1:A:266:VAL:HG13	1:A:267:LEU:N	2.34	0.42
2:B:100:LEU:HD21	2:B:106:ILE:CD1	2.49	0.42
3:D:565:LEU:HD11	6:F:585:LEU:CB	2.45	0.42
3:D:626:ARG:NH1	3:D:628:ASN:HB2	2.34	0.42
4:E:182:ARG:O	4:E:183:TRP:HB2	2.19	0.42
4:E:204:LYS:O	4:E:208:THR:HG23	2.19	0.42
5:T:3731:ARG:H	5:T:3731:ARG:HD2	1.84	0.42
3:D:269:VAL:HG23	6:F:588:ILE:CG1	2.48	0.42
3:D:311:THR:HA	5:T:3728:VAL:HG21	2.02	0.42
5:T:1039:TYR:CZ	5:T:1043:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:2599:ARG:CB	5:T:2631:ASN:ND2	2.83	0.42
5:T:2695:GLU:OE1	5:T:2695:GLU:HA	2.20	0.42
6:F:594:ILE:O	6:F:594:ILE:HG22	2.19	0.42
3:D:347:ARG:CG	3:D:348:PHE:N	2.83	0.41
5:T:3156:LEU:HD23	5:T:3156:LEU:HA	1.93	0.41
5:T:3441:ILE:HD12	5:T:3441:ILE:N	2.35	0.41
1:A:153:LEU:HD11	1:A:274:ILE:HG13	2.01	0.41
2:B:442:THR:HG22	2:B:443:GLY:N	2.35	0.41
3:D:52:LEU:HD23	3:D:52:LEU:H	1.85	0.41
5:T:2643:ILE:HD12	5:T:2643:ILE:HA	1.85	0.41
5:T:2862:LEU:O	5:T:2865:THR:HG22	2.20	0.41
6:F:562:PHE:O	6:F:563:ALA:HB3	2.20	0.41
4:E:191:SER:O	4:E:192:TYR:CG	2.73	0.41
5:T:851:LEU:N	5:T:852:PRO:HD3	2.35	0.41
5:T:2436:MET:HA	5:T:2436:MET:HE3	2.01	0.41
5:T:2770:ASN:OD1	5:T:2770:ASN:N	2.50	0.41
5:T:3168:HIS:ND1	5:T:3168:HIS:C	2.73	0.41
5:T:3349:PHE:O	5:T:3349:PHE:HD1	2.03	0.41
3:D:70:LYS:HZ1	3:D:538:GLU:HA	1.85	0.41
3:D:296:THR:C	3:D:297:LEU:HD22	2.40	0.41
3:D:299:LEU:O	3:D:302:LEU:HB3	2.21	0.41
5:T:914:ASP:HB2	5:T:915:PRO:HD3	2.02	0.41
5:T:2793:MET:HE3	5:T:2848:GLN:HG2	2.01	0.41
1:A:8:LEU:N	1:A:8:LEU:HD12	2.35	0.41
2:B:40:LEU:HD13	2:B:89:GLN:HE21	1.85	0.41
3:D:383:ILE:HG23	3:D:384:CYS:N	2.36	0.41
3:D:543:PHE:O	3:D:544:LYS:C	2.58	0.41
3:D:563:LEU:C	3:D:563:LEU:HD12	2.40	0.41
5:T:1049:SER:HA	5:T:1052:LEU:HD12	2.03	0.41
5:T:1113:LEU:CD1	5:T:2494:LEU:CD1	2.98	0.41
5:T:2560:TRP:CD1	5:T:2560:TRP:C	2.93	0.41
5:T:2575:GLU:OE2	5:T:2575:GLU:N	2.53	0.41
5:T:3678:LEU:HD12	5:T:3678:LEU:HA	1.89	0.41
3:D:380:LYS:O	3:D:383:ILE:HG22	2.20	0.41
4:E:178:LYS:HE2	4:E:178:LYS:HA	2.03	0.41
5:T:859:VAL:O	5:T:863:ILE:HG12	2.20	0.41
5:T:1062:ASP:OD1	5:T:1062:ASP:N	2.53	0.41
5:T:1158:PRO:O	5:T:1162:GLU:HG3	2.19	0.41
5:T:2786:VAL:O	5:T:2786:VAL:CG1	2.69	0.41
5:T:2909:PHE:HA	5:T:2912:ILE:HG22	2.02	0.41
3:D:310:LEU:HD23	3:D:310:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:233:GLU:O	4:E:237:LYS:HG2	2.20	0.41
5:T:1060:ASN:HD21	5:T:1134:LYS:HA	1.86	0.41
5:T:1190:ILE:CG2	5:T:1191:PRO:HD3	2.51	0.41
5:T:2594:ARG:HD3	5:T:2594:ARG:N	2.35	0.41
5:T:3151:MET:SD	5:T:3152:VAL:N	2.93	0.41
5:T:3584:LEU:HD23	5:T:3584:LEU:HA	1.82	0.41
2:B:426:THR:O	2:B:430:LYS:HG2	2.21	0.41
2:B:439:ILE:HG22	2:B:440:LEU:O	2.21	0.41
2:B:451:GLN:O	2:B:454:LEU:HB3	2.20	0.41
2:B:479:GLY:O	2:B:483:LEU:HD12	2.21	0.41
3:D:368:TRP:NE1	6:F:642:VAL:O	2.52	0.41
3:D:629:HIS:CE1	5:T:2591:TYR:CB	2.96	0.41
5:T:1113:LEU:HD13	5:T:2494:LEU:HD13	2.01	0.41
5:T:2662:LEU:HD23	5:T:2662:LEU:C	2.41	0.41
5:T:2783:VAL:HG22	5:T:2783:VAL:O	2.21	0.41
1:A:100:GLU:O	1:A:101:HIS:ND1	2.53	0.41
1:A:242:LEU:HG	1:A:244:ASP:OD1	2.20	0.41
2:B:100:LEU:HD21	2:B:106:ILE:HD13	2.02	0.41
3:D:266:LEU:HD21	3:D:607:ASP:HB2	2.02	0.41
3:D:313:ASN:O	3:D:317:ASN:ND2	2.53	0.41
3:D:560:ILE:HD12	3:D:560:ILE:N	2.35	0.41
3:D:765:ARG:HE	4:E:300:MET:CE	2.34	0.41
5:T:2650:ASP:OD1	5:T:2650:ASP:N	2.54	0.41
5:T:2996:MET:N	5:T:2996:MET:HE3	2.36	0.41
5:T:2996:MET:CE	5:T:2996:MET:CA	2.99	0.41
5:T:3412:HIS:HE1	5:T:3585:GLU:OE1	2.04	0.41
5:T:3499:ASP:N	5:T:3499:ASP:OD1	2.53	0.41
5:T:3516:SER:OG	6:F:562:PHE:CB	2.68	0.41
1:A:202:THR:HG22	1:A:203:THR:H	1.85	0.41
5:T:934:PRO:HD2	5:T:2829:VAL:HG21	2.02	0.41
5:T:993:VAL:HG23	5:T:2541:PHE:CZ	2.56	0.41
1:A:173:HIS:HB2	2:B:39:ILE:HD12	2.03	0.40
3:D:680:LEU:HD23	3:D:680:LEU:N	2.35	0.40
5:T:3268:LYS:HE2	5:T:3268:LYS:HB2	1.97	0.40
5:T:3362:LYS:HA	5:T:3362:LYS:HD2	1.86	0.40
1:A:130:PRO:HA	1:A:359:LYS:HB2	2.03	0.40
1:A:216:LEU:HD12	1:A:216:LEU:N	2.37	0.40
3:D:671:LEU:HD12	5:T:2626:LEU:HD13	2.03	0.40
4:E:292:THR:CB	4:E:295:LEU:HD12	2.52	0.40
5:T:893:LEU:N	5:T:893:LEU:HD22	2.36	0.40
5:T:2618:LEU:HD22	5:T:2618:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:THR:O	2:B:42:SER:OG	2.39	0.40
3:D:263:VAL:HG13	3:D:265:ALA:HB2	2.02	0.40
5:T:2715:ARG:O	5:T:2715:ARG:CG	2.69	0.40
5:T:2854:GLU:OE1	5:T:2884:TRP:NE1	2.45	0.40
5:T:3033:LEU:N	5:T:3033:LEU:CD2	2.85	0.40
1:A:113:LYS:HB2	1:A:371:HIS:NE2	2.36	0.40
2:B:165:CYS:HB3	2:B:183:ASN:OD1	2.22	0.40
2:B:176:LEU:HD21	4:E:185:LEU:HB3	2.04	0.40
2:B:185:ILE:HG22	2:B:292:LEU:CD1	2.51	0.40
3:D:608:GLU:O	3:D:609:GLU:C	2.60	0.40
4:E:102:ILE:H	4:E:102:ILE:HD12	1.86	0.40
5:T:979:ASP:CG	5:T:2489:LYS:HE3	2.41	0.40
5:T:2975:ASN:OD1	5:T:2975:ASN:N	2.52	0.40
5:T:3287:LEU:HD12	5:T:3287:LEU:O	2.22	0.40
1:A:171:LEU:O	1:A:175:ILE:HG13	2.22	0.40
2:B:24:TYR:HD1	2:B:25:THR:HG23	1.86	0.40
2:B:142:THR:HG23	2:B:143:SER:N	2.36	0.40
3:D:43:LEU:HD12	6:F:561:PRO:HB3	2.03	0.40
5:T:2902:VAL:HG13	5:T:2946:VAL:HG12	2.04	0.40
6:F:538:LEU:HD12	6:F:538:LEU:C	2.42	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	370/372 (100%)	331 (90%)	39 (10%)	0	100	100
2	B	398/489 (81%)	361 (91%)	36 (9%)	1 (0%)	41	74
3	D	448/982 (46%)	362 (81%)	85 (19%)	1 (0%)	47	79
4	E	197/476 (41%)	186 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	T	1674/3744 (45%)	1556 (93%)	103 (6%)	15 (1%)	17 54
6	F	120/832 (14%)	97 (81%)	22 (18%)	1 (1%)	19 57
All	All	3207/6895 (46%)	2893 (90%)	296 (9%)	18 (1%)	29 62

