



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:49 PM UTC

PDB ID : 7ZVW / pdb_00007zvw
EMDB ID : EMD-14989
Title : NuA4 Histone Acetyltransferase Complex
Authors : Schultz, P.; Ben-Shem, A.; Frechard, A.
Deposited on : 2022-05-17
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

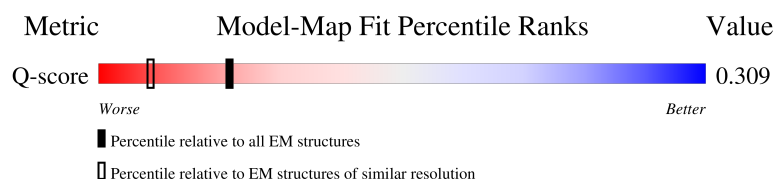
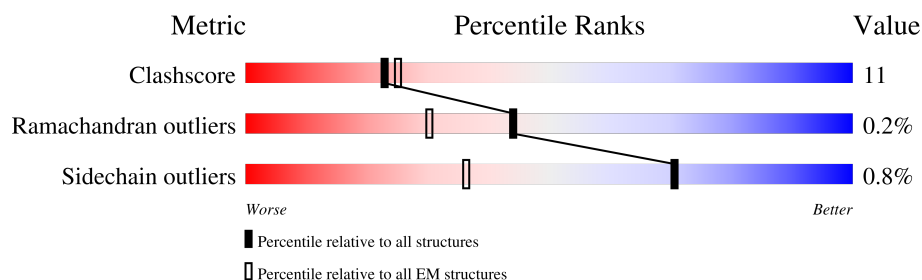
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	3825	
2	B	376	
3	G	468	
4	E	1051	

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Mol	Chain	Length	Quality of chain
4	H	1051	98%
5	F	565	24% 12% 61%
6	C	752	7% 23% 6% 70%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 37905 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 Transcription-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3226	Total	C	N	O	S	0	0
			24052	15394	4173	4395	90		

- Molecule 2 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	350	Total	C	N	O	S	0	0
			2735	1740	457	522	16		

- Molecule 3 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	422	Total	C	N	O	S	0	0
			3310	2110	557	633	10		

- Molecule 4 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	488	Total	C	N	O	S	0	0
			3952	2521	696	724	11		
4	H	22	Total	C	N	O		0	0
			110	66	22	22			

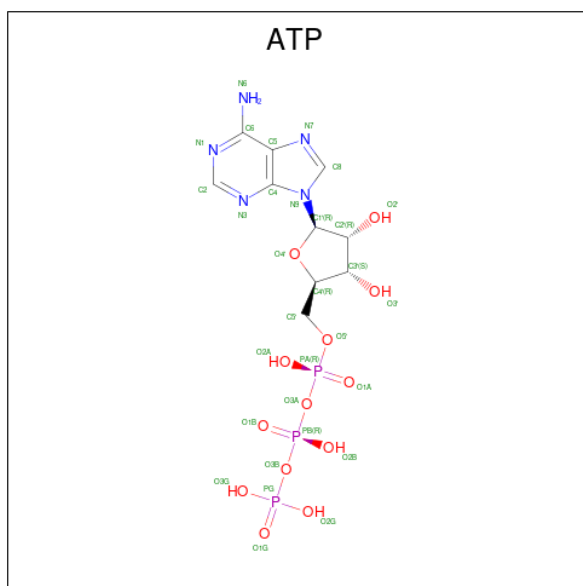
- Molecule 5 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	223	Total	C	N	O	S	0	0
			1877	1189	321	362	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	224	Total	C	N	O	S	0	0
			1805	1135	314	347	9		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

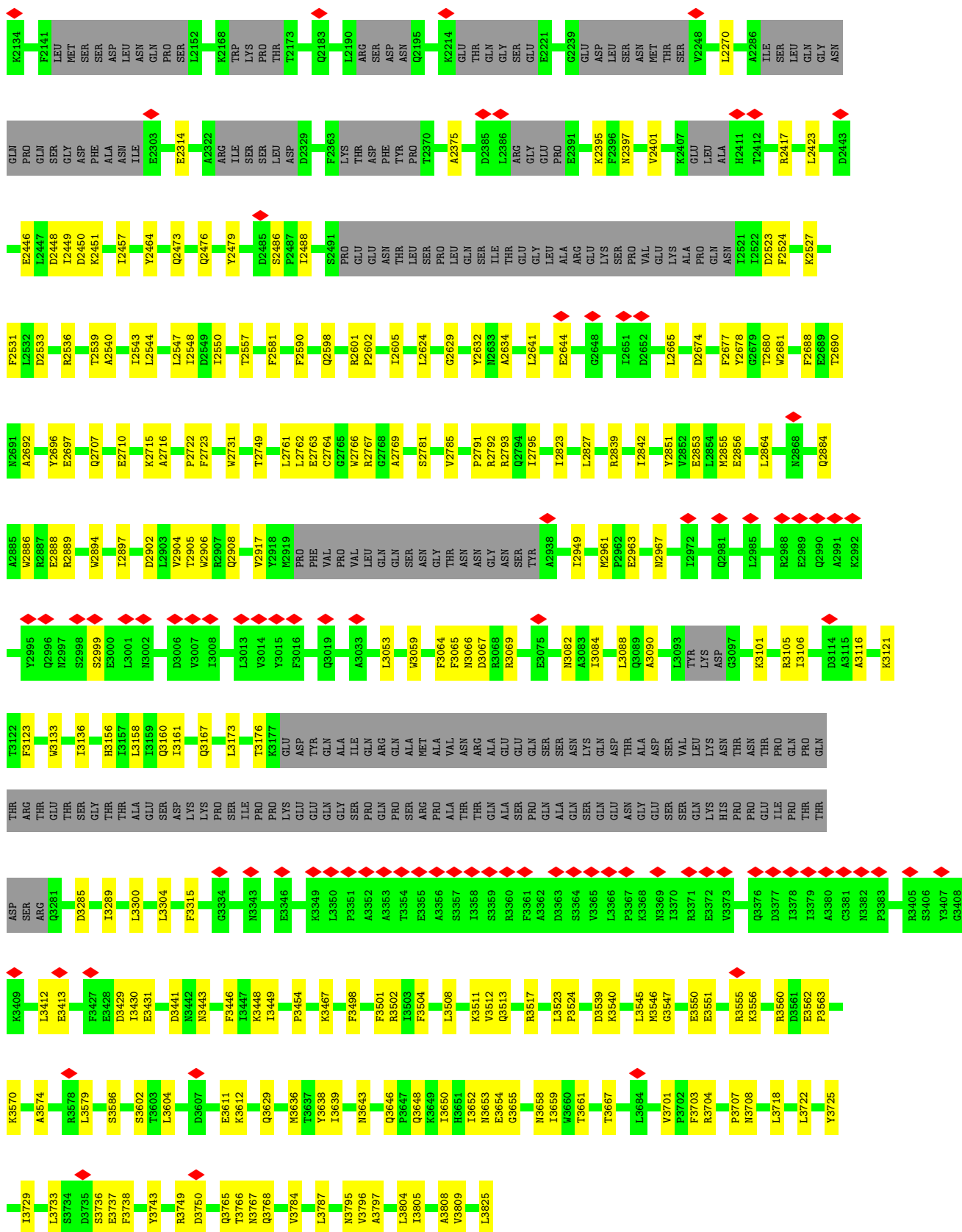


Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

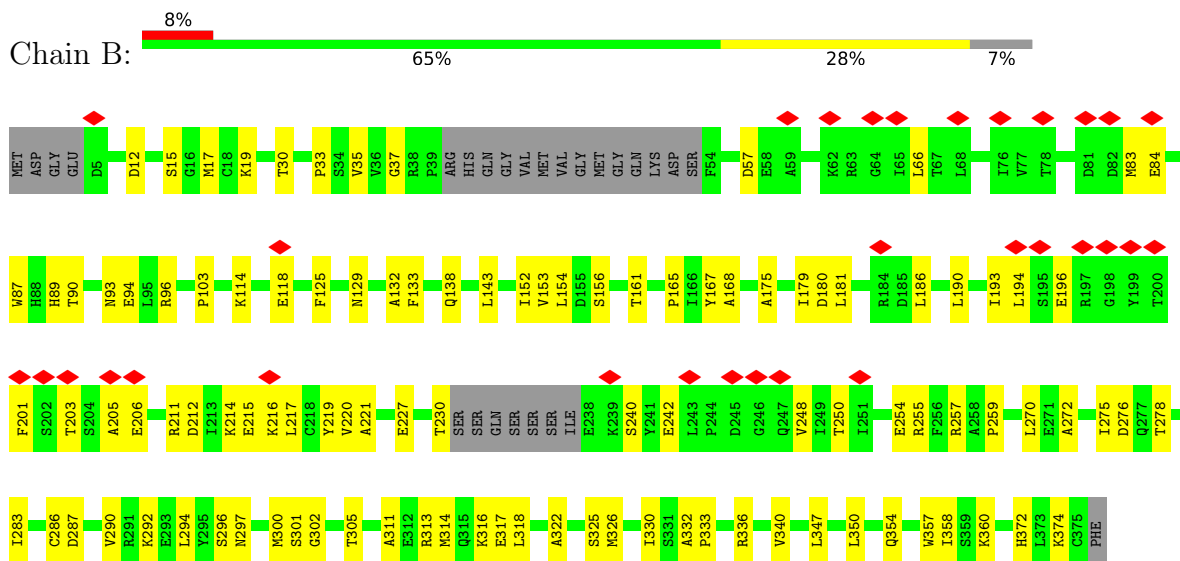
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	
8	G	1	Total	Mg	0
			1	1	

