Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 08:28 am GMT

PDB ID	:	7NFE
EMDB ID	:	EMD-12301
Title	:	Cryo-EM structure of NHEJ super-complex (monomer)
Authors	:	Chaplin, A.K.; Hardwick, S.W.; Kefala Stavridi, A.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on	:	2021-02-06
Resolution	:	4.29 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:

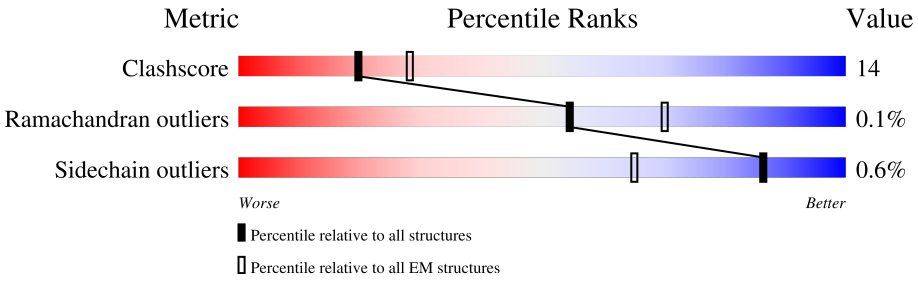
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.29 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	4156	60% 26% 14%
2	B	609	51% 26% 22%
3	C	732	46% 24% 30%
4	F	299	18% 45% 19% 36%
4	G	299	8% 44% 22% 34%
5	H	336	10% 43% 17% 40%
5	I	336	17% 41% 16% 43%
6	J	911	18% 11% 72%

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Mol	Chain	Length	Quality of chain
7	D	24	50% 50%
8	E	24	46% 54%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 44554 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 DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3585	27806	17851	4651	5132	172	0	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	475	3673	2365	610	680	18	0	0

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	513	3999	2557	669	752	21	0	0

- Molecule 4 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	190	1465	936	247	275	7	0	0
4	G	197	Total	C	N	O	S	0	0
			1502	950	253	291	8		

- Molecule 5 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	201	1575	991	271	307	6	0	0
5	I	193	Total	C	N	O	S	0	0
			1521	958	257	300	6		

- Molecule 6 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	258	Total	C	N	O	S	0	0
			2026	1284	345	386	11		

- Molecule 7 is a DNA chain called DNA (5'-D(P*AP*AP*TP*AP*AP*AP*CP*TP*AP*AP*AP*AP*AP*CP*TP*AP*TP*TP*AP*TP*TP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	24	Total	C	N	O	P	0	0
			493	238	92	139	24		

- Molecule 8 is a DNA chain called DNA (5'-D(P*TP*AP*AP*TP*AP*AP*TP*AP*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*AP*G)-3').