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	T	2741	GLN
5	T	2958	ASN
5	T	2974	PRO
5	T	3240	THR
5	T	3263	LEU
5	T	3265	PHE
5	T	3442	GLN
5	T	2574	ASN
5	T	3710	ASN
2	B	414	THR
5	T	3435	GLU
5	T	3716	THR
6	F	542	PRO
3	D	541	PRO
5	T	2721	TYR
5	T	3053	LEU
5	T	3525	ASN
5	T	3408	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	317/317 (100%)	316 (100%)	1 (0%)	92 96
2	B	354/434 (82%)	354 (100%)	0	100 100
3	D	414/892 (46%)	412 (100%)	2 (0%)	88 94
4	E	184/441 (42%)	183 (100%)	1 (0%)	88 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	T	1528/3452 (44%)	1444 (94%)	84 (6%)	21 53
6	F	114/769 (15%)	106 (93%)	8 (7%)	15 46
All	All	2911/6305 (46%)	2815 (97%)	96 (3%)	41 65

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	LYS
3	D	36	ARG
3	D	544	LYS
4	E	189	ARG
5	T	2415	ARG
5	T	2422	VAL
5	T	2424	THR
5	T	2443	LEU
5	T	2459	ASN
5	T	2465	ASP
5	T	2494	LEU
5	T	2500	LEU
5	T	2502	GLU
5	T	2534	CYS
5	T	2539	SER
5	T	2545	LEU
5	T	2547	GLU
5	T	2570	SER
5	T	2574	ASN
5	T	2594	ARG
5	T	2596	ILE
5	T	2600	THR
5	T	2601	ASN
5	T	2602	VAL
5	T	2618	LEU
5	T	2621	HIS
5	T	2626	LEU
5	T	2715	ARG
5	T	2721	TYR
5	T	2746	LEU
5	T	2747	THR
5	T	2753	GLU
5	T	2761	GLU
5	T	2768	ASP

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Mol	Chain	Res	Type
5	T	2782	SER
5	T	2788	THR
5	T	2811	GLN
5	T	2938	ARG
5	T	2943	ILE
5	T	2963	CYS
5	T	2975	ASN
5	T	2984	LYS
5	T	2997	ASN
5	T	3011	LEU
5	T	3053	LEU
5	T	3060	TRP
5	T	3074	ASN
5	T	3098	ARG
5	T	3124	PHE
5	T	3137	ILE
5	T	3151	MET
5	T	3152	VAL
5	T	3157	ILE
5	T	3167	LEU
5	T	3280	LEU
5	T	3309	THR
5	T	3338	CYS
5	T	3342	SER
5	T	3349	PHE
5	T	3365	ASN
5	T	3369	ILE
5	T	3375	LEU
5	T	3412	HIS
5	T	3436	THR
5	T	3442	GLN
5	T	3449	ILE
5	T	3457	ILE
5	T	3460	ASP
5	T	3464	PHE
5	T	3477	LYS
5	T	3494	ASN
5	T	3497	HIS
5	T	3505	ASP
5	T	3519	THR
5	T	3521	PHE
5	T	3526	VAL

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Mol	Chain	Res	Type
5	T	3534	LEU
5	T	3555	PHE
5	T	3563	MET
5	T	3564	ILE
5	T	3572	ILE
5	T	3583	THR
5	T	3624	LEU
5	T	3625	THR
5	T	3680	ARG
5	T	3709	LEU
5	T	3715	VAL
5	T	3721	LEU
6	F	571	GLN
6	F	572	ILE
6	F	574	ARG
6	F	577	TYR
6	F	581	LEU
6	F	584	TYR
6	F	588	ILE
6	F	593	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60	GLN
2	B	248	HIS
2	B	451	GLN
3	D	317	ASN
3	D	567	ASN
4	E	289	GLN
4	E	293	GLN
4	E	302	GLN
5	T	2551	GLN
5	T	2631	ASN
5	T	2638	ASN
5	T	2741	GLN
5	T	2742	HIS
5	T	2792	GLN
5	T	2811	GLN
5	T	2848	GLN
5	T	2899	ASN
5	T	2948	ASN