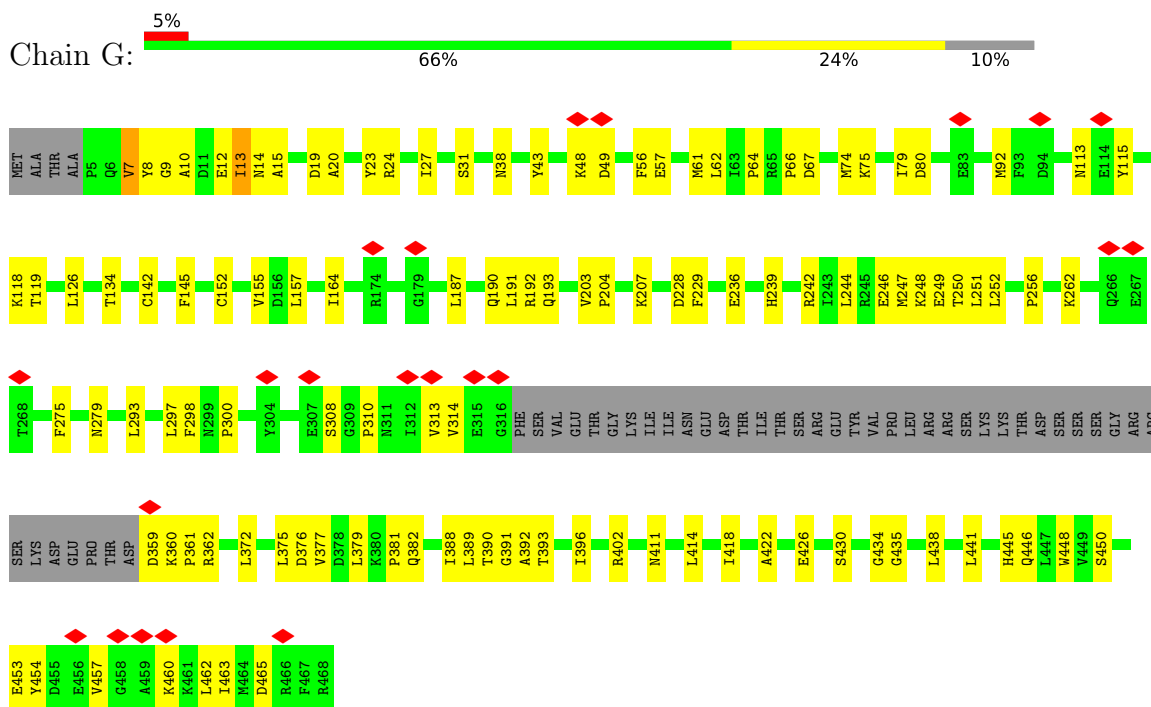




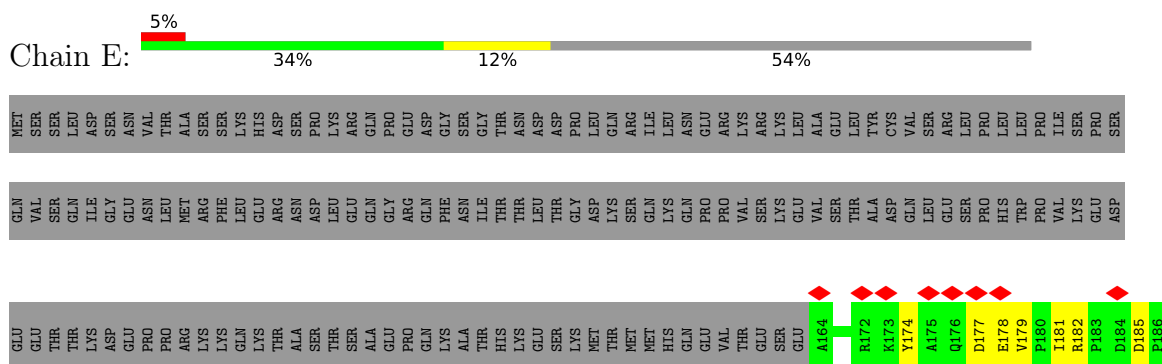
- Molecule 2: Actin

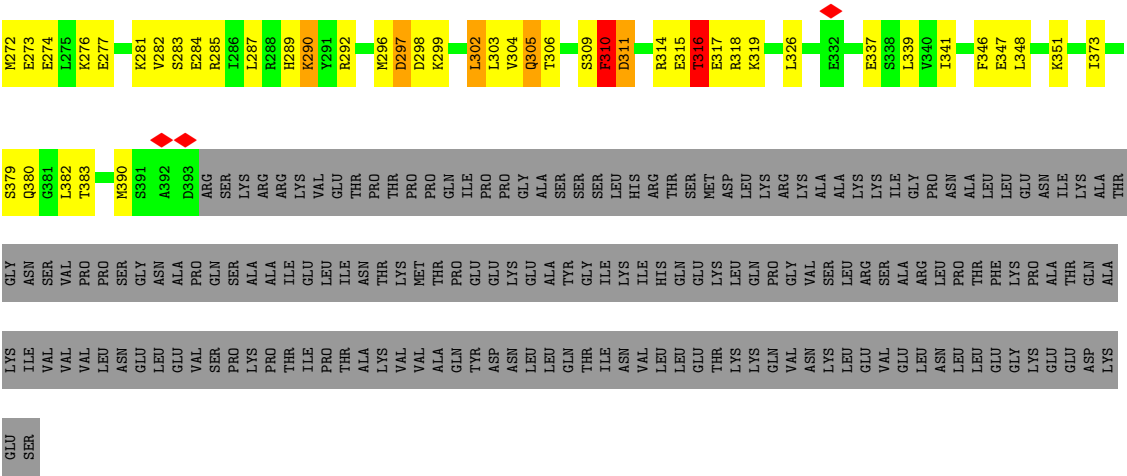


- Molecule 3: Actin

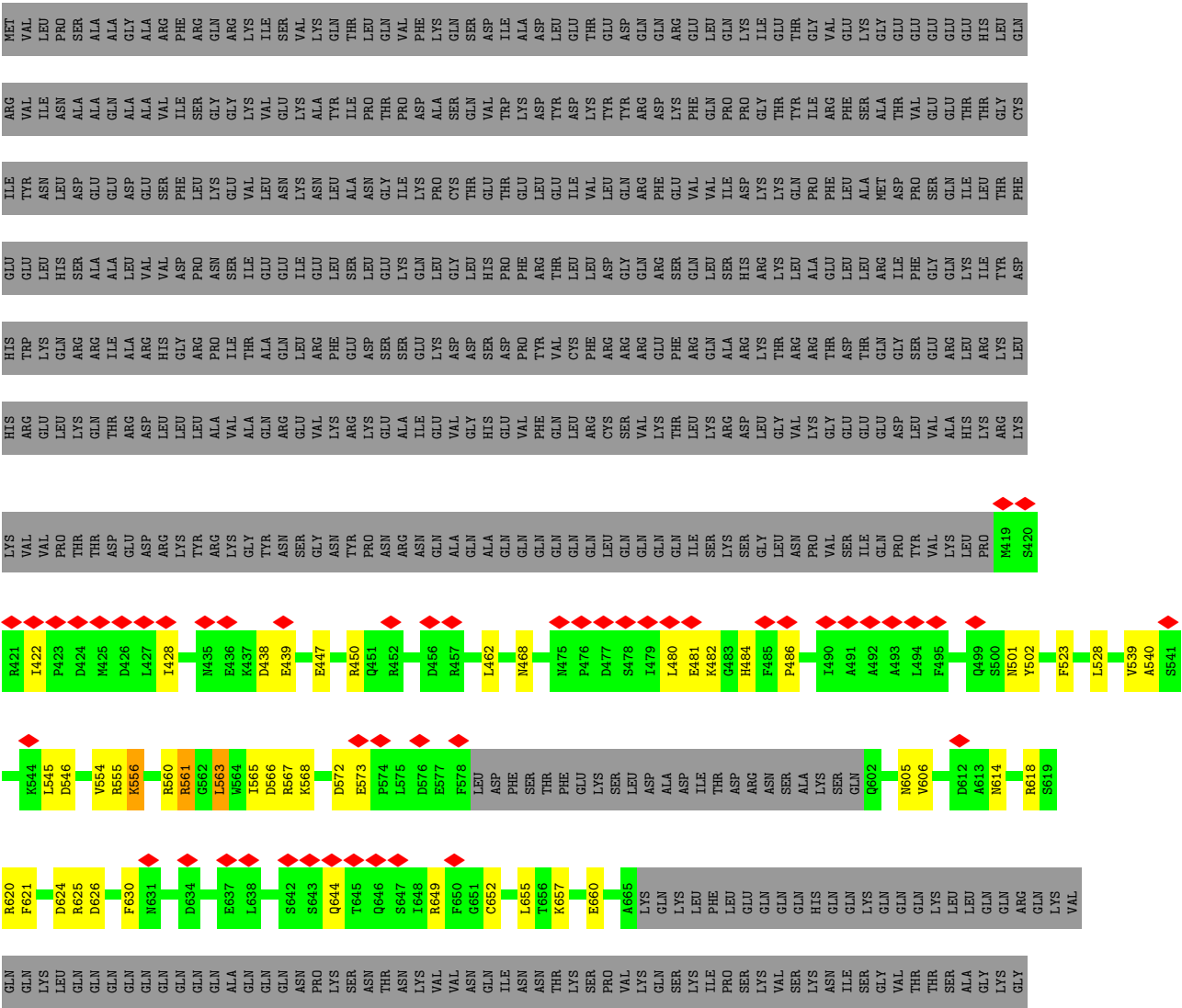


- Molecule 4: Chromatin modification-related protein EAF1





• Molecule 6: Enhancer of polycomb-like protein



ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	518386	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.8	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.005	Depositor
Minimum map value	-2.188	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	386.176, 386.176, 386.176	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.862, 0.862, 0.862	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, MG

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	0.13	0/24505	0.32	0/33321
2	B	0.11	0/2795	0.33	0/3788
3	G	0.24	0/3377	0.43	1/4577 (0.0%)
4	E	0.33	0/4044	0.57	7/5478 (0.1%)
4	H	1.06	0/109	2.33	5/151 (3.3%)
5	F	0.57	1/1916 (0.1%)	1.16	23/2579 (0.9%)
6	C	0.22	0/1842	0.49	0/2495
All	All	0.22	1/38588 (0.0%)	0.47	36/52389 (0.1%)

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
4	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	309	SER	CA-CB	-5.02	1.46	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	310	PHE	CA-CB-CG	10.32	124.12	113.80
4	E	332	GLY	CA-C-O	-10.05	114.58	122.52
5	F	101	GLU	N-CA-C	-9.98	100.37	112.54
4	E	412	PRO	N-CA-CB	9.38	113.10	103.25
4	H	396	GLU	N-CA-C	-8.83	101.65	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	394	PRO	N-CA-C	-8.44	95.08	112.47
5	F	79	PHE	CA-CB-CG	8.30	122.10	113.80
5	F	290	LYS	N-CA-C	-8.11	103.36	113.18
5	F	299	LYS	CB-CA-C	-7.62	107.80	116.63
5	F	104	LYS	N-CA-C	-7.31	102.65	113.40
4	E	415	GLU	CA-C-N	-7.17	110.15	121.62
4	E	415	GLU	C-N-CA	-7.17	110.15	121.62
5	F	108	TYR	N-CA-C	-6.91	100.22	110.23
4	H	400	THR	CB-CA-C	6.67	116.44	109.83
5	F	290	LYS	CA-C-N	-6.65	112.18	122.49
5	F	290	LYS	C-N-CA	-6.65	112.18	122.49
5	F	316	THR	N-CA-C	-6.46	104.24	111.28
4	H	398	ASN	N-CA-C	-6.37	105.46	112.72
3	G	10	ALA	N-CA-CB	-6.30	100.38	110.46
5	F	85	GLU	CA-C-O	-6.27	114.59	121.87
5	F	297	ASP	CB-CA-C	-6.27	98.95	109.48
5	F	113	TYR	CA-C-N	-6.03	110.02	121.54
5	F	113	TYR	C-N-CA	-6.03	110.02	121.54
5	F	111	GLU	N-CA-C	-5.99	105.80	113.23
5	F	110	PHE	CB-CA-C	5.93	118.60	110.06
4	H	390	GLU	N-CA-C	5.93	116.07	108.24
4	E	330	THR	CB-CA-C	-5.79	100.63	110.88
5	F	310	PHE	N-CA-CB	-5.73	100.81	110.49
5	F	112	LYS	N-CA-C	-5.66	105.21	111.71
5	F	78	GLU	N-CA-C	5.61	117.48	111.36
5	F	102	LEU	N-CA-C	-5.54	106.37	113.02
4	E	415	GLU	CB-CA-C	-5.33	99.82	110.42
5	F	316	THR	CA-C-N	-5.26	113.23	120.28
5	F	316	THR	C-N-CA	-5.26	113.23	120.28
5	F	78	GLU	CA-C-O	-5.24	114.87	120.42
4	E	303	LEU	N-CA-C	-5.13	105.77	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	300	MET	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24052	0	22457	498	0
2	B	2735	0	2704	84	0
3	G	3310	0	3269	84	0
4	E	3952	0	3937	109	0
4	H	110	0	51	1	0
5	F	1877	0	1848	81	0
6	C	1805	0	1782	42	0
7	B	31	0	12	3	0
7	G	31	0	12	3	0
8	B	1	0	0	0	0
8	G	1	0	0	0	0
All	All	37905	0	36072	827	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 11.