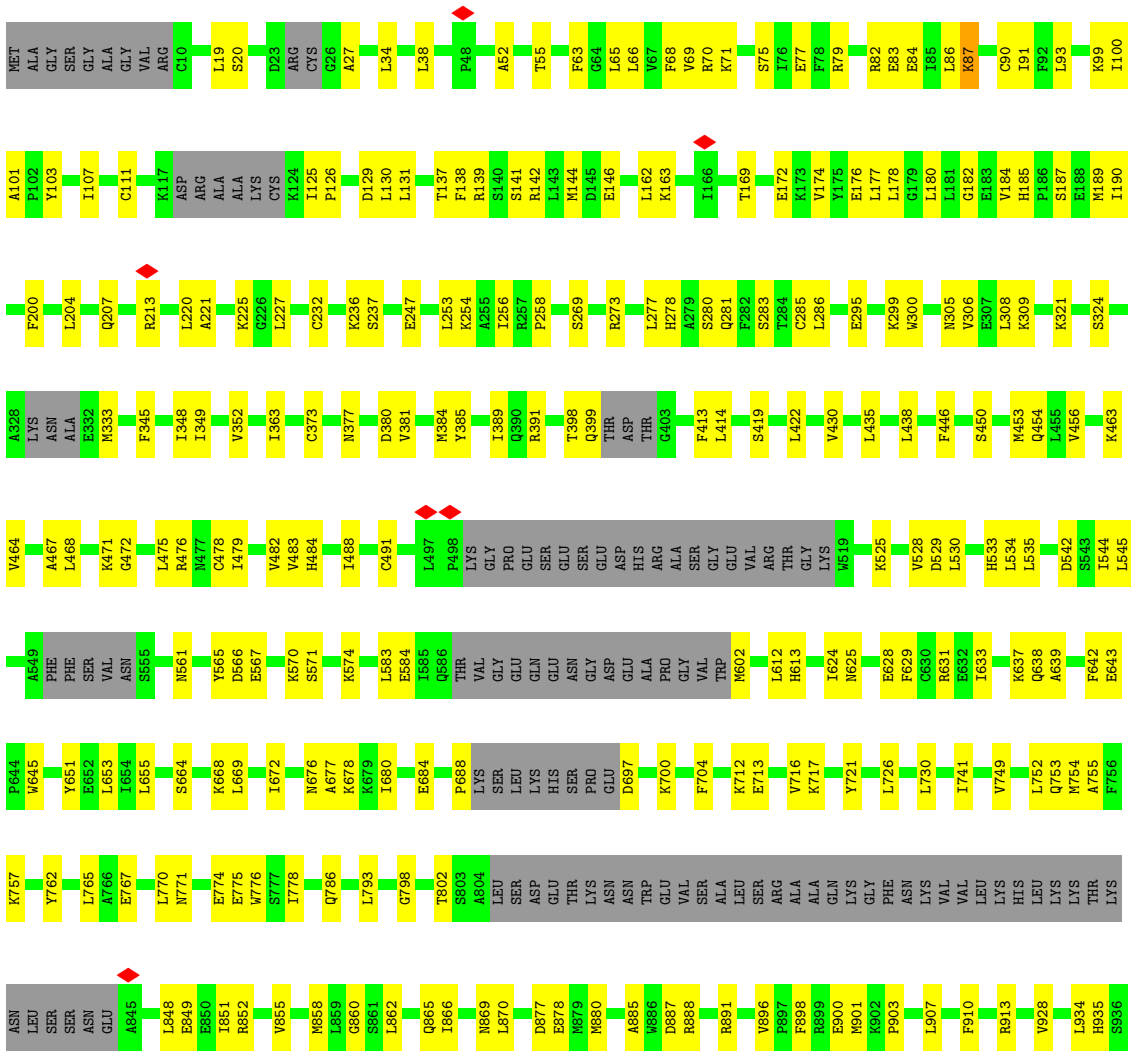
Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	24	Total	C	N	O	P	0	0
			494	240	81	149	24		