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Mol	Chain	Res	Type
5	T	3119	ASN
5	T	3570	HIS
5	T	3627	ASN
5	T	3693	GLN
5	T	3695	ASN
5	T	3732	ASN
6	F	544	ASN
6	F	559	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
7	ATP	B	501	2	26,33,33	0.90	1 (3%)	31,52,52	1.57	5 (16%)

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
7	ATP	B	501	2	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	ATP	C5-C4	2.28	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	501	ATP	PA-O3A-PB	-3.76	119.92	132.83
7	B	501	ATP	N3-C2-N1	-3.66	122.96	128.68
7	B	501	ATP	PB-O3B-PG	-3.38	121.22	132.83
7	B	501	ATP	C3'-C2'-C1'	2.94	105.41	100.98
7	B	501	ATP	C4-C5-N7	-2.60	106.69	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	501	ATP	C5'-O5'-PA-O3A
7	B	501	ATP	O4'-C4'-C5'-O5'
7	B	501	ATP	C5'-O5'-PA-O1A
7	B	501	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

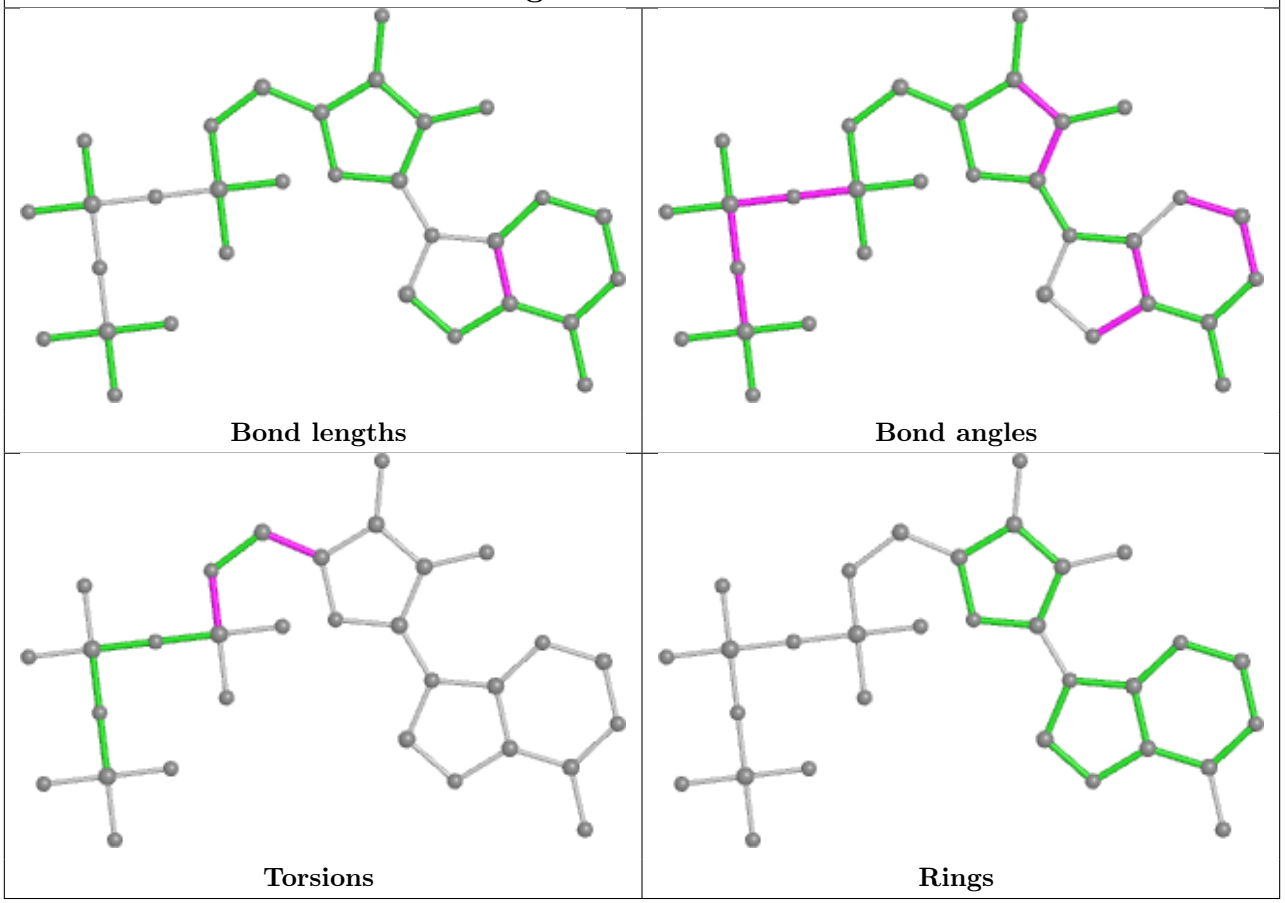
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 501



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.

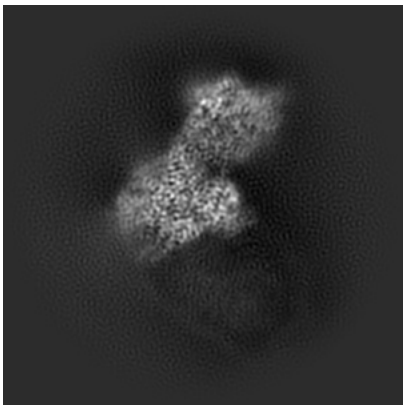
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33794. These allow visual inspection of the internal detail of the map and identification of artifacts.

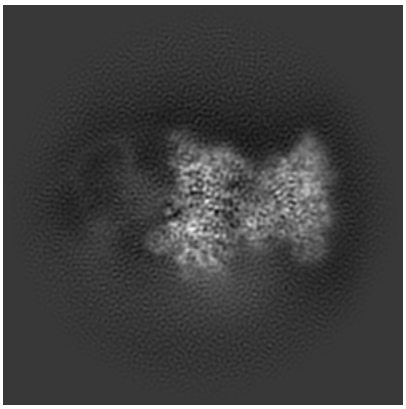
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