All (827) 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)
4:E:411:ASN:CB	4:E:444:GLY:H	1.57	1.17
4:E:411:ASN:CB	4:E:444:GLY:N	2.17	1.07
1:A:744:LYS:HG2	1:A:748:MET:HE1	1.56	0.88
1:A:1872:TYR:HA	1:A:1875:LEU:HD23	1.56	0.86
2:B:129:ASN:HD21	5:F:70:LYS:HB3	1.40	0.85
1:A:2894:TRP:HA	1:A:3512:VAL:HG23	1.56	0.84
1:A:2853:GLU:HB3	1:A:2906:TRP:HH2	1.43	0.83
5:F:271:SER:HB3	5:F:276:LYS:HD3	1.62	0.82
1:A:1410:ALA:O	1:A:1413:ARG:NH1	2.13	0.81
3:G:256:PRO:HA	3:G:402:ARG:HE	1.44	0.80
1:A:1913:HIS:HE1	1:A:1963:ILE:HG13	1.48	0.77
1:A:686:MET:HG3	1:A:690:MET:HE1	1.67	0.77
5:F:289:HIS:CE1	5:F:305:GLN:HG3	2.21	0.76
1:A:1914:GLN:O	1:A:1918:ARG:N	2.20	0.74
4:E:316:ALA:HB2	4:E:421:LEU:HD22	1.69	0.74
2:B:129:ASN:ND2	5:F:70:LYS:HB3	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1507:LEU:O	1:A:1511:GLN:NE2	2.20	0.73
2:B:190:LEU:HD13	2:B:193:ILE:HD11	1.69	0.72
1:A:688:LYS:HA	1:A:691:LEU:HD12	1.71	0.72
3:G:445:HIS:HD2	3:G:448:TRP:HE1	1.35	0.72
4:E:411:ASN:CB	4:E:444:GLY:CA	2.67	0.72
1:A:576:MET:HG3	1:A:666:MET:HB2	1.71	0.72
3:G:313:VAL:HA	3:G:362:ARG:HH12	1.53	0.72
1:A:3602:SER:O	1:A:3708:ASN:ND2	2.25	0.70
1:A:2476:GLN:HG2	1:A:2548:ILE:HD12	1.73	0.70
3:G:441:LEU:HD22	4:E:299:GLU:HB3	1.73	0.69
1:A:1518:LEU:HD11	1:A:1526:ASN:HD22	1.55	0.69
2:B:180:ASP:HB3	2:B:270:LEU:HD21	1.75	0.69
2:B:286:CYS:SG	2:B:287:ASP:N	2.65	0.68
4:E:295:HIS:ND1	5:F:113:TYR:HB3	2.09	0.68
1:A:3707:PRO:HG3	4:E:245:THR:HG21	1.74	0.68
4:E:535:LYS:O	4:E:537:PRO:HD3	1.93	0.68
3:G:392:ALA:HB3	7:G:501:ATP:H5'1	1.76	0.68
2:B:179:ILE:HD11	2:B:278:THR:HG21	1.75	0.68
1:A:1611:ASP:HA	1:A:1617:ARG:HH22	1.59	0.68
1:A:3431:GLU:OE2	1:A:3448:LYS:NZ	2.27	0.68
1:A:1726:ASP:O	1:A:1730:LYS:NZ	2.26	0.68
1:A:3084:ILE:HD11	1:A:3106:ILE:HG23	1.75	0.68
1:A:325:HIS:O	1:A:329:HIS:ND1	2.23	0.67
1:A:1549:PHE:HB2	1:A:1552:ASP:HB2	1.76	0.67
3:G:64:PRO:HB2	3:G:229:PHE:HZ	1.60	0.67
4:E:421:LEU:HD12	4:E:422:PRO:HD2	1.76	0.67
1:A:546:PRO:HB2	1:A:547:ILE:HD12	1.76	0.67
2:B:161:THR:HB	2:B:179:ILE:HB	1.75	0.67
2:B:179:ILE:HG22	2:B:181:LEU:H	1.60	0.67
2:B:300:MET:HE1	2:B:336:ARG:HD3	1.75	0.66
1:A:1599:GLU:HG2	1:A:1600:ILE:HD12	1.76	0.66
5:F:81:ASN:C	5:F:83:ALA:H	2.03	0.66
1:A:3646:GLN:OE1	1:A:3648:GLN:NE2	2.27	0.66
1:A:773:LEU:HD13	1:A:815:LEU:HD13	1.76	0.66
5:F:123:THR:OG1	5:F:126:GLU:OE1	2.14	0.66
1:A:1069:VAL:HG21	1:A:1142:MET:HG2	1.77	0.66
4:E:671:MET:HG3	5:F:382:LEU:HD12	1.78	0.66
1:A:2792:ARG:NH2	1:A:2902:ASP:OD1	2.28	0.66
4:E:411:ASN:CB	4:E:444:GLY:HA3	2.26	0.65
1:A:2766:TRP:NE1	1:A:2902:ASP:OD1	2.29	0.65
1:A:2375:ALA:HB1	1:A:2417:ARG:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:CYS:O	1:A:749:SER:OG	2.13	0.65
1:A:1226:ARG:NH2	1:A:1275:ASP:OD1	2.30	0.65
3:G:248:LYS:HA	3:G:252:LEU:HD23	1.78	0.65
3:G:390:THR:HG22	3:G:391:GLY:H	1.60	0.65
3:G:422:ALA:N	6:C:624:ASP:OD2	2.30	0.65
4:E:182:ARG:HH12	6:C:630:PHE:HA	1.62	0.65
4:E:653:ARG:NH2	4:E:658:LEU:O	2.31	0.64
4:E:665:ASP:OD1	4:E:668:ARG:NH2	2.30	0.64
2:B:201:PHE:HB3	2:B:206:GLU:HB3	1.78	0.64
1:A:2598:GLN:O	1:A:2601:ARG:NH2	2.31	0.64
1:A:2665:LEU:HD21	1:A:2680:THR:HB	1.80	0.64
2:B:37:GLY:HA3	2:B:66:LEU:HD13	1.78	0.64
1:A:416:LEU:HD11	1:A:574:THR:HB	1.79	0.63
1:A:620:LEU:HG	1:A:623:ARG:HH21	1.63	0.63
1:A:1915:ILE:HA	1:A:1918:ARG:HG2	1.79	0.63
1:A:3116:ALA:O	1:A:3121:LYS:NZ	2.31	0.63
2:B:242:GLU:HA	2:B:248:VAL:HA	1.80	0.63
1:A:1205:ILE:HA	1:A:1207:MET:HE3	1.80	0.63
4:E:297:LEU:O	4:E:300:MET:HB3	1.98	0.63
1:A:1255:LEU:HB3	1:A:1261:PHE:HE1	1.64	0.63
2:B:360:LYS:HG2	5:F:71:PRO:HG3	1.80	0.63
1:A:1659:LYS:NZ	1:A:1660:GLU:OE2	2.32	0.62
4:E:664:LEU:HA	4:E:667:MET:HG3	1.81	0.62
1:A:1591:PHE:HD2	1:A:1604:PHE:HD1	1.47	0.62
1:A:2710:GLU:HA	4:E:667:MET:HE1	1.81	0.62
2:B:84:GLU:HA	2:B:87:TRP:CE3	2.35	0.62
2:B:168:ALA:HB2	4:E:430:LYS:HZ3	1.64	0.62
3:G:191:LEU:HD22	3:G:293:LEU:HD21	1.80	0.62
3:G:446:GLN:HA	5:F:84:ARG:HG2	1.81	0.62
3:G:300:PRO:HG2	3:G:361:PRO:HB2	1.81	0.62
4:E:332:GLY:C	4:E:334:ILE:H	2.08	0.62
1:A:394:TYR:HE1	1:A:414:LEU:HD13	1.64	0.62
1:A:1605:VAL:HG22	1:A:1650:LEU:HD23	1.81	0.62
4:E:448:PHE:HB3	4:E:452:ASP:HB2	1.81	0.62
1:A:1703:LEU:HA	1:A:1706:LEU:HD12	1.81	0.62
1:A:388:TRP:CZ3	1:A:1691:PRO:HD2	2.35	0.61
1:A:1209:TYR:OH	1:A:1213:ARG:NH1	2.32	0.61
1:A:1747:VAL:HA	1:A:1787:ILE:HD13	1.81	0.61
1:A:811:LEU:HD11	1:A:1382:LYS:HG3	1.81	0.61
4:E:417:ILE:HG13	6:C:563:LEU:HB2	1.80	0.61
1:A:1352:GLU:HB3	1:A:1356:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2665:LEU:HD13	1:A:2681:TRP:CE2	2.35	0.61
4:E:535:LYS:HE2	4:E:616:ARG:HB3	1.83	0.61
1:A:2446:GLU:HG3	1:A:2448:ASP:H	1.65	0.61
1:A:2690:THR:OG1	1:A:2731:TRP:NE1	2.23	0.61
1:A:1079:LYS:HG3	1:A:1142:MET:HE1	1.82	0.60
4:E:597:TRP:NE1	4:E:601:GLU:OE2	2.34	0.60
1:A:2855:MET:HE3	1:A:2855:MET:HA	1.83	0.60
1:A:3639:ILE:HD12	1:A:3784:VAL:HG22	1.83	0.60
4:E:414:ASP:O	4:E:415:GLU:C	2.43	0.60
4:E:546:GLU:O	4:E:639:ARG:NH1	2.34	0.60
1:A:1925:LEU:HB3	1:A:1967:ILE:HD13	1.84	0.59
1:A:420:GLU:HA	1:A:423:MET:HE2	1.84	0.59
1:A:1023:MET:HA	1:A:1026:ILE:HG12	1.84	0.59
1:A:1398:LEU:HD12	1:A:1420:ILE:HD12	1.85	0.59
1:A:1792:SER:HA	1:A:1795:HIS:HB3	1.84	0.59
3:G:9:GLY:HA2	4:E:302:TRP:CH2	2.38	0.59
1:A:689:GLN:HB3	1:A:696:LEU:HD13	1.84	0.59
1:A:1727:LYS:HA	1:A:1730:LYS:HE2	1.83	0.59
1:A:416:LEU:O	1:A:419:ILE:HG22	2.03	0.59
1:A:1063:GLU:HG3	1:A:1130:TYR:CD2	2.38	0.59
1:A:1964:TYR:HA	1:A:1967:ILE:HG22	1.84	0.59
3:G:376:ASP:OD1	3:G:377:VAL:N	2.35	0.59
2:B:89:HIS:HD2	2:B:93:ASN:HB2	1.67	0.59
1:A:1004:LEU:HD13	1:A:2488:ILE:HG22	1.83	0.59
1:A:1918:ARG:HA	1:A:1921:VAL:HG22	1.84	0.59
4:E:332:GLY:O	4:E:334:ILE:N	2.36	0.59
2:B:96:ARG:NE	4:E:345:LEU:O	2.30	0.58
1:A:1574:GLU:HG3	1:A:1575:PRO:HD3	1.85	0.58
1:A:3502:ARG:NH2	1:A:3524:PRO:O	2.36	0.58
1:A:3511:LYS:NZ	1:A:3737:GLU:OE2	2.35	0.58
1:A:3513:GLN:OE1	1:A:3517:ARG:NH1	2.32	0.58
1:A:3703:PHE:HE2	1:A:3804:LEU:HB3	1.66	0.58
1:A:1352:GLU:HB3	1:A:1356:ARG:NH1	2.18	0.58
1:A:802:GLU:HB2	1:A:844:VAL:HG23	1.86	0.58
1:A:1144:LEU:HB3	1:A:1198:MET:HE1	1.85	0.58
1:A:1523:LEU:HD11	1:A:1564:LEU:HD21	1.84	0.58
1:A:331:LEU:HD13	1:A:373:ASP:HB2	1.85	0.58
1:A:432:ARG:NH1	1:A:582:SER:O	2.36	0.58
4:E:499:TRP:HE1	6:C:555:ARG:NH2	2.02	0.58
1:A:1680:LEU:HB2	1:A:1700:PHE:HZ	1.69	0.57
1:A:3443:ASN:O	1:A:3443:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:48:LYS:HD3	3:G:66:PRO:HB2	1.86	0.57
3:G:251:LEU:HD11	3:G:275:PHE:HB2	1.85	0.57
4:E:651:ILE:HG21	4:E:657:ARG:HB2	1.84	0.57
1:A:444:LYS:O	1:A:448:MET:HG3	2.05	0.57
2:B:114:LYS:NZ	3:G:31:SER:OG	2.36	0.57
2:B:132:ALA:HB1	2:B:357:TRP:HB3	1.86	0.57
5:F:390:MET:HE1	6:C:422:ILE:HG12	1.85	0.57
1:A:3570:LYS:HD3	6:C:644:GLN:HE21	1.69	0.57
2:B:103:PRO:HB3	2:B:132:ALA:HB3	1.86	0.57
1:A:435:LEU:HA	1:A:438:ILE:HD12	1.87	0.57
3:G:75:LYS:NZ	3:G:80:ASP:OD2	2.38	0.57
4:E:542:ILE:HD11	4:E:548:ARG:HD2	1.87	0.57
1:A:1793:GLU:C	1:A:1794:MET:HE2	2.30	0.57
1:A:2856:GLU:OE1	1:A:2889:ARG:NH2	2.38	0.57
1:A:764:HIS:NE2	1:A:1525:ASN:OD1	2.28	0.57
4:E:245:THR:O	4:E:249:GLU:HG2	2.03	0.57
1:A:1677:SER:HA	1:A:1730:LYS:HD2	1.86	0.57
4:H:403:VAL:HA	4:H:406:LEU:CB	2.34	0.57
3:G:145:PHE:HA	4:E:300:MET:HE1	1.87	0.56
3:G:157:LEU:O	3:G:393:THR:OG1	2.22	0.56
3:G:204:PRO:HD2	3:G:207:LYS:HD2	1.86	0.56
3:G:24:ARG:HD3	3:G:38:ASN:HB2	1.88	0.56
3:G:155:VAL:HG23	3:G:164:ILE:HG12	1.87	0.56
1:A:325:HIS:O	1:A:328:ARG:HG3	2.06	0.56
1:A:2853:GLU:HB3	1:A:2906:TRP:CH2	2.31	0.56
1:A:1189:LYS:HE2	1:A:1227:ASP:HB3	1.87	0.56
1:A:1861:MET:O	1:A:1865:ILE:HG13	2.06	0.56
2:B:220:VAL:HG22	2:B:259:PRO:HB3	1.87	0.56
3:G:74:MET:HA	3:G:74:MET:HE3	1.86	0.56
1:A:428:LYS:HZ3	1:A:430:GLU:HB2	1.70	0.56
1:A:1817:ASP:HA	1:A:1821:TRP:CZ3	2.41	0.56
1:A:3643:ASN:OD1	1:A:3667:THR:OG1	2.24	0.56
2:B:152:ILE:HD11	2:B:283:ILE:HD13	1.86	0.56
3:G:48:LYS:HB2	3:G:67:ASP:HB3	1.86	0.56
1:A:394:TYR:CE1	1:A:414:LEU:HD13	2.41	0.56
1:A:1652:GLU:OE2	1:A:1702:THR:HB	2.05	0.56
1:A:1886:VAL:HG22	1:A:1924:ALA:HB2	1.88	0.56
4:E:194:GLU:HG3	4:E:201:THR:HG21	1.87	0.56
4:E:419:PRO:HB2	6:C:567:ARG:HH21	1.71	0.56
1:A:1411:GLN:HE22	1:A:1417:ARG:HB3	1.71	0.56
6:C:556:LYS:HZ1	6:C:563:LEU:HB3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:HG12	1:A:557:LEU:HB3	1.86	0.56
1:A:3508:LEU:HD11	1:A:3729:ILE:HG12	1.88	0.56
1:A:704:LEU:HD13	1:A:749:SER:HB3	1.87	0.56
1:A:428:LYS:HG3	1:A:431:SER:H	1.71	0.55
2:B:314:MET:HE3	2:B:314:MET:O	2.05	0.55
5:F:292:ARG:CG	5:F:297:ASP:HB2	2.35	0.55
1:A:1200:LEU:HD12	1:A:1243:LEU:HD21	1.87	0.55
3:G:113:ASN:HB3	3:G:118:LYS:HE3	1.89	0.55
1:A:314:SER:HA	1:A:320:ARG:HH12	1.72	0.55
1:A:1327:PHE:HB3	1:A:1386:GLN:NE2	2.21	0.55
4:E:209:ILE:HD11	4:E:496:ASP:HA	1.87	0.55
1:A:687:TYR:CZ	1:A:691:LEU:HD21	2.41	0.55
1:A:3156:HIS:ND1	1:A:3160:GLN:OE1	2.39	0.55
2:B:270:LEU:HG	2:B:272:ALA:H	1.72	0.55
1:A:1639:GLU:O	1:A:1643:ARG:NH2	2.40	0.55
1:A:2897:ILE:HG21	1:A:2961:MET:HE1	1.88	0.55
2:B:167:TYR:CE1	4:E:430:LYS:HE3	2.42	0.55
1:A:961:GLY:HA3	1:A:2449:ILE:HG22	1.89	0.55
1:A:1878:ASN:OD1	1:A:1879:THR:N	2.39	0.55
1:A:1591:PHE:CD2	1:A:1604:PHE:HD1	2.24	0.55
1:A:2710:GLU:OE2	4:E:674:ARG:NH2	2.40	0.55
1:A:3167:GLN:HE21	1:A:3300:LEU:HD12	1.71	0.55
1:A:3629:GLN:HG3	1:A:3658:ASN:HA	1.88	0.55
2:B:87:TRP:HA	2:B:90:THR:HG22	1.89	0.55
6:C:438:ASP:OD1	6:C:439:GLU:N	2.40	0.55
1:A:825:GLU:OE1	1:A:832:ARG:NH1	2.39	0.55
2:B:347:LEU:HD12	2:B:350:LEU:HD12	1.89	0.55
1:A:1515:LEU:HD22	1:A:1564:LEU:HB2	1.89	0.54
1:A:774:LYS:O	1:A:777:THR:OG1	2.19	0.54
1:A:1762:THR:O	1:A:1765:ARG:HG3	2.07	0.54
1:A:3701:VAL:HG23	1:A:3808:ALA:HA	1.90	0.54
2:B:325:SER:HB2	6:C:605:ASN:HD22	1.72	0.54
1:A:2749:THR:OG1	1:A:2763:GLU:OE1	2.24	0.54
1:A:3550:GLU:OE2	1:A:3560:ARG:NH1	2.39	0.54
1:A:691:LEU:HD22	1:A:735:LYS:HG2	1.90	0.54
5:F:310:PHE:CG	5:F:311:ASP:N	2.74	0.54
2:B:30:THR:HG21	2:B:94:GLU:HB3	1.90	0.54
4:E:494:PRO:HB3	6:C:501:ASN:HD21	1.72	0.54
1:A:1518:LEU:HD13	1:A:1521:GLN:HB2	1.89	0.54
1:A:3429:ASP:HB2	1:A:3448:LYS:HD3	1.90	0.54
1:A:1913:HIS:CD2	1:A:1921:VAL:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:465:ASP:O	5:F:253:LYS:NZ	2.36	0.54
1:A:934:ARG:HD2	1:A:2842:ILE:HG12	1.90	0.53
1:A:1133:SER:HB2	1:A:1191:ALA:HB2	1.89	0.53
1:A:3136:ILE:HD13	1:A:3161:ILE:HD11	1.88	0.53
1:A:3767:ASN:OD1	1:A:3768:GLN:N	2.41	0.53
2:B:12:ASP:HB3	2:B:19:LYS:HB2	1.90	0.53
1:A:2908:GLN:NE2	1:A:2949:ILE:HD11	2.23	0.53
5:F:106:SER:O	5:F:108:TYR:N	2.42	0.53
6:C:620:ARG:HH21	6:C:621:PHE:HZ	1.56	0.53
1:A:765:LEU:HD11	1:A:792:LEU:HD11	1.89	0.53
5:F:292:ARG:HB3	5:F:297:ASP:HB2	1.91	0.53
1:A:2762:LEU:HG	1:A:2767:ARG:HH12	1.72	0.53
2:B:296:SER:OG	2:B:297:ASN:OD1	2.25	0.53
1:A:3574:ALA:O	6:C:649:ARG:NH1	2.42	0.53
5:F:237:ALA:HB1	5:F:239:TRP:CD1	2.43	0.53
1:A:1432:SER:O	1:A:1436:ILE:HG12	2.09	0.53
1:A:1890:TYR:HE1	1:A:1927:LEU:HG	1.73	0.53
5:F:304:VAL:O	5:F:305:GLN:C	2.51	0.53
1:A:1664:ASP:OD1	1:A:1665:LYS:NZ	2.36	0.53
1:A:1763:ILE:O	1:A:1780:TYR:OH	2.27	0.53
1:A:1915:ILE:HD12	1:A:1918:ARG:HD2	1.90	0.53
1:A:2764:CYS:O	1:A:2769:ALA:N	2.41	0.53
1:A:837:GLU:O	1:A:841:THR:OG1	2.19	0.53
1:A:970:ILE:HD11	1:A:2543:ILE:HG21	1.91	0.53
1:A:2823:ILE:O	1:A:2827:LEU:HD23	2.09	0.53
1:A:3539:ASP:OD1	1:A:3540:LYS:N	2.42	0.53
2:B:143:LEU:HB2	2:B:153:VAL:HG21	1.91	0.53
1:A:1660:GLU:HA	1:A:1663:LYS:HD3	1.91	0.52
4:E:592:GLU:OE2	4:E:656:ARG:NH2	2.42	0.52
1:A:1704:GLN:O	1:A:1708:ILE:HG12	2.10	0.52
1:A:1748:VAL:HG22	1:A:1790:TYR:HE2	1.74	0.52
1:A:1881:LYS:O	1:A:1885:TYR:HD1	1.92	0.52
1:A:2884:GLN:NE2	1:A:2888:GLU:OE2	2.35	0.52
1:A:2601:ARG:HB2	1:A:2602:PRO:HD3	1.91	0.52
6:C:568:LYS:HB2	6:C:626:ASP:HB3	1.91	0.52
1:A:350:ARG:CZ	1:A:367:ALA:HB1	2.39	0.52
1:A:2457:ILE:HG13	1:A:2581:PHE:HE1	1.74	0.52
1:A:3579:LEU:HD11	6:C:649:ARG:NE	2.25	0.52
1:A:1068:ALA:HB1	1:A:1074:VAL:HG11	1.92	0.52
3:G:23:TYR:N	7:G:501:ATP:O2B	2.27	0.52
3:G:119:THR:HB	3:G:460:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1813:LEU:HA	1:A:1816:PHE:HB3	1.90	0.52
3:G:228:ASP:OD1	3:G:229:PHE:N	2.42	0.52
1:A:691:LEU:HD22	1:A:735:LYS:HE3	1.92	0.52
1:A:905:LEU:HD22	1:A:922:THR:HG23	1.91	0.52
1:A:3066:ASN:HD21	1:A:3082:ASN:HB2	1.75	0.52
3:G:411:ASN:HD21	3:G:414:LEU:HD23	1.75	0.52
4:E:220:LEU:N	5:F:347:GLU:OE2	2.43	0.52
4:E:535:LYS:NZ	4:E:614:ASP:O	2.26	0.52
1:A:685:PHE:HE1	1:A:689:GLN:HE21	1.56	0.52
1:A:2791:PRO:O	1:A:2795:ILE:HD12	2.10	0.52
2:B:211:ARG:O	2:B:215:GLU:HG3	2.09	0.52
3:G:13:ILE:HG22	3:G:15:ALA:HB2	1.92	0.52
1:A:883:ASP:OD1	1:A:884:ASN:ND2	2.42	0.52
3:G:190:GLN:O	3:G:193:GLN:HG3	2.10	0.52
6:C:657:LYS:O	6:C:660:GLU:HG3	2.10	0.52
1:A:364:ARG:HD2	1:A:403:LEU:HD21	1.92	0.51
1:A:3064:PHE:HZ	1:A:3101:LYS:HD2	1.75	0.51
2:B:165:PRO:HG2	2:B:175:ALA:HB1	1.93	0.51
1:A:1147:VAL:HA	1:A:1150:ILE:HD12	1.92	0.51
1:A:1399:SER:O	1:A:1403:THR:OG1	2.17	0.51
4:E:280:ARG:HH22	4:E:480:GLU:HG3	1.75	0.51
1:A:1079:LYS:HG2	1:A:1083:ARG:NE	2.26	0.51
2:B:84:GLU:HA	2:B:87:TRP:HE3	1.72	0.51
1:A:1325:LEU:HD12	1:A:1329:MET:HG2	1.92	0.51
1:A:1747:VAL:HG12	1:A:1790:TYR:HD2	1.75	0.51
1:A:3704:ARG:NH2	1:A:3825:LEU:O	2.39	0.51
3:G:308:SER:O	3:G:310:PRO:HD3	2.11	0.51
4:E:336:CYS:SG	4:E:337:ILE:N	2.83	0.51
1:A:375:ILE:HG23	1:A:382:LEU:HD11	1.91	0.51
1:A:1140:ARG:O	1:A:1144:LEU:HG	2.11	0.51
1:A:1913:HIS:CE1	1:A:1963:ILE:HG13	2.38	0.51
1:A:2605:ILE:HG21	1:A:2632:TYR:HD2	1.76	0.51
3:G:454:TYR:HE1	3:G:460:LYS:HD2	1.74	0.51
1:A:1680:LEU:HB2	1:A:1700:PHE:CZ	2.45	0.51
2:B:311:ALA:HA	2:B:330:ILE:HD13	1.93	0.51
1:A:411:SER:O	1:A:415:LEU:HD23	2.11	0.51
1:A:2692:ALA:HA	1:A:3796:VAL:HG23	1.93	0.51
4:E:197:ASP:OD1	4:E:198:ARG:N	2.44	0.51
4:E:246:ASP:OD1	6:C:484:HIS:NE2	2.35	0.51
1:A:1688:VAL:HG13	1:A:1691:PRO:HD3	1.93	0.51
3:G:250:THR:HB	6:C:606:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:292:ARG:CB	5:F:297:ASP:HB2	2.40	0.51
1:A:880:LEU:O	1:A:884:ASN:ND2	2.43	0.50
1:A:1554:MET:HE3	1:A:1591:PHE:CZ	2.46	0.50
1:A:717:LEU:HD22	1:A:746:CYS:HB2	1.92	0.50
1:A:3653:ASN:OD1	1:A:3654:GLU:N	2.44	0.50
5:F:268:ASP:OD2	5:F:270:ARG:HG3	2.11	0.50
5:F:390:MET:HE3	5:F:390:MET:HA	1.93	0.50
1:A:721:LEU:HB3	1:A:743:PHE:CZ	2.46	0.50
1:A:899:ASP:OD1	1:A:900:ASP:N	2.44	0.50
1:A:1097:MET:HE2	1:A:1167:PHE:HB3	1.92	0.50
1:A:1661:TRP:O	1:A:1665:LYS:NZ	2.34	0.50
1:A:1680:LEU:HD22	1:A:1730:LYS:HA	1.93	0.50
1:A:3652:ILE:HG22	1:A:3659:ILE:HD12	1.92	0.50
5:F:237:ALA:HB1	5:F:239:TRP:HD1	1.76	0.50
6:C:614:ASN:OD1	6:C:618:ARG:NH2	2.41	0.50
1:A:2904:VAL:O	1:A:2908:GLN:HG2	2.11	0.50
1:A:3059:TRP:HB3	1:A:3090:ALA:HB2	1.93	0.50
1:A:3517:ARG:HD3	1:A:3725:TYR:CE1	2.47	0.50
4:E:416:ILE:HG22	4:E:444:GLY:HA3	1.93	0.50
1:A:312:CYS:SG	1:A:320:ARG:NH2	2.85	0.50
1:A:1020:LYS:HA	1:A:1023:MET:HE3	1.94	0.50
1:A:1648:VAL:O	1:A:1652:GLU:OE1	2.30	0.50
1:A:956:MET:HE3	1:A:956:MET:HA	1.93	0.50
1:A:1322:LEU:O	1:A:1330:GLN:NE2	2.43	0.50
5:F:83:ALA:HB3	5:F:114:ASN:HD22	1.76	0.50
1:A:439:ILE:O	1:A:443:THR:HG23	2.10	0.50
1:A:583:ASN:HD21	1:A:601:ARG:HH21	1.58	0.50
1:A:1257:ARG:HE	1:A:1258:ASN:H	1.60	0.50
1:A:1503:LEU:HD22	1:A:1549:PHE:CD2	2.47	0.50
1:A:1262:SER:HA	1:A:1266:GLN:HB2	1.94	0.49
4:E:487:ILE:HD11	5:F:326:LEU:HD22	1.94	0.49
1:A:846:LEU:HD22	1:A:880:LEU:HG	1.93	0.49
1:A:1554:MET:HE3	1:A:1591:PHE:HZ	1.76	0.49
1:A:3064:PHE:CZ	1:A:3101:LYS:HD2	2.47	0.49
3:G:7:VAL:HG11	5:F:109:LEU:HD13	1.94	0.49
1:A:790:ARG:HB2	1:A:838:LEU:HD21	1.93	0.49
2:B:301:SER:OG	2:B:302:GLY:N	2.45	0.49
2:B:318:LEU:HD23	2:B:322:ALA:HB2	1.94	0.49
1:A:1574:GLU:O	1:A:1578:LYS:NZ	2.44	0.49
1:A:1760:LEU:HD21	1:A:1787:ILE:HG21	1.94	0.49
1:A:1915:ILE:O	1:A:1918:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1960:VAL:HG12	1:A:1964:TYR:CE2	2.48	0.49
1:A:3067:ASP:CG	1:A:3105:ARG:HH21	2.20	0.49
3:G:66:PRO:HA	3:G:229:PHE:CG	2.46	0.49
1:A:3501:PHE:HB2	1:A:3523:LEU:HD21	1.92	0.49
2:B:227:GLU:O	2:B:230:THR:OG1	2.30	0.49
3:G:74:MET:HE1	3:G:79:ILE:HA	1.94	0.49
4:E:458:LYS:HD2	6:C:523:PHE:CE1	2.48	0.49
1:A:1315:ALA:HB3	1:A:1316:PRO:HD3	1.95	0.49
1:A:1531:ILE:O	1:A:1535:ILE:HG12	2.12	0.49
1:A:3501:PHE:CE1	1:A:3636:MET:HG3	2.48	0.49
2:B:276:ASP:OD2	2:B:317:GLU:HB3	2.13	0.49
1:A:1333:ASN:O	1:A:1337:ILE:HG12	2.13	0.49
1:A:2270:LEU:HA	1:A:2314:GLU:HA	1.95	0.49
2:B:138:GLN:HB2	2:B:340:VAL:HG21	1.95	0.49
1:A:346:LEU:HB2	1:A:349:LEU:HD23	1.95	0.49
1:A:1557:LEU:HD22	1:A:1576:LEU:HG	1.94	0.49
1:A:3586:SER:OG	6:C:652:CYS:SG	2.47	0.49
3:G:49:ASP:N	3:G:49:ASP:OD1	2.46	0.49
1:A:1174:CYS:HA	1:A:1199:MET:HE1	1.95	0.49
2:B:114:LYS:HB2	2:B:372:HIS:NE2	2.28	0.49
2:B:240:SER:HB3	2:B:250:THR:HG22	1.94	0.49
4:E:447:ASP:OD1	4:E:448:PHE:N	2.46	0.49
3:G:145:PHE:HA	4:E:300:MET:CE	2.42	0.48
4:E:332:GLY:C	4:E:334:ILE:N	2.71	0.48
1:A:341:PRO:HD3	1:A:374:PHE:HZ	1.78	0.48
1:A:2674:ASP:OD1	1:A:2839:ARG:NH1	2.46	0.48
2:B:33:PRO:HB2	2:B:35:VAL:HG23	1.95	0.48
1:A:407:VAL:O	1:A:410:MET:HG3	2.13	0.48
1:A:1311:HIS:HA	1:A:1314:LEU:HB2	1.94	0.48
1:A:1753:ILE:HG22	1:A:1755:THR:HG22	1.95	0.48
1:A:1763:ILE:O	1:A:1767:THR:OG1	2.27	0.48
1:A:3586:SER:HB2	6:C:655:LEU:HD22	1.96	0.48
5:F:113:TYR:C	5:F:115:GLN:H	2.21	0.48
1:A:928:LYS:HG3	1:A:2889:ARG:NH1	2.29	0.48
3:G:372:LEU:HA	3:G:375:LEU:HD12	1.94	0.48
5:F:85:GLU:CD	5:F:85:GLU:H	2.21	0.48
5:F:315:GLU:OE1	5:F:318:ARG:HD3	2.14	0.48
1:A:2523:ASP:O	1:A:2527:LYS:HG2	2.13	0.48
1:A:2696:TYR:CE2	1:A:3797:ALA:HB2	2.49	0.48
1:A:3431:GLU:HA	1:A:3448:LYS:HA	1.95	0.48
1:A:1278:ASN:O	1:A:1284:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1792:SER:O	1:A:1795:HIS:ND1	2.25	0.48
2:B:118:GLU:HG2	2:B:372:HIS:HE1	1.79	0.48
5:F:103:ALA:O	5:F:104:LYS:HB2	2.12	0.48
1:A:1237:THR:HG22	1:A:1241:LYS:HE2	1.96	0.48
3:G:445:HIS:CD2	3:G:448:TRP:HE1	2.25	0.48
3:G:453:GLU:HG3	5:F:88:ASP:OD2	2.13	0.48
1:A:416:LEU:O	1:A:416:LEU:HD23	2.13	0.48
1:A:1221:LEU:HD11	1:A:1243:LEU:HD22	1.95	0.48
1:A:1416:ILE:O	1:A:1420:ILE:HG12	2.14	0.48
3:G:389:LEU:HD13	3:G:418:ILE:HD11	1.94	0.48
1:A:301:ILE:O	1:A:305:ILE:HG12	2.14	0.48
3:G:191:LEU:CD2	3:G:247:MET:HE3	2.44	0.48
1:A:1598:ARG:HA	1:A:1646:ASN:HD21	1.77	0.48
1:A:2681:TRP:CZ2	4:E:583:PRO:HB2	2.49	0.48
1:A:1507:LEU:C	1:A:1511:GLN:HE22	2.22	0.47
1:A:1645:SER:HA	1:A:1648:VAL:HG22	1.96	0.47
4:E:553:TRP:CD2	4:E:602:ARG:HG2	2.49	0.47
5:F:130:PHE:HZ	5:F:287:LEU:HB2	1.79	0.47
1:A:2688:PHE:HZ	1:A:3795:ASN:HA	1.79	0.47
2:B:217:LEU:HD13	2:B:255:ARG:HG2	1.94	0.47
5:F:292:ARG:HE	5:F:292:ARG:HA	1.79	0.47
1:A:1762:THR:O	1:A:1766:MET:HG3	2.13	0.47
4:E:339:ARG:HH21	4:E:342:LEU:HD21	1.79	0.47
5:F:272:MET:HE1	5:F:274:GLU:HB2	1.96	0.47
1:A:434:LEU:O	1:A:438:ILE:HG13	2.15	0.47
1:A:3555:ARG:NH1	1:A:3611:GLU:OE2	2.48	0.47
1:A:3703:PHE:CE2	1:A:3804:LEU:HB3	2.49	0.47
3:G:142:CYS:SG	3:G:435:GLY:N	2.87	0.47
4:E:273:TRP:NE1	4:E:275:LEU:HB2	2.29	0.47
4:E:499:TRP:HE1	6:C:555:ARG:CZ	2.27	0.47
1:A:836:VAL:HG12	1:A:859:PRO:HB3	1.95	0.47
1:A:1525:ASN:HA	1:A:1530:GLN:HE22	1.79	0.47
1:A:1572:PHE:C	1:A:1575:PRO:HD2	2.40	0.47
1:A:3082:ASN:HB3	4:E:699:PRO:CG	2.44	0.47