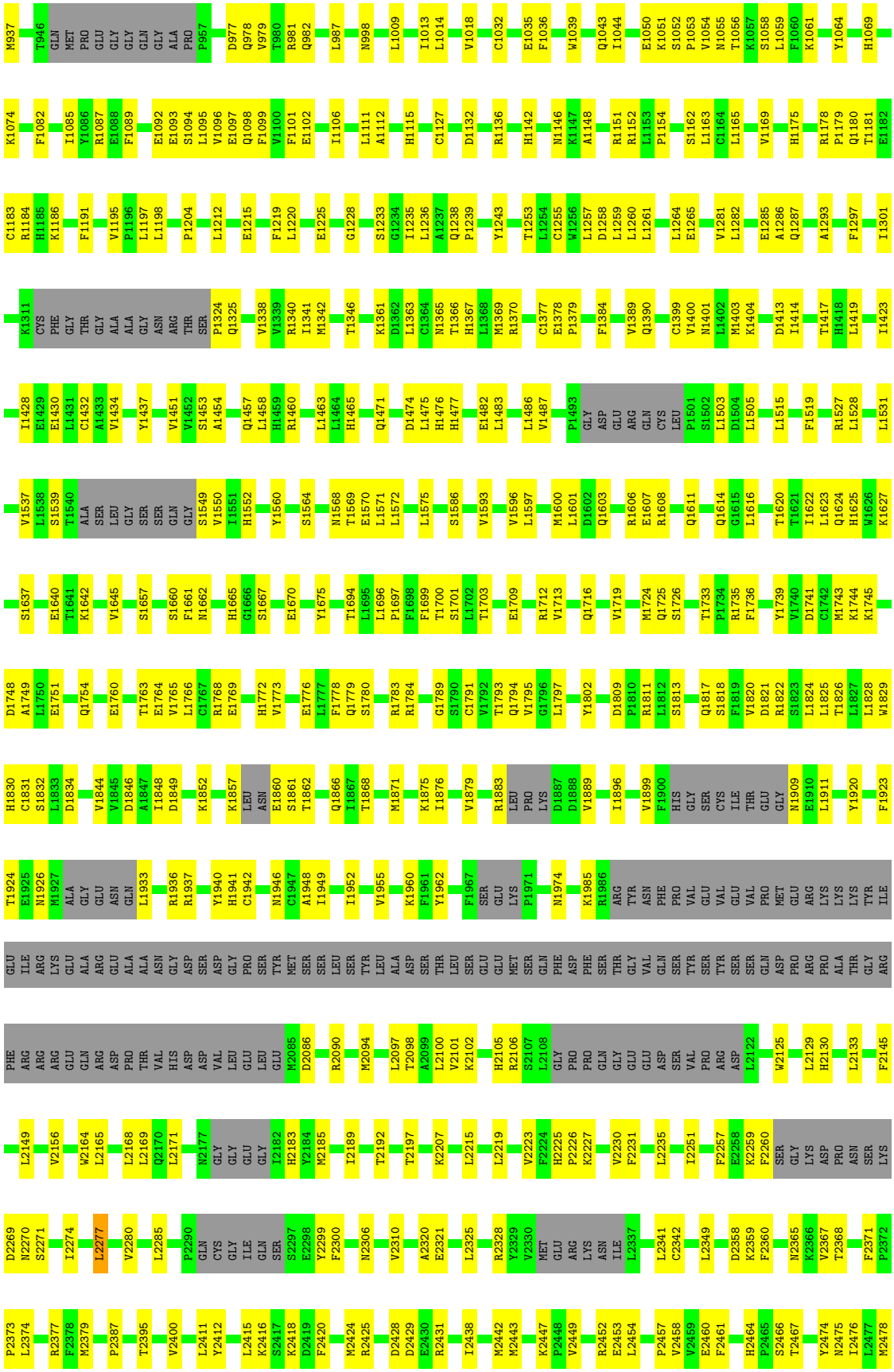
3 Residue-property plots (i)