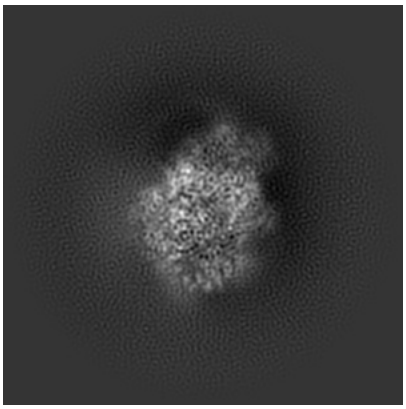
6.1.1 Primary map



X

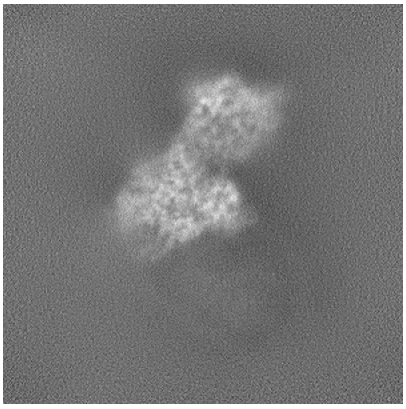


Y

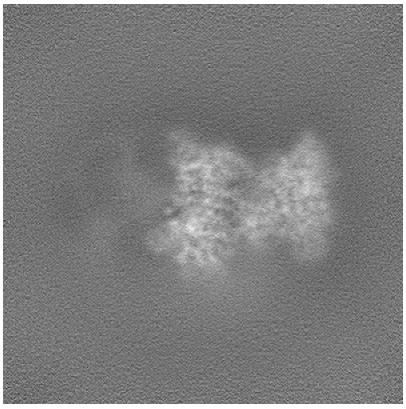


Z

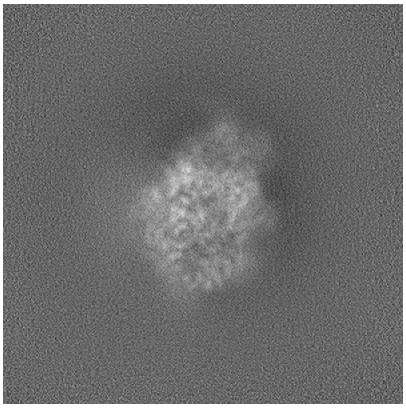
6.1.2 Raw map



X



Y

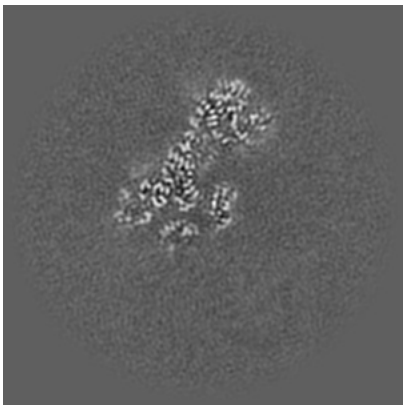


Z

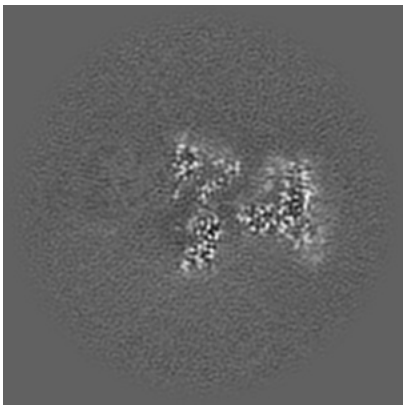
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

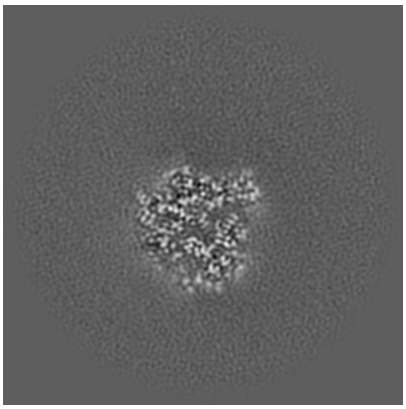
6.2.1 Primary map



X Index: 250

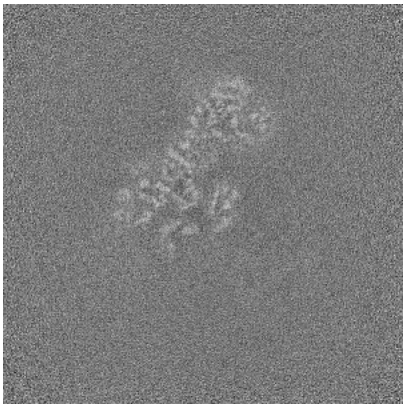


Y Index: 250

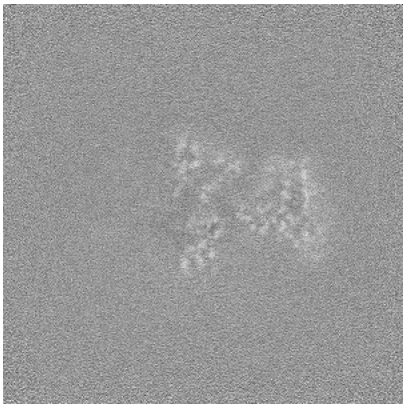


Z Index: 250

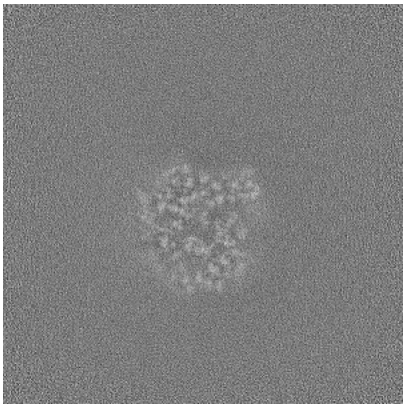
6.2.2 Raw map



X Index: 250



Y Index: 250

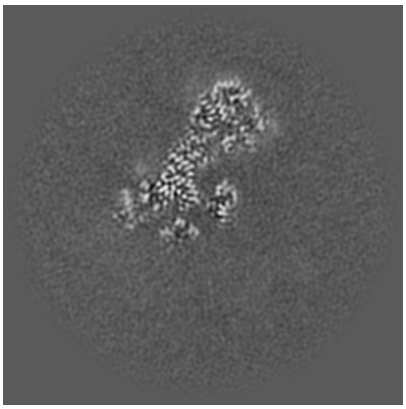


Z Index: 250

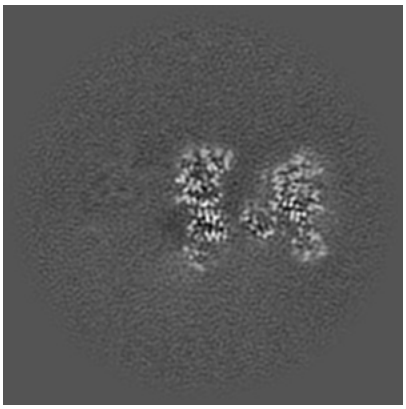
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