2:B:17:MET:HE1	7:B:401:ATP:H5'1	1.97	0.47
2:B:156:SER:HB2	2:B:161:THR:HG23	1.97	0.47
1:A:1392:VAL:HG23	1:A:1438:ALA:HB2	1.97	0.47
1:A:3133:TRP:HE1	1:A:3441:ASP:HA	1.80	0.47
4:E:540:PRO:HG3	4:E:619:TYR:CE2	2.50	0.47
1:A:1323:ARG:NH1	1:A:1323:ARG:HA	2.29	0.47
1:A:1357:LEU:O	1:A:1360:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3053:LEU:HB3	4:E:706:LYS:HD3	1.96	0.47
3:G:145:PHE:CD1	4:E:300:MET:HE1	2.50	0.47
5:F:272:MET:O	5:F:276:LYS:HG2	2.15	0.47
1:A:2795:ILE:HG13	1:A:2851:TYR:CE1	2.50	0.47
4:E:640:ARG:HG2	4:E:644:LEU:HD23	1.96	0.47
6:C:545:LEU:HD23	6:C:545:LEU:H	1.80	0.47
1:A:367:ALA:O	1:A:370:THR:OG1	2.23	0.47
1:A:580:LYS:HD2	1:A:669:HIS:HB3	1.96	0.47
1:A:1334:ILE:HG13	1:A:1397:LEU:HD22	1.97	0.47
1:A:1854:ALA:HB2	1:A:1894:ARG:HD2	1.97	0.47
3:G:382:GLN:HA	4:E:479:TYR:CE2	2.50	0.47
1:A:447:LYS:HE2	1:A:617:GLU:OE2	2.15	0.47
1:A:2707:GLN:HA	1:A:2710:GLU:OE1	2.14	0.47
5:F:79:PHE:O	5:F:80:SER:HB3	2.14	0.47
6:C:482:LYS:HD2	6:C:540:ALA:HA	1.97	0.47
1:A:376:HIS:O	1:A:379:ARG:NH1	2.48	0.46
1:A:1314:LEU:HD21	1:A:1347:PHE:CE1	2.50	0.46
1:A:1704:GLN:NE2	1:A:1734:PRO:HA	2.30	0.46
5:F:109:LEU:O	5:F:110:PHE:HB2	2.15	0.46
1:A:415:LEU:HD12	1:A:438:ILE:HG12	1.96	0.46
2:B:347:LEU:HD21	4:E:321:LEU:HD21	1.97	0.46
4:E:658:LEU:HD13	6:C:422:ILE:HB	1.98	0.46
5:F:282:VAL:HA	5:F:285:ARG:HG2	1.96	0.46
5:F:298:ASP:HA	5:F:302:LEU:HB3	1.98	0.46
1:A:583:ASN:HB2	1:A:597:ASN:HA	1.97	0.46
1:A:2767:ARG:HG2	1:A:2905:THR:HG21	1.97	0.46
1:A:3545:LEU:HD13	1:A:3650:ILE:HG13	1.98	0.46
2:B:167:TYR:CZ	4:E:430:LYS:HE3	2.50	0.46
3:G:145:PHE:HE2	3:G:438:LEU:HD13	1.79	0.46
4:E:345:LEU:HD13	4:E:349:GLU:HB2	1.97	0.46
6:C:468:ASN:C	6:C:468:ASN:HD22	2.22	0.46
1:A:1258:ASN:HA	1:A:1261:PHE:HB2	1.98	0.46
1:A:3430:ILE:O	1:A:3449:ILE:HG22	2.16	0.46
4:E:263:ARG:HG3	5:F:339:LEU:HD21	1.97	0.46
5:F:110:PHE:HA	5:F:113:TYR:HD2	1.79	0.46
1:A:620:LEU:HD12	1:A:623:ARG:HE	1.79	0.46
2:B:211:ARG:O	2:B:214:LYS:HG3	2.15	0.46
3:G:426:GLU:O	3:G:430:SER:OG	2.21	0.46
5:F:90:LEU:HD13	5:F:92:LEU:HD11	1.97	0.46
1:A:840:LEU:HD23	1:A:856:LEU:HD22	1.97	0.46
1:A:1317:ILE:HG13	1:A:1333:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1536:LEU:HD12	1:A:1576:LEU:HD21	1.97	0.46
1:A:1601:THR:HG21	1:A:1646:ASN:HB3	1.97	0.46
1:A:2856:GLU:CD	1:A:2889:ARG:HH22	2.24	0.46
1:A:3285:ASP:O	1:A:3289:ILE:HD12	2.16	0.46
1:A:3650:ILE:HG22	1:A:3661:THR:HB	1.98	0.46
2:B:83:MET:HE3	2:B:87:TRP:CE2	2.50	0.46
1:A:1591:PHE:HD2	1:A:1604:PHE:CD1	2.31	0.46
1:A:3412:LEU:N	1:A:3454:PRO:O	2.41	0.46
5:F:90:LEU:HD23	5:F:90:LEU:HA	1.59	0.46
1:A:712:SER:O	1:A:716:ILE:HD12	2.16	0.46
1:A:1082:ILE:HA	1:A:1085:THR:HG22	1.98	0.46
1:A:1171:ASN:OD1	1:A:1209:TYR:OH	2.31	0.46
1:A:1644:PHE:HE1	1:A:1672:LEU:HD22	1.81	0.46
1:A:1728:ILE:HG13	1:A:1729:SER:N	2.31	0.46
1:A:1881:LYS:HG2	1:A:1885:TYR:HE1	1.80	0.46
1:A:2547:LEU:HA	1:A:2550:ILE:HG22	1.97	0.46
5:F:96:ILE:HD12	5:F:96:ILE:HA	1.73	0.46
1:A:2598:GLN:HG2	1:A:2632:TYR:HE1	1.81	0.45
2:B:129:ASN:HD21	5:F:70:LYS:CB	2.19	0.45
2:B:212:ASP:O	2:B:216:LYS:HG3	2.16	0.45
3:G:204:PRO:HG3	3:G:236:GLU:HG2	1.97	0.45
3:G:379:LEU:HD23	3:G:379:LEU:H	1.81	0.45
4:E:177:ASP:CG	4:E:178:GLU:H	2.24	0.45
5:F:81:ASN:C	5:F:83:ALA:N	2.64	0.45
5:F:120:PRO:HD2	5:F:284:GLU:OE2	2.15	0.45
1:A:399:GLN:HE22	1:A:444:LYS:HB3	1.81	0.45
1:A:1882:GLN:O	1:A:1886:VAL:HG23	2.16	0.45
2:B:300:MET:SD	2:B:305:THR:OG1	2.71	0.45
1:A:853:LEU:HD12	1:A:856:LEU:HD12	1.98	0.45
1:A:1443:LEU:HA	1:A:1446:VAL:HG22	1.97	0.45
1:A:3082:ASN:HB3	4:E:699:PRO:HG2	1.97	0.45
1:A:1739:PHE:O	1:A:1743:ILE:HG12	2.16	0.45
1:A:1961:ALA:O	1:A:1965:GLN:HG2	2.16	0.45
1:A:2864:LEU:HG	1:A:2917:VAL:HG11	1.99	0.45
2:B:313:ARG:HA	2:B:316:LYS:HG2	1.98	0.45
4:E:251:ALA:O	4:E:254:GLU:HG3	2.16	0.45
4:E:348:GLU:O	4:E:351:LYS:HB2	2.15	0.45
4:E:663:MET:O	4:E:667:MET:HG3	2.17	0.45
5:F:257:ARG:O	5:F:260:ILE:HG22	2.16	0.45
1:A:615:PHE:HD1	1:A:667:PHE:HE2	1.64	0.45
1:A:834:ILE:O	1:A:838:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2450:ASP:OD1	1:A:2451:LYS:N	2.49	0.45
2:B:190:LEU:HA	2:B:193:ILE:HG12	1.97	0.45
2:B:290:VAL:HG12	2:B:294:LEU:HG	1.98	0.45
1:A:148:SER:O	1:A:151:PRO:HD2	2.17	0.45
1:A:372:ALA:HA	1:A:414:LEU:HD12	1.98	0.45
1:A:959:ILE:HB	1:A:962:LEU:HB2	1.97	0.45
1:A:2397:ASN:O	1:A:2401:VAL:HG23	2.16	0.45
3:G:155:VAL:O	3:G:155:VAL:HG13	2.17	0.45
1:A:3315:PHE:HD1	1:A:3467:LYS:HG3	1.81	0.45
5:F:348:LEU:HB3	6:C:539:VAL:HG21	1.99	0.45
1:A:548:GLN:OE1	1:A:548:GLN:N	2.49	0.45
1:A:717:LEU:O	1:A:721:LEU:HD23	2.16	0.45
1:A:923:LEU:HD13	1:A:2823:ILE:HG23	1.99	0.45
1:A:1844:MET:N	1:A:1844:MET:HE2	2.31	0.45
1:A:1893:SER:HA	1:A:1931:VAL:HG21	1.99	0.45
1:A:3508:LEU:HB2	1:A:3733:LEU:HD11	1.99	0.45
1:A:3612:LYS:NZ	1:A:3654:GLU:OE1	2.50	0.45
2:B:358:ILE:HD11	2:B:374:LYS:HB3	1.98	0.45
4:E:178:GLU:OE1	4:E:179:VAL:N	2.47	0.45
4:E:458:LYS:NZ	6:C:528:LEU:HB2	2.32	0.45
1:A:823:ILE:HG12	1:A:831:GLU:HG3	1.98	0.45
1:A:1480:LEU:HD12	1:A:1538:VAL:HG11	1.98	0.45
1:A:1604:PHE:HD2	1:A:1650:LEU:HD21	1.80	0.45
1:A:1668:LEU:O	1:A:1672:LEU:HG	2.17	0.45
2:B:15:SER:H	7:B:401:ATP:PG	2.40	0.45
1:A:1693:TYR:O	1:A:1696:VAL:HG12	2.17	0.45
2:B:203:THR:HG22	2:B:205:ALA:H	1.81	0.45
1:A:303:ASP:HB3	1:A:307:ARG:HH21	1.83	0.44
1:A:576:MET:HA	1:A:576:MET:HE2	1.98	0.44
1:A:1556:ALA:O	1:A:1560:LEU:HD23	2.18	0.44
1:A:2423:LEU:HD12	1:A:2464:TYR:HE2	1.82	0.44
2:B:374:LYS:HE2	6:C:561:ARG:HH11	1.82	0.44
5:F:272:MET:SD	5:F:273:GLU:N	2.90	0.44
5:F:379:SER:OG	5:F:380:GLN:OE1	2.35	0.44
1:A:3765:GLN:NE2	1:A:3766:THR:OG1	2.50	0.44
3:G:313:VAL:HG12	3:G:314:VAL:N	2.32	0.44
1:A:815:LEU:HG	1:A:1231:GLU:HB3	2.00	0.44
1:A:1776:ARG:HD3	1:A:1776:ARG:HA	1.70	0.44
1:A:2590:PHE:HE2	4:E:568:TYR:CG	2.35	0.44
1:A:3546:MET:O	1:A:3550:GLU:HG2	2.17	0.44
4:E:448:PHE:O	4:E:449:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:80:SER:O	5:F:81:ASN:C	2.59	0.44
1:A:302:PRO:HB3	1:A:340:ILE:HD11	2.00	0.44
1:A:943:LEU:HB2	1:A:3655:GLY:O	2.17	0.44
1:A:973:GLY:HA2	1:A:2557:THR:HG22	1.99	0.44
1:A:3066:ASN:ND2	1:A:3082:ASN:HB2	2.32	0.44
1:A:2665:LEU:HA	1:A:2665:LEU:HD23	1.72	0.44
1:A:3604:LEU:HD23	1:A:3825:LEU:HD13	1.99	0.44
5:F:277:GLU:O	5:F:281:LYS:HG2	2.17	0.44
5:F:346:PHE:CD1	6:C:486:PRO:HB3	2.53	0.44
1:A:1314:LEU:HA	1:A:1317:ILE:HG22	2.00	0.44
1:A:1547:HIS:HD2	1:A:1550:MET:N	2.15	0.44
1:A:1648:VAL:O	1:A:1651:CYS:HB2	2.16	0.44
1:A:3718:LEU:HD23	1:A:3722:LEU:HD23	1.99	0.44
2:B:156:SER:HA	2:B:161:THR:HA	2.00	0.44
1:A:312:CYS:O	1:A:320:ARG:NH2	2.50	0.44
1:A:1443:LEU:HD21	1:A:1489:LEU:HD12	1.99	0.44
1:A:2488:ILE:HD11	1:A:2540:ALA:HA	2.00	0.44
1:A:3431:GLU:HG2	1:A:3446:PHE:HB3	1.98	0.44
1:A:3562:GLU:OE1	4:E:174:TYR:OH	2.21	0.44
3:G:27:ILE:HB	3:G:92:MET:SD	2.58	0.44
3:G:249:GLU:HG2	7:G:501:ATP:N6	2.32	0.44
3:G:457:VAL:HG11	3:G:463:ILE:HG13	1.99	0.44
4:E:256:LYS:HA	4:E:259:VAL:HG12	2.00	0.44
1:A:704:LEU:HD12	1:A:745:LEU:HG	2.00	0.44
1:A:2523:ASP:OD1	1:A:2523:ASP:N	2.50	0.44
3:G:457:VAL:HG13	3:G:462:LEU:HD23	2.00	0.44
4:E:668:ARG:HD2	4:E:672:ARG:HH21	1.83	0.44
5:F:79:PHE:HB2	5:F:94:HIS:CD2	2.52	0.44
1:A:200:LEU:O	1:A:204:PRO:HD3	2.18	0.43
3:G:152:CYS:SG	3:G:388:ILE:HD12	2.58	0.43
4:E:454:VAL:HA	4:E:457:GLU:HG2	2.00	0.43
1:A:1391:ARG:O	1:A:1395:ILE:HG12	2.18	0.43
1:A:1527:SER:O	1:A:1531:ILE:HG12	2.18	0.43
1:A:2716:ALA:HB1	1:A:2723:PHE:HD1	1.84	0.43
2:B:318:LEU:O	2:B:322:ALA:N	2.52	0.43
2:B:332:ALA:HB1	2:B:336:ARG:NH1	2.33	0.43
4:E:418:PRO:HA	4:E:419:PRO:HD3	1.91	0.43
1:A:331:LEU:O	1:A:337:LYS:NZ	2.33	0.43
1:A:3736:SER:C	1:A:3738:PHE:H	2.26	0.43
2:B:181:LEU:HD22	2:B:270:LEU:HD23	1.98	0.43
2:B:186:LEU:O	2:B:190:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:LEU:O	2:B:194:LEU:HD23	2.19	0.43
3:G:190:GLN:OE1	3:G:293:LEU:HD12	2.18	0.43
3:G:359:ASP:OD1	3:G:360:LYS:N	2.51	0.43
4:E:538:LYS:HG3	4:E:620:ALA:HA	2.01	0.43
6:C:447:GLU:HA	6:C:450:ARG:HG2	1.99	0.43
1:A:374:PHE:O	1:A:378:VAL:HG12	2.18	0.43
1:A:403:LEU:HD12	1:A:407:VAL:HG21	2.01	0.43
1:A:842:VAL:HG12	1:A:844:VAL:HG12	2.01	0.43
1:A:1279:ALA:HB1	1:A:1328:GLN:HB3	2.00	0.43
1:A:1665:LYS:HD2	1:A:1668:LEU:HD22	2.00	0.43
1:A:2479:TYR:HD2	1:A:2548:ILE:HD11	1.82	0.43
1:A:3736:SER:O	1:A:3737:GLU:HG2	2.19	0.43
5:F:258:TRP:CE2	5:F:277:GLU:HG2	2.53	0.43
1:A:388:TRP:CH2	1:A:1691:PRO:HD2	2.54	0.43
1:A:683:LEU:N	1:A:684:PRO:HD2	2.33	0.43
1:A:1325:LEU:HD13	1:A:1326:PRO:HD2	2.00	0.43
1:A:2963:GLU:OE2	1:A:2967:ASN:HB2	2.19	0.43
1:A:3805:ILE:O	1:A:3809:VAL:HG23	2.19	0.43
4:E:191:LEU:HD21	6:C:546:ASP:C	2.44	0.43
5:F:83:ALA:HB2	5:F:111:GLU:HG3	2.00	0.43
5:F:113:TYR:C	5:F:115:GLN:N	2.76	0.43
5:F:382:LEU:HD23	5:F:382:LEU:HA	1.79	0.43
1:A:769:ILE:HD11	1:A:792:LEU:HD23	1.99	0.43
1:A:1059:VAL:HG22	1:A:1123:CYS:HB2	2.00	0.43
1:A:1659:LYS:O	1:A:1663:LYS:NZ	2.51	0.43
1:A:1958:THR:N	1:A:1961:ALA:HB3	2.33	0.43
1:A:2486:SER:HB3	1:A:2539:THR:HA	2.00	0.43
5:F:337:GLU:O	5:F:341:ILE:HG12	2.18	0.43
1:A:3065:PHE:HZ	1:A:3069:ARG:HH21	1.67	0.43
3:G:13:ILE:O	3:G:14:ASN:HB2	2.19	0.43
4:E:443:ILE:HD12	4:E:448:PHE:CE1	2.54	0.43
4:E:547:LEU:H	4:E:547:LEU:HD23	1.84	0.43
4:E:548:ARG:HH21	4:E:598:GLN:HE22	1.66	0.43
1:A:2886:TRP:CD1	1:A:2889:ARG:HH21	2.37	0.43
2:B:333:PRO:O	2:B:336:ARG:HG3	2.18	0.43
1:A:1540:HIS:CE1	1:A:1578:LYS:HB2	2.54	0.43
1:A:2590:PHE:HE1	1:A:2624:LEU:HD22	1.84	0.43
2:B:292:LYS:HA	2:B:326:MET:SD	2.59	0.43
2:B:354:GLN:HA	2:B:357:TRP:CD1	2.54	0.43
4:E:612:PHE:HD2	4:E:624:GLN:HG3	1.83	0.43
6:C:572:ASP:OD1	6:C:573:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:MET:HG2	1:A:936:PHE:CE1	2.54	0.42
1:A:1094:PHE:O	1:A:1098:VAL:HG23	2.19	0.42
1:A:1146:SER:O	1:A:1150:ILE:HG13	2.19	0.42
1:A:1513:ARG:HH21	1:A:1516:GLN:CB	2.32	0.42
1:A:1789:ILE:O	1:A:1793:GLU:HG2	2.19	0.42
1:A:1895:PHE:O	1:A:1935:ARG:NH2	2.52	0.42
2:B:89:HIS:CD2	2:B:93:ASN:HD22	2.35	0.42
3:G:19:ASP:OD1	3:G:20:ALA:N	2.52	0.42
3:G:450:SER:HB2	5:F:90:LEU:HG	2.01	0.42
4:E:196:LEU:HD23	4:E:196:LEU:H	1.84	0.42
1:A:1295:SER:CB	1:A:1302:ILE:HG13	2.49	0.42
1:A:1774:ASP:OD1	1:A:1775:ALA:N	2.52	0.42
1:A:1868:PHE:CE1	1:A:1872:TYR:HE2	2.37	0.42
1:A:2710:GLU:HG2	4:E:667:MET:HE2	2.01	0.42
2:B:143:LEU:HB2	2:B:153:VAL:CG2	2.48	0.42
1:A:721:LEU:HD12	1:A:743:PHE:CE2	2.54	0.42
1:A:957:PHE:HE2	1:A:2544:LEU:HD21	1.84	0.42
1:A:1226:ARG:HG2	1:A:1283:VAL:HG21	2.01	0.42
1:A:1783:ILE:O	1:A:1786:PRO:HD2	2.19	0.42
1:A:2533:ASP:HA	1:A:2536:ARG:HG2	2.00	0.42
1:A:3643:ASN:CG	1:A:3667:THR:HG1	2.26	0.42
2:B:125:PHE:CE2	2:B:133:PHE:HB3	2.54	0.42
2:B:219:TYR:O	2:B:259:PRO:HG2	2.19	0.42
3:G:57:GLU:O	3:G:61:MET:HG3	2.19	0.42
1:A:1915:ILE:HG23	1:A:1916:ASP:N	2.34	0.42
1:A:697:LEU:HD21	1:A:741:ARG:HB3	2.02	0.42
1:A:1698:GLN:HA	1:A:1701:GLU:OE2	2.19	0.42
1:A:3158:LEU:HA	1:A:3161:ILE:HG22	2.01	0.42
4:E:257:ILE:HD13	5:F:346:PHE:HD2	1.85	0.42
5:F:85:GLU:O	5:F:86:SER:CB	2.68	0.42
1:A:1440:HIS:NE2	1:A:1488:LYS:HD3	2.35	0.42
1:A:1673:LEU:HD12	1:A:1673:LEU:HA	1.89	0.42
1:A:2423:LEU:HD12	1:A:2464:TYR:CE2	2.54	0.42
1:A:1157:LEU:HD21	1:A:2524:PHE:CE2	2.54	0.42
1:A:1839:TYR:O	1:A:1842:GLU:HG3	2.20	0.42
1:A:2999:SER:HA	4:E:685:ARG:HA	2.02	0.42
1:A:3088:LEU:HD11	1:A:3123:PHE:CD1	2.55	0.42
3:G:187:LEU:HD11	3:G:297:LEU:HD11	2.01	0.42
5:F:100:SER:HB3	5:F:103:ALA:HB2	2.02	0.42
1:A:1317:ILE:HD11	1:A:1337:ILE:HD13	2.01	0.42
1:A:1960:VAL:HG12	1:A:1964:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:479:TYR:CE1	4:E:493:PRO:HG2	2.55	0.42
5:F:101:GLU:H	5:F:101:GLU:HG3	1.60	0.42
1:A:316:LEU:HB3	1:A:319:ALA:HB3	2.02	0.42
1:A:360:TYR:O	1:A:364:ARG:NH2	2.53	0.42
1:A:1483:LEU:HD23	1:A:1487:LEU:HD23	2.01	0.42
1:A:1863:LYS:O	1:A:1866:ILE:HG22	2.20	0.42
1:A:3167:GLN:HG2	1:A:3304:LEU:HD11	2.01	0.42
3:G:192:ARG:HG3	3:G:244:LEU:HD21	2.02	0.42
6:C:554:VAL:HA	6:C:566:ASP:O	2.20	0.42
1:A:605:ASN:ND2	1:A:1567:CYS:HB3	2.34	0.42
1:A:687:TYR:O	1:A:691:LEU:HG	2.19	0.42
1:A:773:LEU:HD23	1:A:773:LEU:HA	1.92	0.42
1:A:852:HIS:HB3	1:A:855:TYR:HD2	1.85	0.42
1:A:1247:SER:HB2	1:A:1251:TRP:CH2	2.55	0.42
1:A:3749:ARG:NH2	1:A:3750:ASP:OD1	2.39	0.42
2:B:89:HIS:CD2	2:B:93:ASN:HB2	2.53	0.42
3:G:298:PHE:CD2	3:G:402:ARG:HD3	2.55	0.42
5:F:130:PHE:HE2	5:F:283:SER:HB3	1.85	0.42
1:A:327:THR:O	1:A:330:ILE:HB	2.20	0.41
1:A:616:ARG:HD3	1:A:685:PHE:CE2	2.55	0.41
1:A:1442:GLY:O	1:A:1446:VAL:HG13	2.20	0.41
1:A:1786:PRO:HA	1:A:1789:ILE:HG22	2.01	0.41
1:A:2761:LEU:HD21	1:A:2781:SER:HB2	2.01	0.41
2:B:212:ASP:O	2:B:215:GLU:HB2	2.20	0.41
3:G:262:LYS:HE3	3:G:262:LYS:HB2	1.81	0.41
3:G:382:GLN:HA	4:E:479:TYR:HE2	1.84	0.41
4:E:423:THR:H	6:C:626:ASP:CG	2.27	0.41
5:F:289:HIS:NE2	5:F:305:GLN:HG3	2.33	0.41
5:F:292:ARG:HG3	5:F:297:ASP:HB2	2.01	0.41
1:A:615:PHE:HD2	1:A:682:GLU:HG2	1.84	0.41
1:A:1084:GLY:HA3	1:A:2531:PHE:CE1	2.55	0.41
1:A:1178:ILE:HD11	1:A:1217:ILE:HG12	2.01	0.41
1:A:1352:GLU:HA	1:A:1355:ASN:HB2	2.02	0.41
1:A:1354:LEU:HD23	1:A:1354:LEU:HA	1.92	0.41
3:G:142:CYS:O	3:G:434:GLY:HA3	2.20	0.41
4:E:270:GLN:HB3	4:E:272:LYS:HE3	2.02	0.41
6:C:480:LEU:HD12	6:C:481:GLU:N	2.36	0.41
1:A:409:ILE:HD12	1:A:409:ILE:HA	1.81	0.41
1:A:616:ARG:HD3	1:A:685:PHE:HE2	1.85	0.41
1:A:1261:PHE:O	1:A:1265:PHE:HB3	2.19	0.41
1:A:1302:ILE:H	1:A:1302:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3547:GLY:O	1:A:3551:GLU:HG2	2.20	0.41
2:B:254:GLU:HG3	2:B:257:ARG:HH21	1.84	0.41
3:G:376:ASP:OD2	5:F:319:LYS:NZ	2.53	0.41
6:C:572:ASP:OD1	6:C:625:ARG:NH2	2.53	0.41
1:A:338:MET:O	1:A:342:LYS:NZ	2.34	0.41
1:A:350:ARG:NH1	1:A:371:VAL:HG23	2.35	0.41
1:A:366:LEU:O	1:A:370:THR:HG23	2.20	0.41
1:A:1561:GLU:OE1	1:A:1603:ARG:NE	2.40	0.41
1:A:2629:GLY:HA2	1:A:2634:ALA:HB3	2.03	0.41
1:A:3504:PHE:HB3	1:A:3733:LEU:HD21	2.01	0.41
4:E:473:LYS:HD2	4:E:473:LYS:HA	1.72	0.41
5:F:79:PHE:HE1	5:F:108:TYR:CZ	2.38	0.41
5:F:110:PHE:HA	5:F:113:TYR:CD2	2.56	0.41
5:F:113:TYR:O	5:F:115:GLN:N	2.50	0.41
1:A:613:SER:O	1:A:616:ARG:HB3	2.21	0.41
1:A:747:PHE:CE1	1:A:792:LEU:HD13	2.56	0.41
1:A:1145:GLU:O	1:A:1149:LEU:HD23	2.21	0.41
1:A:1688:VAL:HG22	1:A:1689:VAL:H	1.85	0.41
1:A:2715:LYS:HG2	5:F:373:ILE:HG13	2.02	0.41
1:A:3562:GLU:HB3	1:A:3563:PRO:HD3	2.02	0.41
2:B:154:LEU:HD11	2:B:275:ILE:CG2	2.51	0.41
5:F:297:ASP:OD2	5:F:302:LEU:N	2.53	0.41
1:A:135:LYS:C	1:A:138:PRO:HD2	2.46	0.41
1:A:603:PHE:HB3	1:A:607:ASP:HB2	2.02	0.41
1:A:734:ILE:HG13	1:A:735:LYS:N	2.35	0.41
1:A:1816:PHE:CE1	1:A:1820:VAL:HG21	2.55	0.41
1:A:1914:GLN:N	1:A:1917:THR:OG1	2.48	0.41
1:A:1970:PHE:HB3	1:A:1971:PRO:HD3	2.02	0.41
4:E:185:ASP:O	4:E:187:THR:HG23	2.20	0.41
4:E:266:GLU:OE2	4:E:270:GLN:NE2	2.54	0.41
5:F:315:GLU:O	5:F:316:THR:C	2.61	0.41
1:A:822:LEU:HD23	1:A:1232:LEU:HD21	2.02	0.41
3:G:62:LEU:O	3:G:239:HIS:NE2	2.47	0.41
4:E:230:PHE:CE2	4:E:235:LEU:HD21	2.55	0.41
4:E:494:PRO:HD3	6:C:502:TYR:O	2.20	0.41
1:A:350:ARG:NH1	1:A:367:ALA:HB1	2.35	0.41
1:A:405:LEU:HD22	1:A:560:ASP:OD1	2.21	0.41
1:A:1129:ILE:HD13	1:A:1180:CYS:SG	2.61	0.41
1:A:2395:LYS:HB3	1:A:2395:LYS:HE3	1.74	0.41
1:A:2681:TRP:HZ2	4:E:583:PRO:HB2	1.85	0.41
3:G:43:TYR:HB2	3:G:56:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:285:PHE:HZ	5:F:284:GLU:HG2	1.84	0.41
1:A:314:SER:OG	1:A:1833:SER:OG	2.37	0.41
1:A:359:ALA:HA	1:A:362:THR:HG22	2.02	0.41
1:A:415:LEU:HD12	1:A:438:ILE:HG23	2.03	0.41
1:A:415:LEU:CD1	1:A:438:ILE:HG12	2.51	0.41
1:A:445:ARG:HD2	1:A:445:ARG:HA	1.75	0.41
1:A:766:ASN:HB2	1:A:804:LEU:HD21	2.02	0.41
1:A:858:LYS:HA	1:A:858:LYS:HD3	1.84	0.41
1:A:1087:ASN:O	1:A:1090:ILE:HG22	2.20	0.41
1:A:1157:LEU:HD21	1:A:2524:PHE:CD2	2.56	0.41
1:A:1182:PHE:CZ	1:A:3413:GLU:HG2	2.56	0.41
1:A:1640:LYS:HA	1:A:1643:ARG:HH22	1.86	0.41
1:A:1680:LEU:HD13	1:A:1730:LYS:HG3	2.03	0.41
1:A:1817:ASP:HA	1:A:1821:TRP:HZ3	1.85	0.41
1:A:1879:THR:OG1	1:A:1916:ASP:OD2	2.39	0.41
1:A:1894:ARG:HE	1:A:1894:ARG:HB2	1.69	0.41
1:A:2722:PRO:HA	6:C:428:ILE:HG13	2.02	0.41
1:A:2785:VAL:HG22	1:A:2793:ARG:HE	1.85	0.41
1:A:3101:LYS:HG3	1:A:3743:TYR:CE2	2.55	0.41
1:A:3498:PHE:HD1	1:A:3523:LEU:HD23	1.85	0.41
2:B:154:LEU:HD23	2:B:154:LEU:O	2.21	0.41
3:G:115:TYR:O	3:G:119:THR:HG23	2.21	0.41
3:G:126:LEU:HD21	3:G:134:THR:HG21	2.03	0.41
3:G:381:PRO:HA	3:G:414:LEU:HD11	2.03	0.41
4:E:271:ARG:NH2	5:F:317:GLU:OE2	2.46	0.41
5:F:379:SER:O	5:F:383:THR:HG23	2.21	0.41
1:A:388:TRP:HA	1:A:391:VAL:HG12	2.02	0.41
1:A:842:VAL:HA	1:A:843:PRO:HD3	1.95	0.41
1:A:1293:THR:O	1:A:1296:GLU:HG3	2.21	0.41
1:A:1382:LYS:HD3	1:A:1385:GLU:HG3	2.02	0.41
1:A:1515:LEU:HD11	1:A:1560:LEU:HD13	2.03	0.41
1:A:2674:ASP:HA	1:A:2677:PHE:HB3	2.03	0.41
2:B:57:ASP:OD1	2:B:57:ASP:N	2.53	0.41
4:E:667:MET:O	4:E:671:MET:HG2	2.21	0.41
1:A:394:TYR:HD1	1:A:414:LEU:HD22	1.86	0.40
1:A:412:ALA:HB1	1:A:442:TYR:OH	2.21	0.40
1:A:997:TYR:CZ	1:A:1001:ILE:HD11	2.56	0.40
1:A:2590:PHE:CE1	1:A:2624:LEU:HD22	2.57	0.40
3:G:145:PHE:CE2	3:G:438:LEU:HD13	2.55	0.40
3:G:191:LEU:HD21	3:G:247:MET:HE3	2.04	0.40
1:A:299:GLN:C	1:A:302:PRO:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:MET:HG3	1:A:666:MET:HE3	2.03	0.40
1:A:1878:ASN:O	1:A:1881:LYS:N	2.54	0.40
1:A:2641:LEU:O	1:A:2644:GLU:HG2	2.22	0.40
1:A:2785:VAL:HG22	1:A:2793:ARG:NE	2.36	0.40
3:G:252:LEU:HB2	3:G:396:ILE:HD12	2.03	0.40
1:A:663:PHE:HA	1:A:666:MET:HG2	2.03	0.40
1:A:752:LEU:HD23	1:A:752:LEU:HA	1.95	0.40
1:A:765:LEU:HD12	1:A:765:LEU:HA	1.97	0.40
1:A:858:LYS:HB3	1:A:859:PRO:HD3	2.03	0.40
1:A:1248:LEU:HD11	1:A:1268:LEU:HD21	2.03	0.40
3:G:203:VAL:HG22	3:G:279:ASN:HB2	2.02	0.40
3:G:298:PHE:HD2	3:G:402:ARG:HD3	1.85	0.40
5:F:351:LYS:HB2	5:F:351:LYS:HE2	1.81	0.40
1:A:2473:GLN:OE1	1:A:2473:GLN:N	2.54	0.40
1:A:2678:TYR:OH	1:A:2697:GLU:OE2	2.35	0.40
1:A:3556:LYS:HE2	1:A:3556:LYS:HB2	1.80	0.40
1:A:3638:TYR:HE2	1:A:3787:LEU:HD11	1.85	0.40
2:B:193:ILE:O	2:B:196:GLU:HG3	2.22	0.40
2:B:215:GLU:HG2	7:B:401:ATP:C2	2.57	0.40
2:B:221:ALA:O	2:B:313:ARG:HD2	2.21	0.40
3:G:242:ARG:O	3:G:246:GLU:OE1	2.39	0.40
4:E:181:ILE:HG21	4:E:187:THR:HG22	2.03	0.40
4:E:345:LEU:HD11	4:E:350:ILE:HG23	2.03	0.40
4:E:476:LEU:H	4:E:481:LYS:HZ1	1.68	0.40
5:F:79:PHE:CE1	5:F:108:TYR:CZ	3.10	0.40
1:A:925:ILE:HD13	1:A:925:ILE:HA	1.89	0.40
1:A:1221:LEU:O	1:A:1224:VAL:HG12	2.21	0.40
1:A:1601:THR:O	1:A:1605:VAL:HG23	2.21	0.40
1:A:3167:GLN:NE2	1:A:3430:ILE:HD13	2.37	0.40
1:A:3173:LEU:O	1:A:3176:THR:HG22	2.22	0.40
4:E:275:LEU:HD12	6:C:462:LEU:HB2	2.04	0.40
5:F:348:LEU:HD13	6:C:539:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3148/3825 (82%)	3050 (97%)	98 (3%)	0	100	100
2	B	344/376 (92%)	330 (96%)	14 (4%)	0	100	100
3	G	418/468 (89%)	404 (97%)	14 (3%)	0	100	100
4	E	482/1051 (46%)	448 (93%)	29 (6%)	5 (1%)	12	40
4	H	20/1051 (2%)	16 (80%)	2 (10%)	2 (10%)	0	3
5	F	219/565 (39%)	201 (92%)	15 (7%)	3 (1%)	9	31
6	C	220/752 (29%)	211 (96%)	9 (4%)	0	100	100
All	All	4851/8088 (60%)	4660 (96%)	181 (4%)	10 (0%)	44	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	333	LYS
4	E	412	PRO
5	F	311	ASP
4	H	393	GLN
4	E	300	MET
4	E	415	GLU
5	F	86	SER
4	E	414	ASP
5	F	310	PHE
4	H	392	ASN