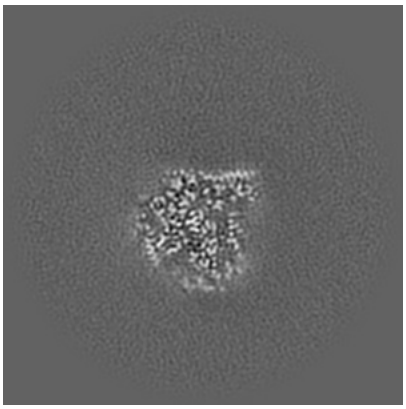
6.3.1 Primary map



X Index: 247

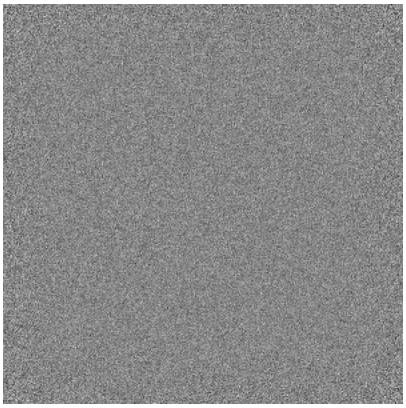


Y Index: 264

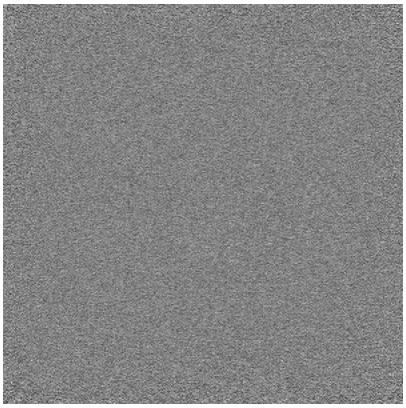


Z Index: 257

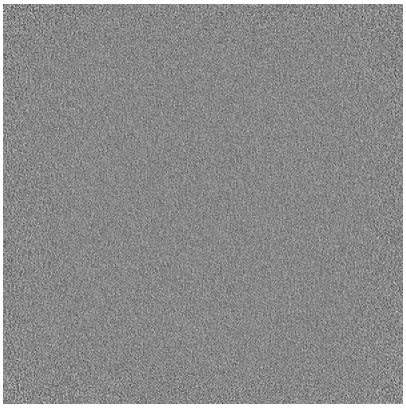
6.3.2 Raw map



X Index: 0



Y Index: 0

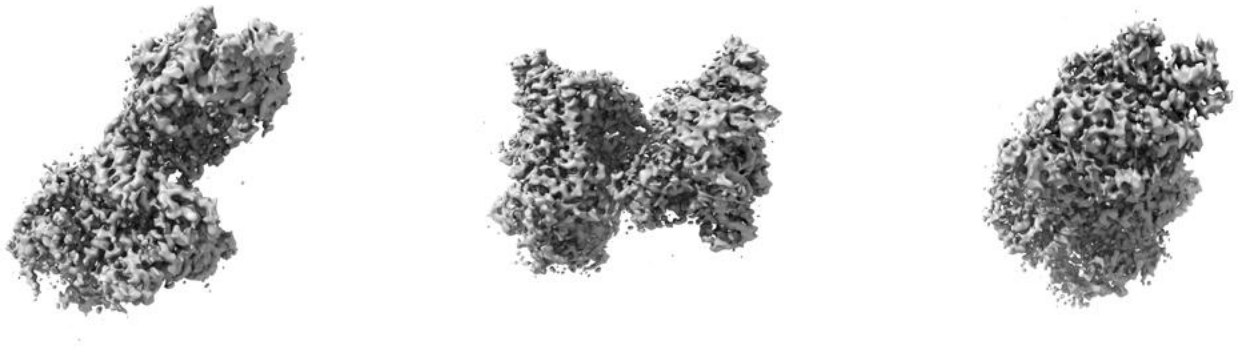


Z Index: 0

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

6.4 Orthogonal surface views (i)

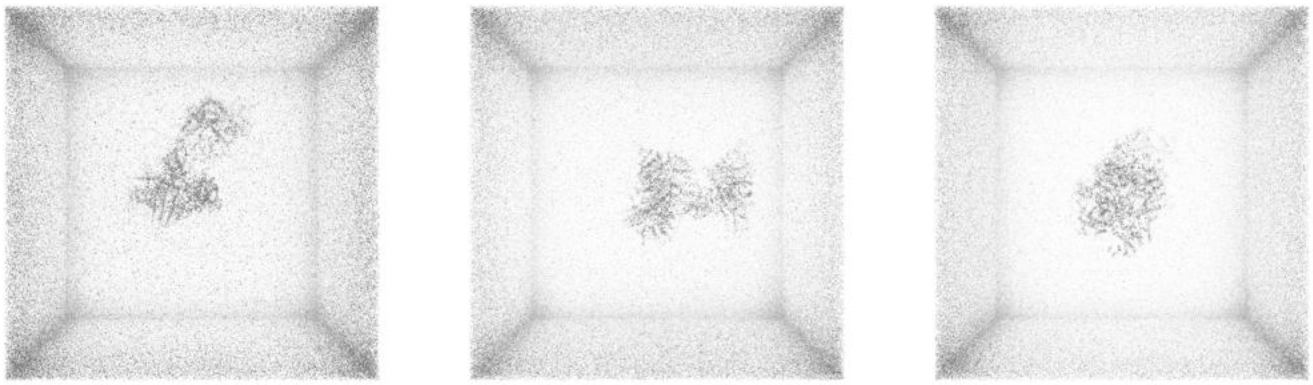
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0396. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

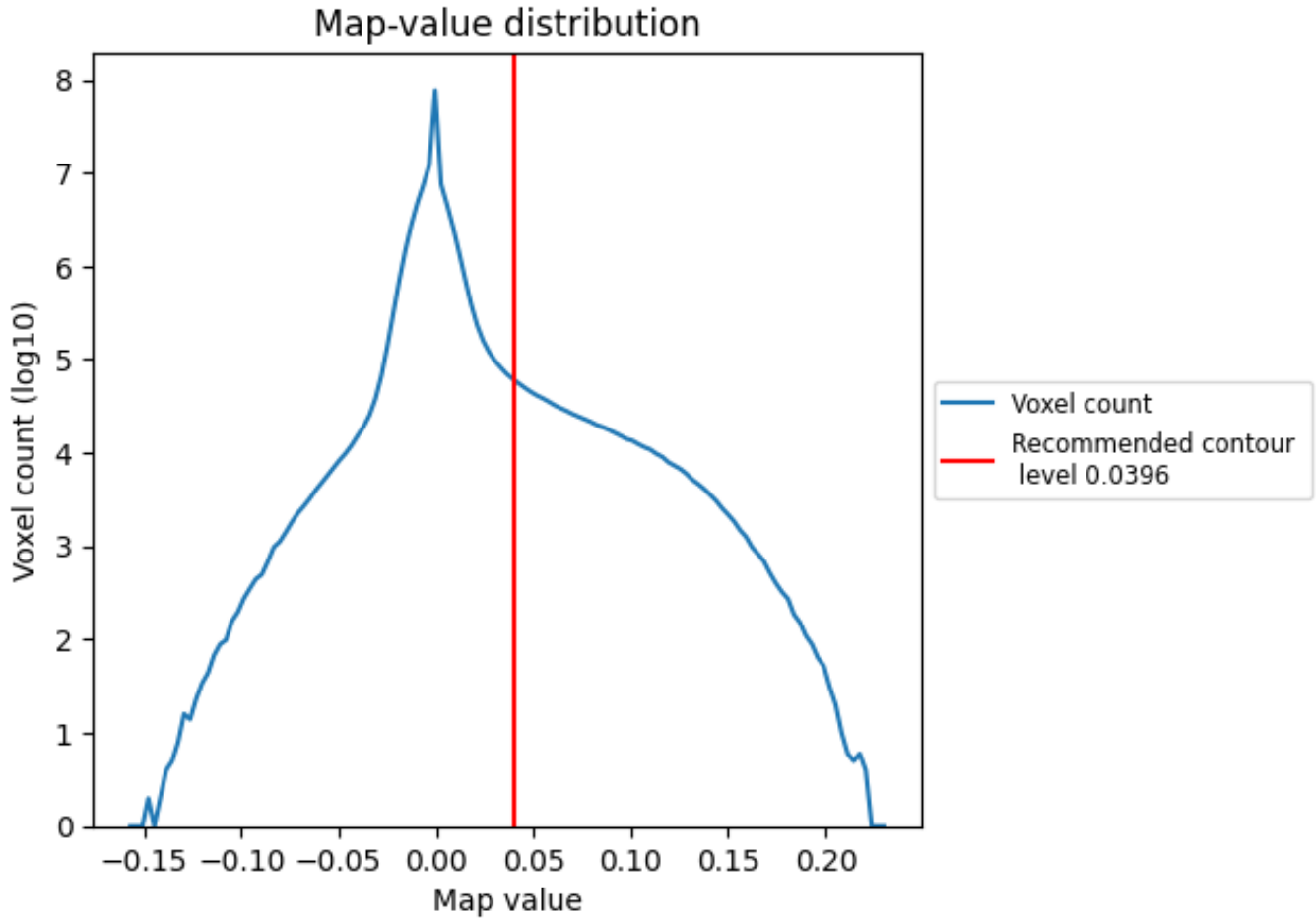
6.5 Mask visualisation (i)