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	2299/3450 (67%)	2299 (100%)	0	100	100
2	B	300/322 (93%)	300 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	362/419 (86%)	358 (99%)	4 (1%)	65	74
4	E	422/940 (45%)	419 (99%)	3 (1%)	76	78
5	F	209/520 (40%)	190 (91%)	19 (9%)	9	30
6	C	206/682 (30%)	201 (98%)	5 (2%)	43	62
All	All	3798/6333 (60%)	3767 (99%)	31 (1%)	70	77

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	7	VAL
3	G	8	TYR
3	G	12	GLU
3	G	13	ILE
4	E	330	THR
4	E	460	PRO
4	E	696	VAL
5	F	69	ASN
5	F	70	LYS
5	F	79	PHE
5	F	85	GLU
5	F	90	LEU
5	F	96	ILE
5	F	100	SER
5	F	101	GLU
5	F	102	LEU
5	F	105	ASN
5	F	109	LEU
5	F	290	LYS
5	F	296	MET
5	F	302	LEU
5	F	303	LEU
5	F	305	GLN
5	F	306	THR
5	F	314	ARG
5	F	316	THR
6	C	556	LYS
6	C	560	ARG
6	C	561	ARG
6	C	563	LEU
6	C	565	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	GLN
1	A	417	ASN
1	A	597	ASN
1	A	609	ASN
1	A	803	ASN
1	A	993	ASN
1	A	1179	HIS
1	A	1238	ASN
1	A	1511	GLN
1	A	1526	ASN
1	A	1555	ASN
1	A	1565	HIS
1	A	1769	GLN
1	A	1913	HIS
1	A	2545	ASN
1	A	2871	ASN
1	A	3167	GLN
1	A	3170	HIS
1	A	3313	GLN
1	A	3318	ASN
1	A	3418	HIS
1	A	3484	GLN
1	A	3629	GLN
1	A	3765	GLN
1	A	3786	GLN
1	A	3799	GLN
2	B	93	ASN
2	B	355	GLN
3	G	14	ASN
3	G	411	ASN
3	G	445	HIS
4	E	611	GLN
5	F	69	ASN
5	F	93	HIS
5	F	94	HIS
5	F	114	ASN
6	C	509	GLN
6	C	542	ASN
6	C	644	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ATP	B	401	8	32,33,33	0.26	0	48,52,52	0.28	0
7	ATP	G	501	8	32,33,33	0.30	0	48,52,52	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	B	401	8	-	5/22/38/38	0/3/3/3
7	ATP	G	501	8	-	13/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

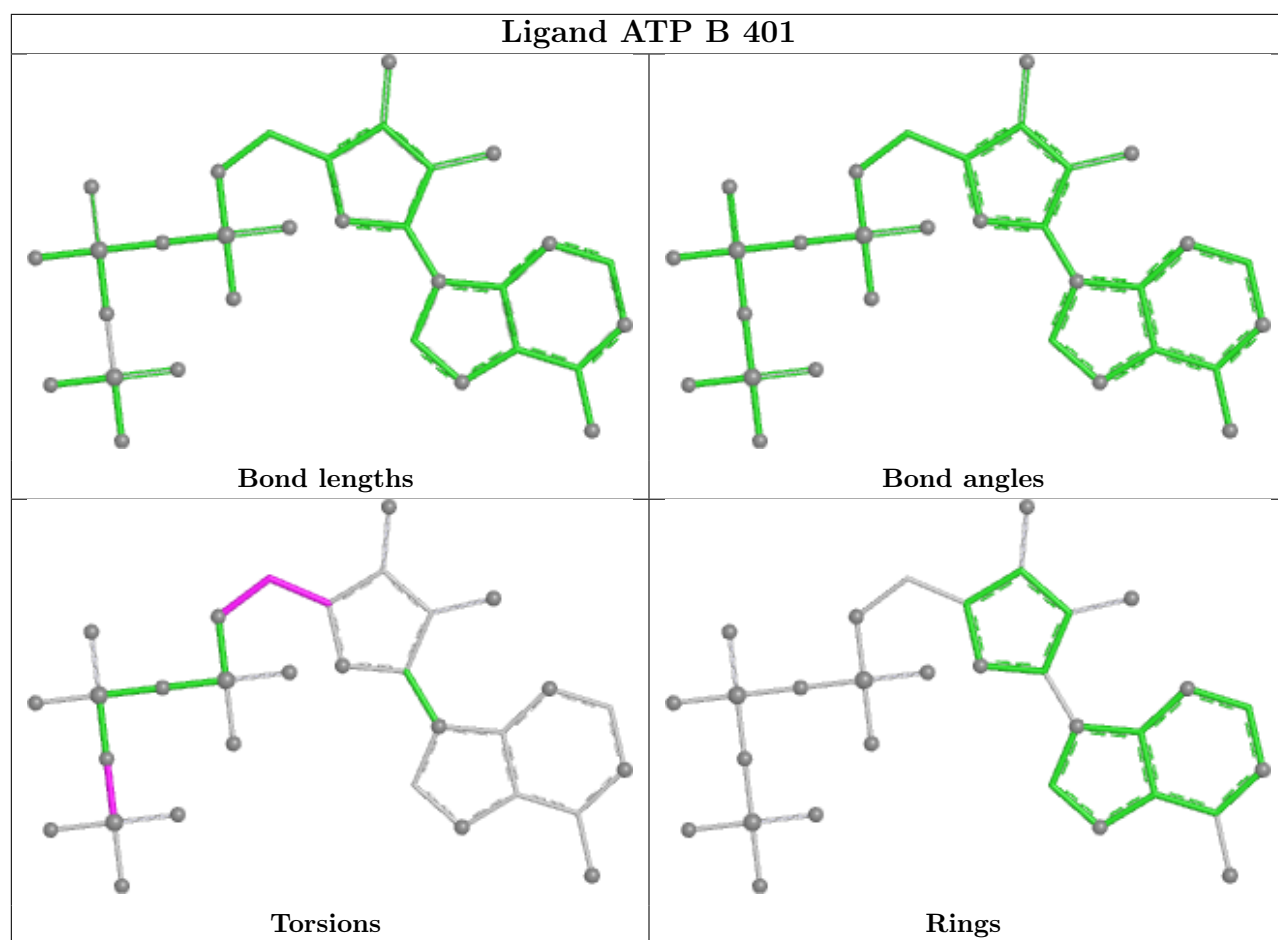
Mol	Chain	Res	Type	Atoms
7	B	401	ATP	PB-O3B-PG-O3G
7	G	501	ATP	PB-O3B-PG-O2G
7	G	501	ATP	C5'-O5'-PA-O1A
7	G	501	ATP	C5'-O5'-PA-O2A
7	G	501	ATP	C5'-O5'-PA-O3A
7	B	401	ATP	C3'-C4'-C5'-O5'
7	B	401	ATP	O4'-C4'-C5'-O5'
7	G	501	ATP	O4'-C4'-C5'-O5'
7	B	401	ATP	C4'-C5'-O5'-PA
7	G	501	ATP	C2'-C1'-N9-C8
7	G	501	ATP	PB-O3B-PG-O3G
7	G	501	ATP	C2'-C1'-N9-C4
7	B	401	ATP	PB-O3B-PG-O1G
7	G	501	ATP	PB-O3B-PG-O1G
7	G	501	ATP	PA-O3A-PB-O1B
7	G	501	ATP	O4'-C1'-N9-C8
7	G	501	ATP	O4'-C1'-N9-C4
7	G	501	ATP	PA-O3A-PB-O2B