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

7 Map analysis

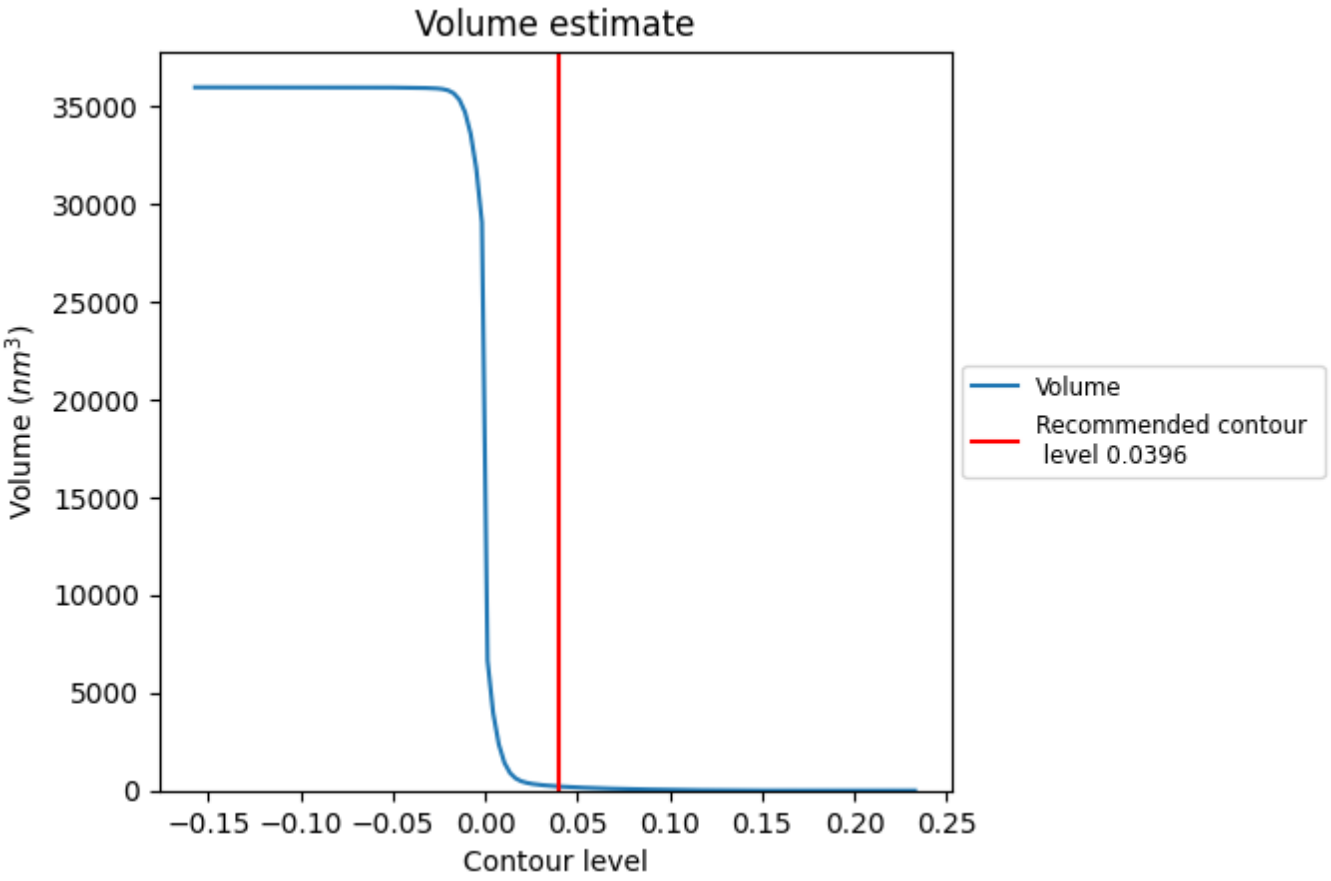
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