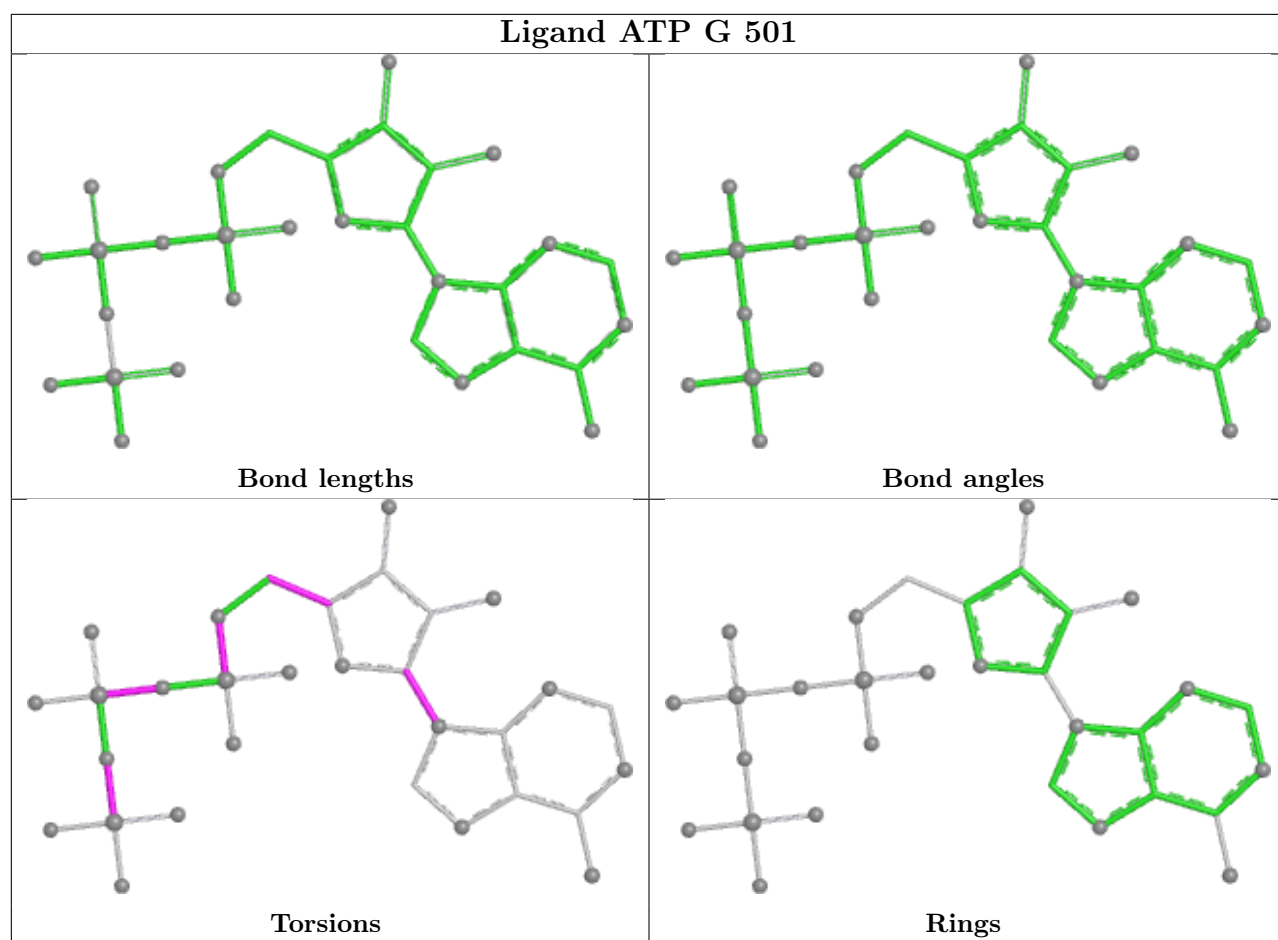
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	401	ATP	3	0
7	G	501	ATP	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

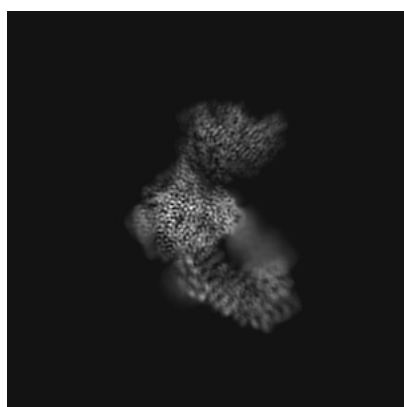
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14989. These allow visual inspection of the internal detail of the map and identification of artifacts.

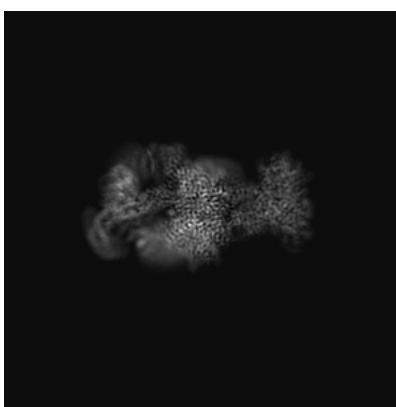
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

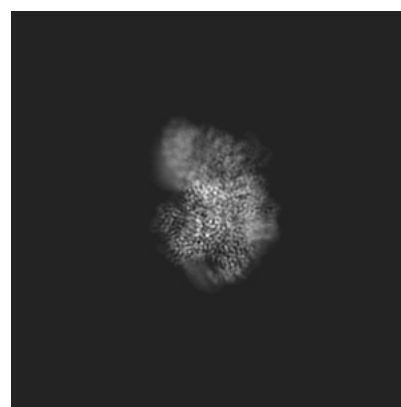
6.1.1 Primary map



X



Y

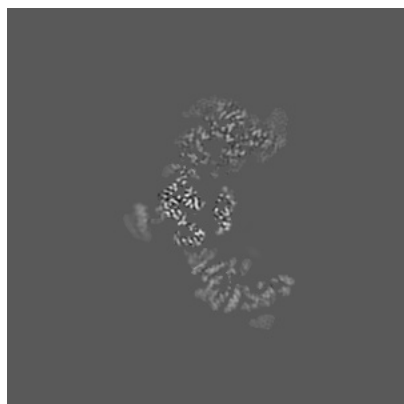


Z

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

6.2 Central slices [i](#)

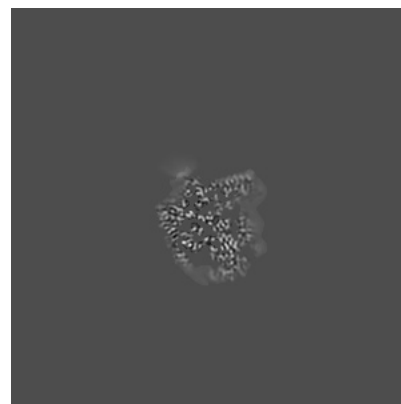
6.2.1 Primary map



X Index: 224



Y Index: 224

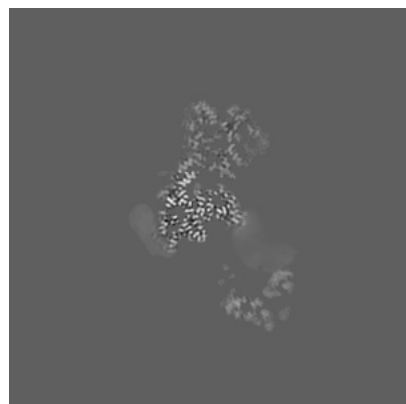


Z Index: 224

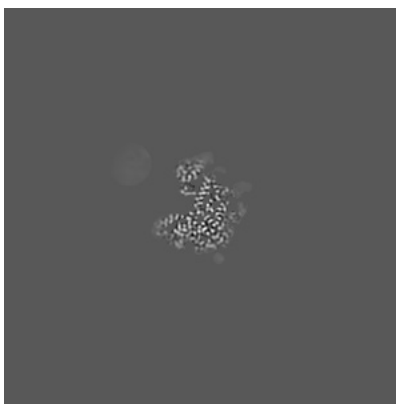
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

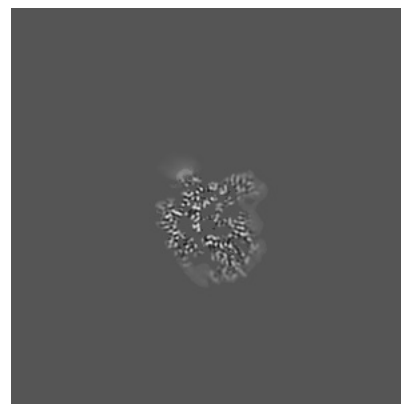
6.3.1 Primary map



X Index: 209



Y Index: 182

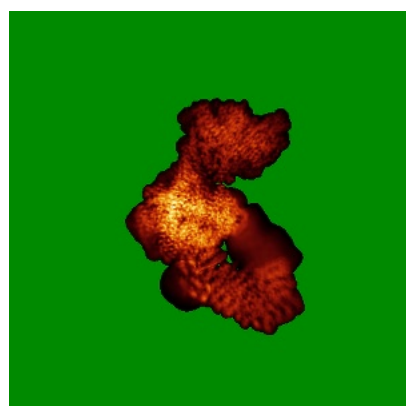


Z Index: 221

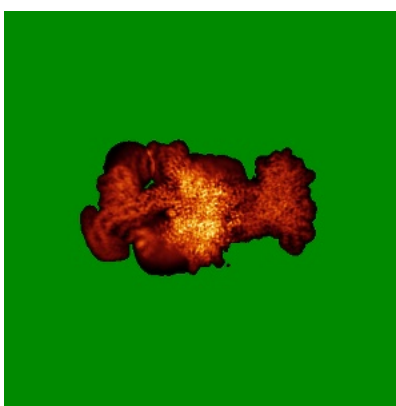
The images above show the largest variance slices of the map in three orthogonal directions.

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

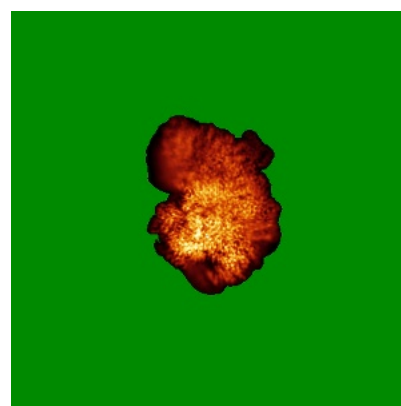
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