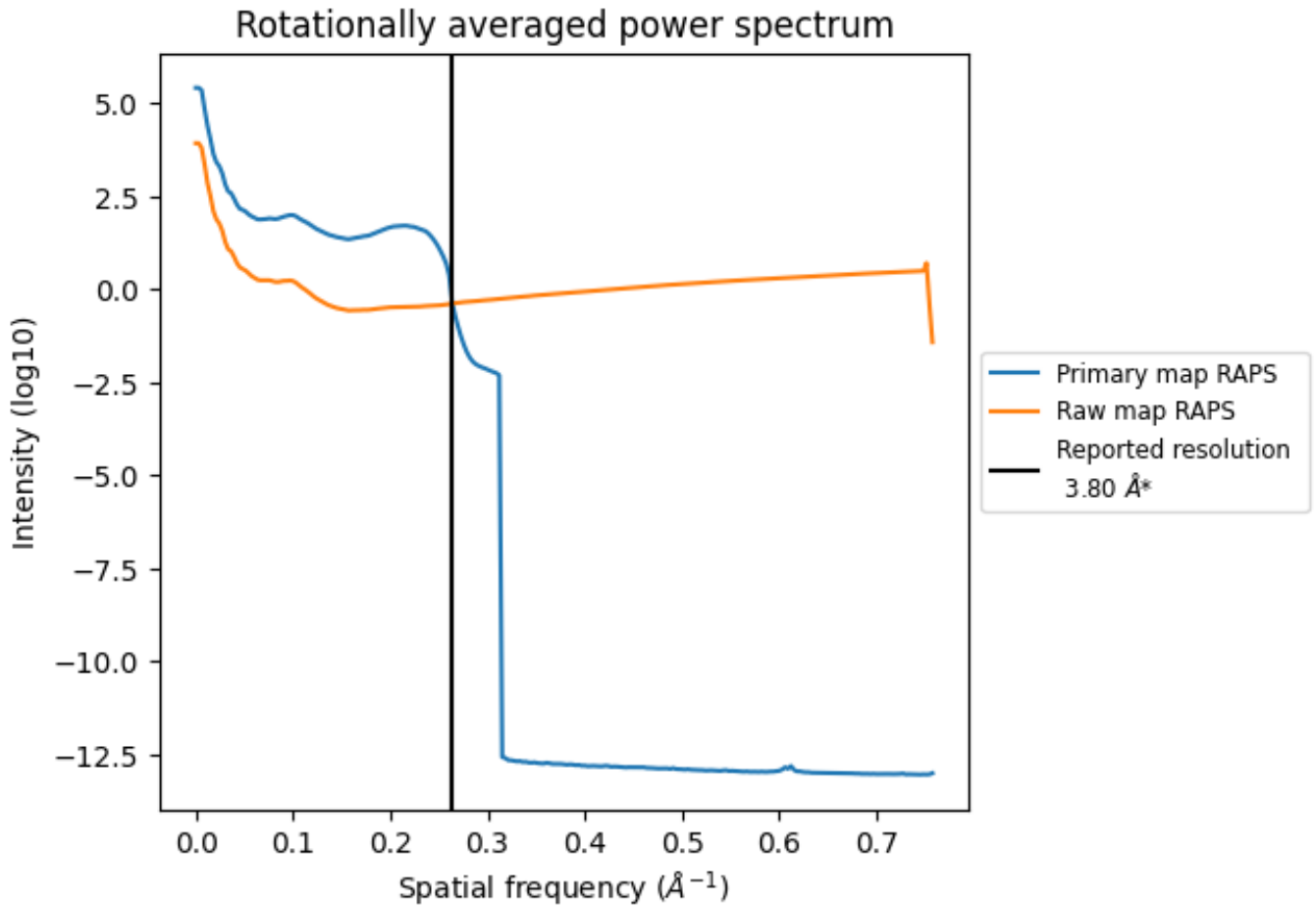
7.2 Volume estimate



The volume at the recommended contour level is 213 nm^3; this corresponds to an approximate mass of 193 kDa.

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

7.3 Rotationally averaged power spectrum (i)

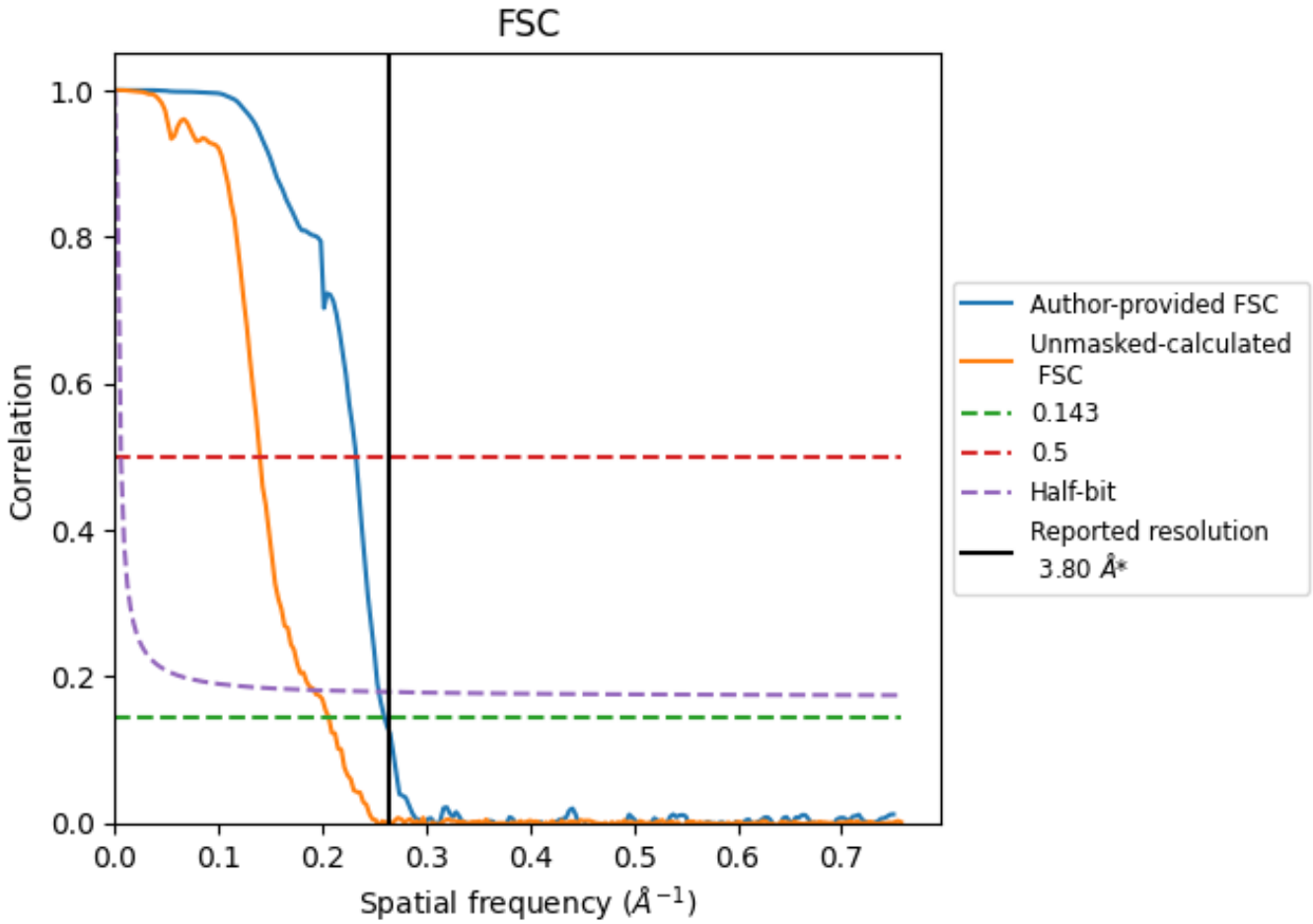


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

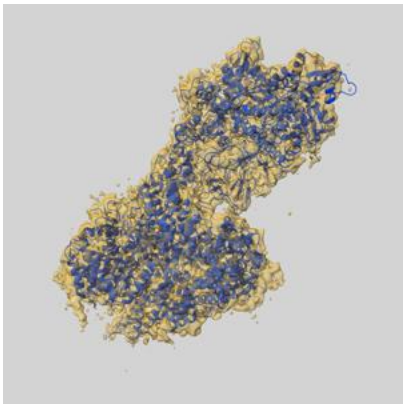
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.85	4.30	3.93
Unmasked-calculated*	4.85	7.15	5.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.85 differs from the reported value 3.8 by more than 10 %

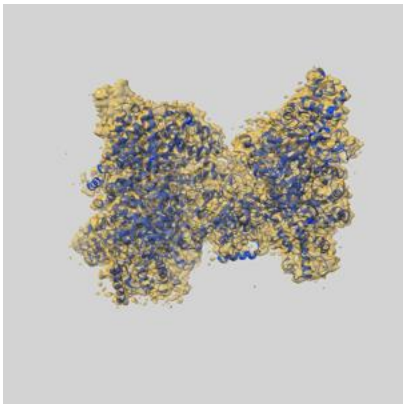
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33794 and PDB model 7YFN. Per-residue inclusion information can be found in section 3 on page 5.