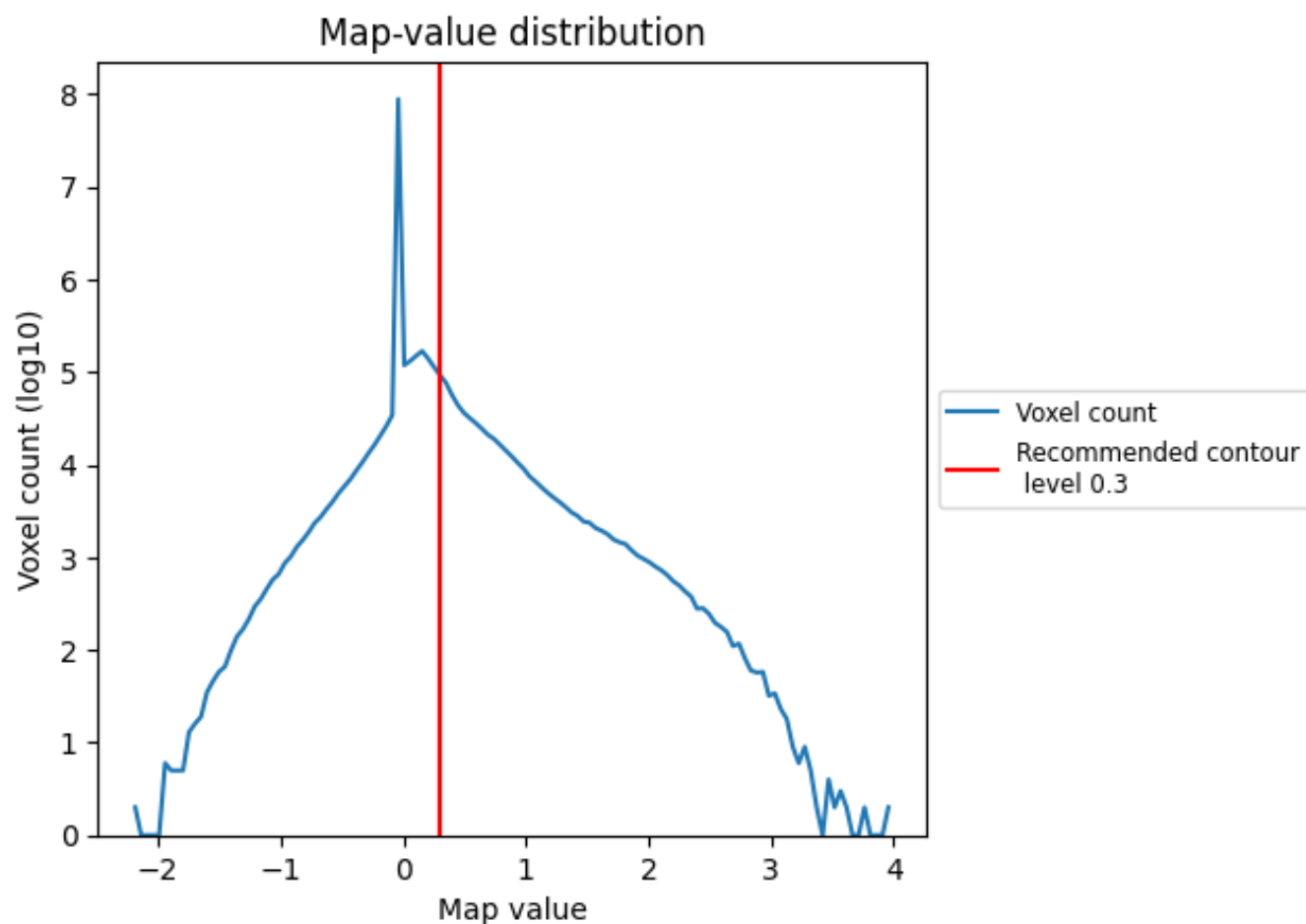
6.6 Mask visualisation

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

7 Map analysis [i](#)

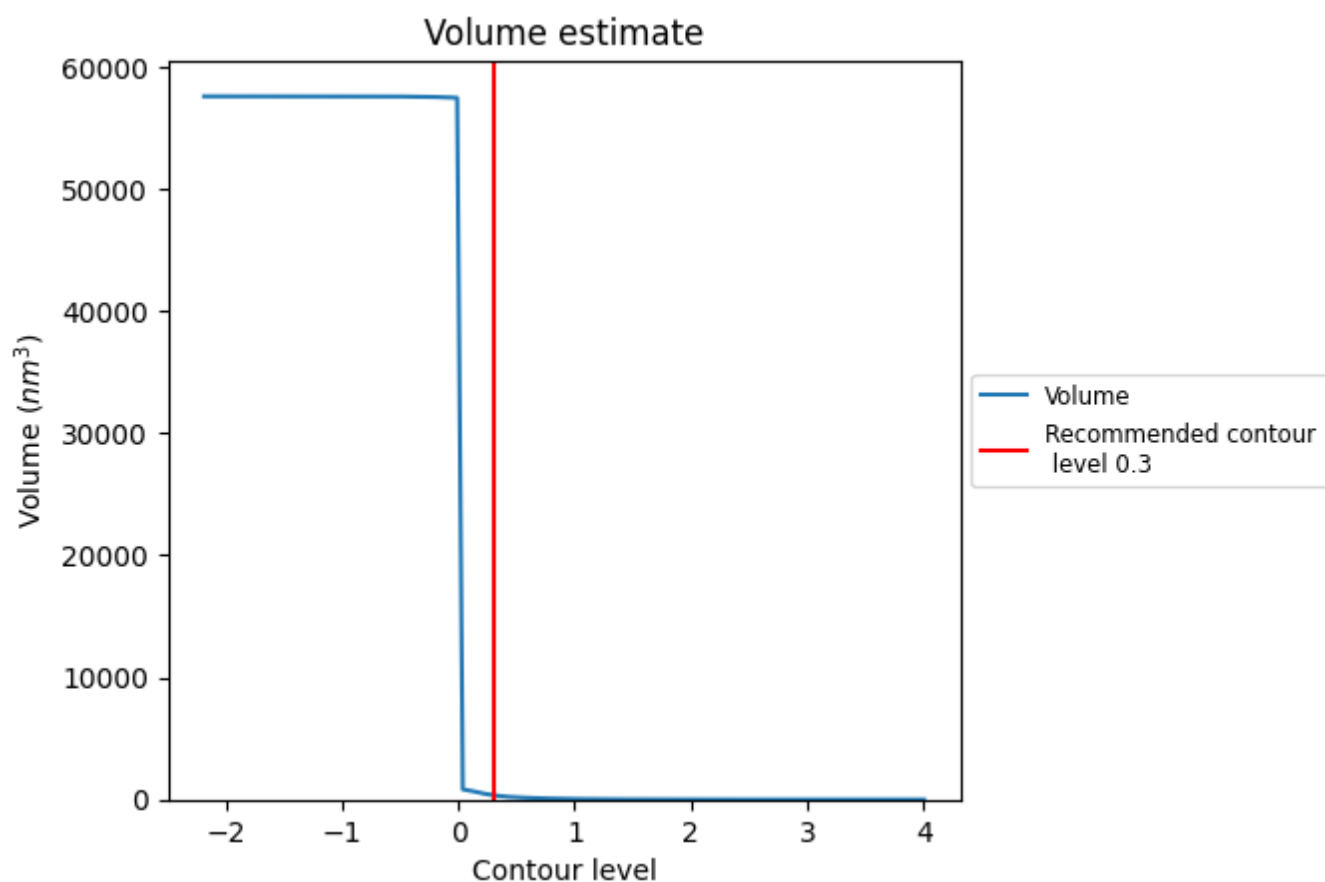
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

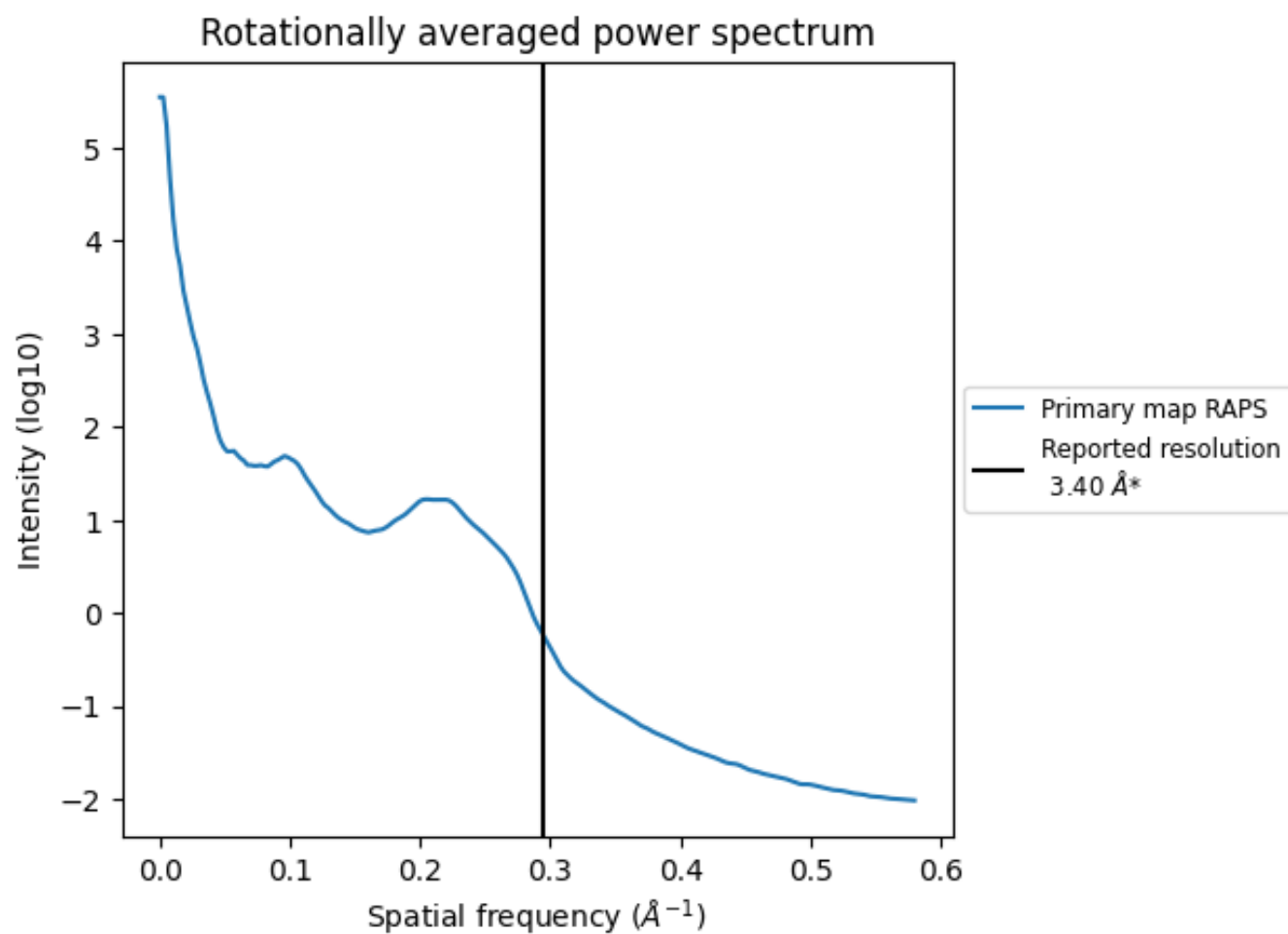
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 358 nm³; this corresponds to an approximate mass of 323 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 0.294 Å⁻¹

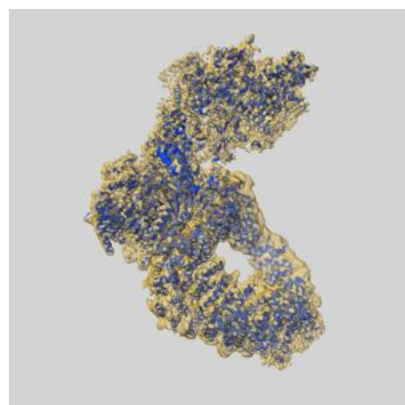
8 Fourier-Shell correlation

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

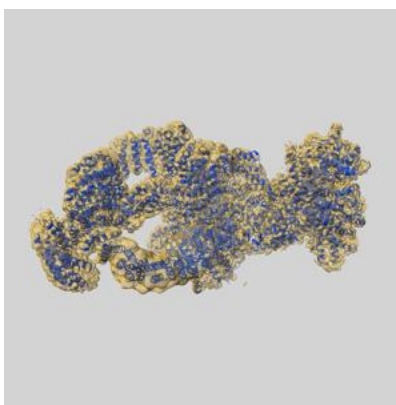
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14989 and PDB model 7ZVW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

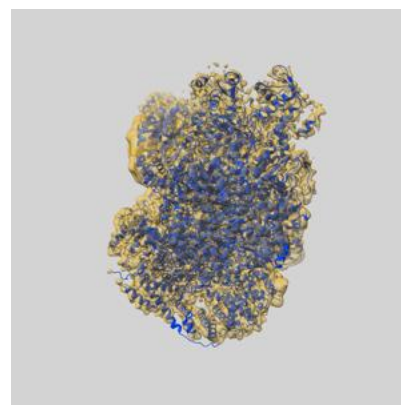
9.1 Map-model overlay [i](#)



X



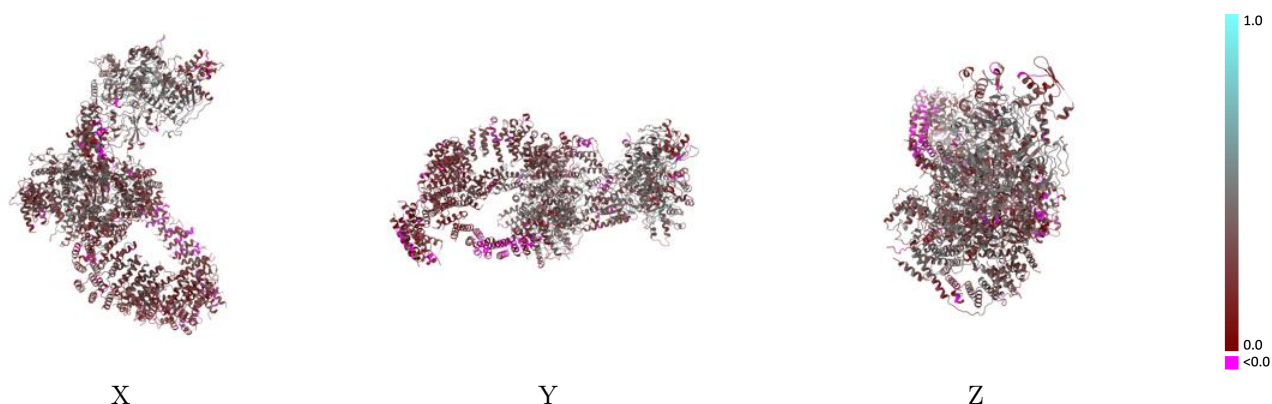
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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](#)

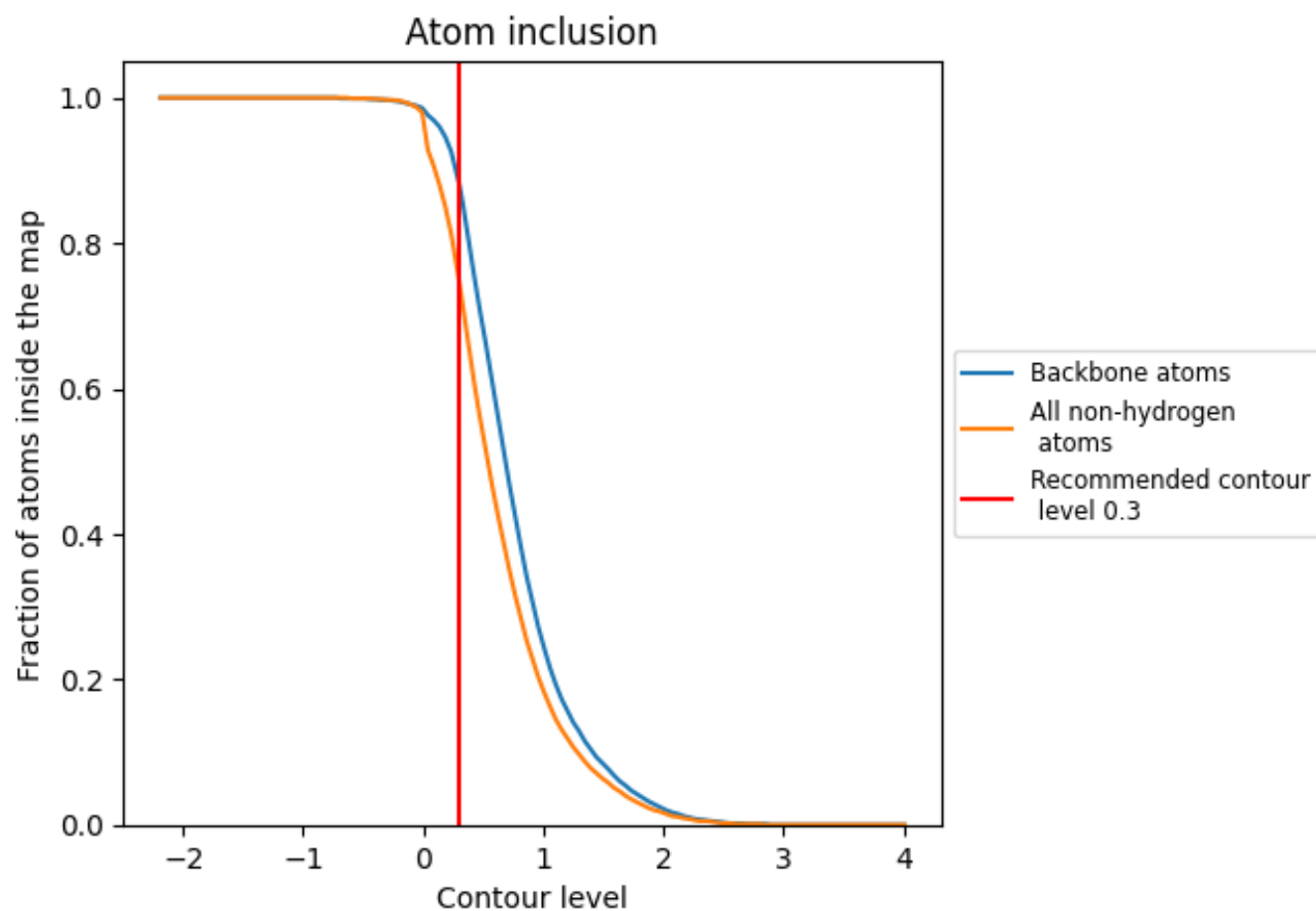


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 75% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.3090
A	0.7740	0.2840
B	0.6900	0.3500
C	0.5820	0.2910
E	0.6980	0.3340
F	0.7400	0.3760
G	0.7390	0.3920
H	0.7000	0.4500

1.0

0.0

<0.0