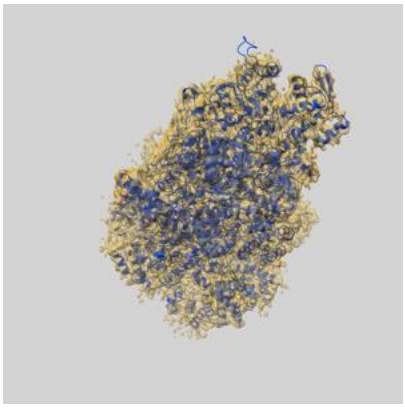
9.1 Map-model overlay



X



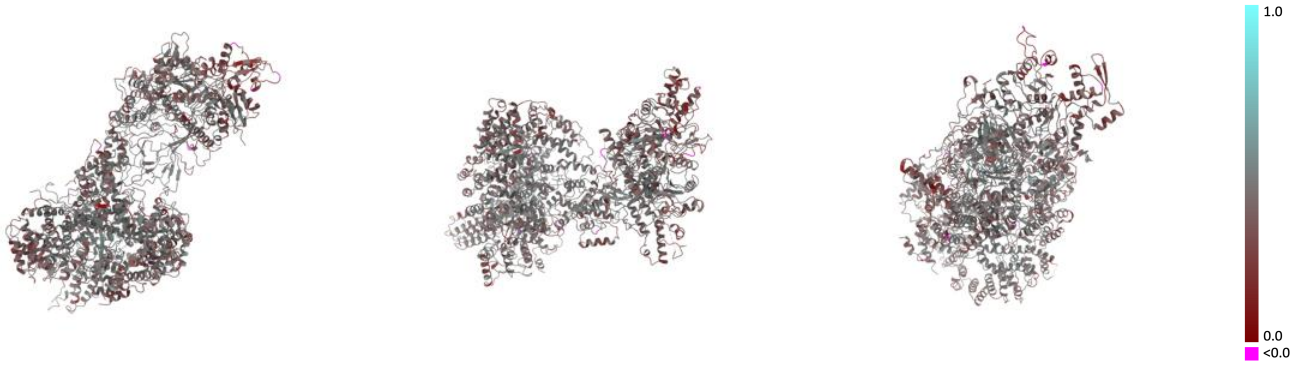
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0396 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.

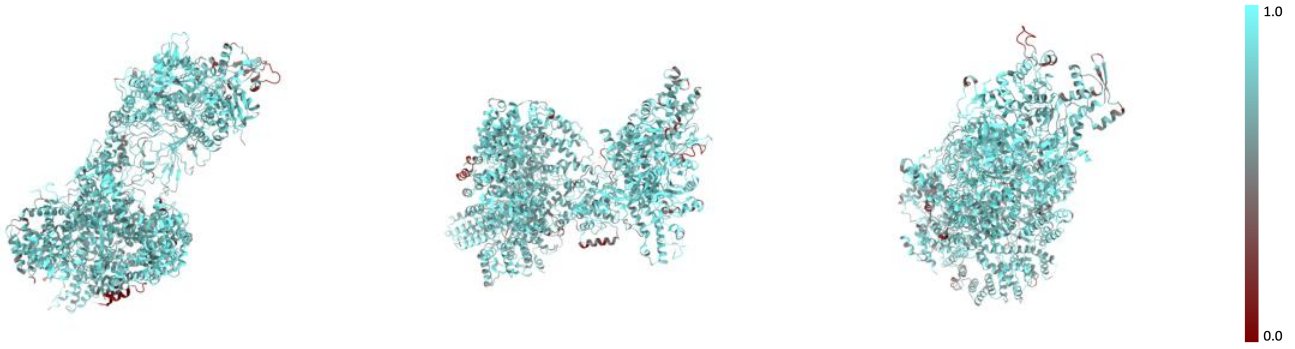
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

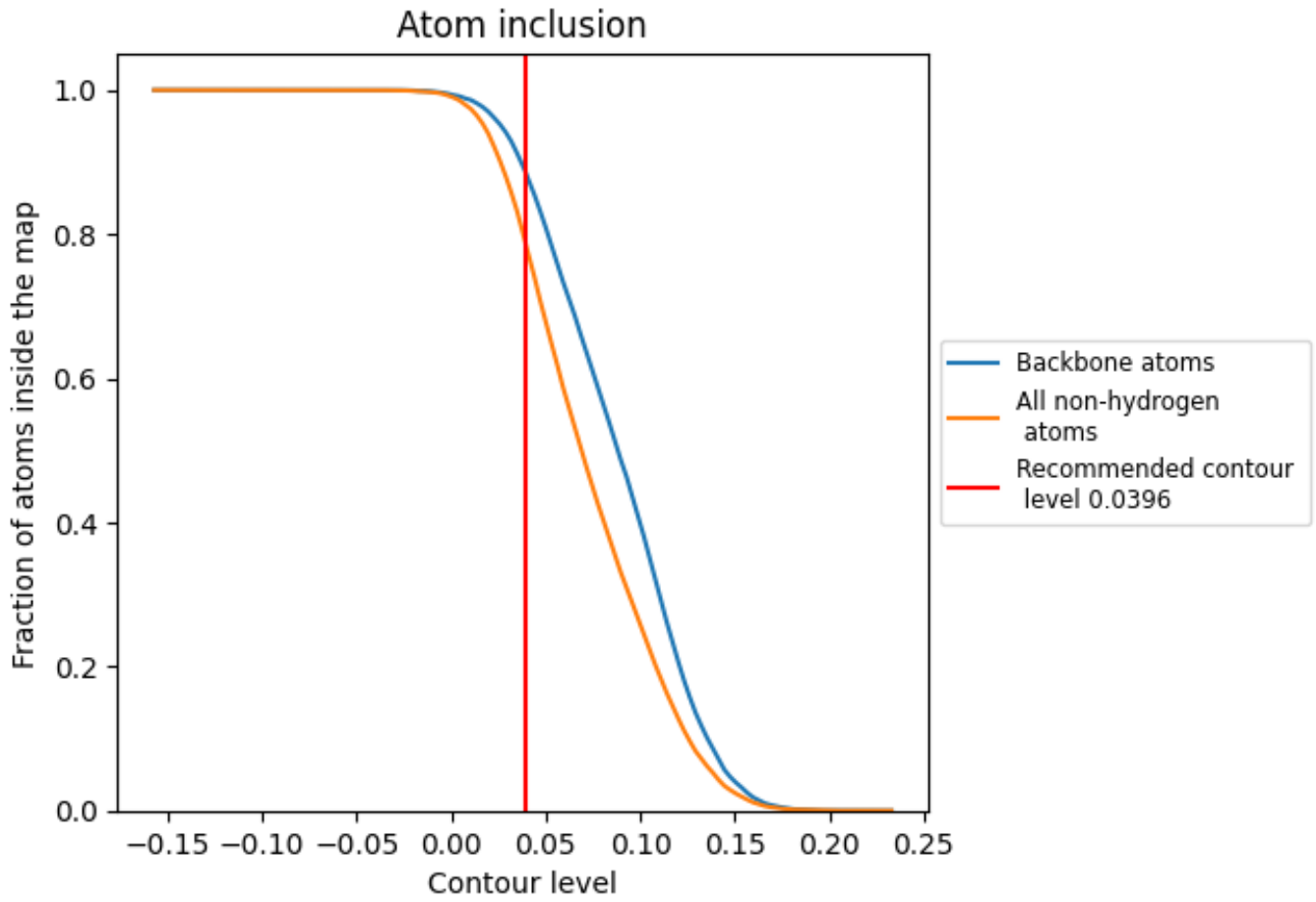
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0396).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0396) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7857	0.4140
A	0.7537	0.3800
B	0.8481	0.4410
D	0.7659	0.4070
E	0.7940	0.3820
F	0.7380	0.4150
T	0.7857	0.4210