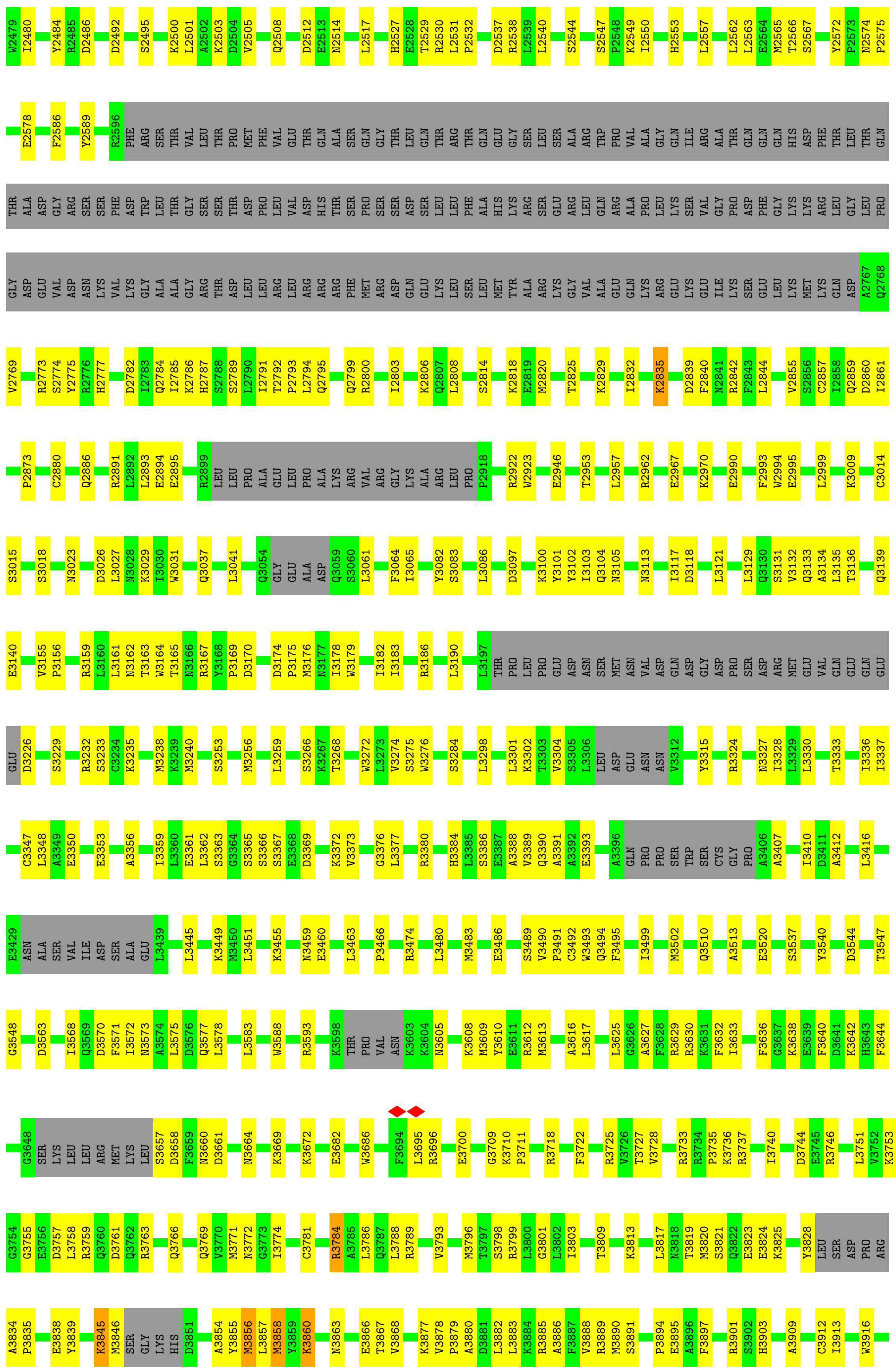
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

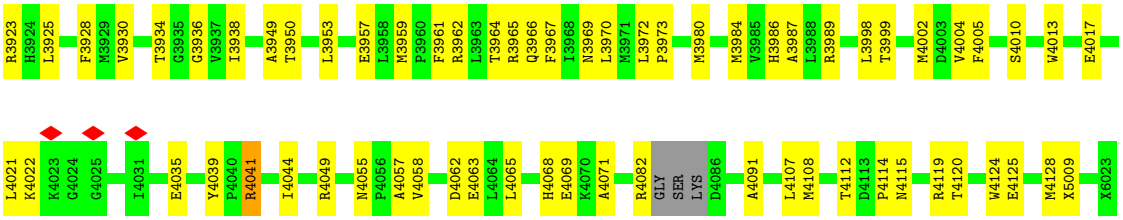
• Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit

Chain A:



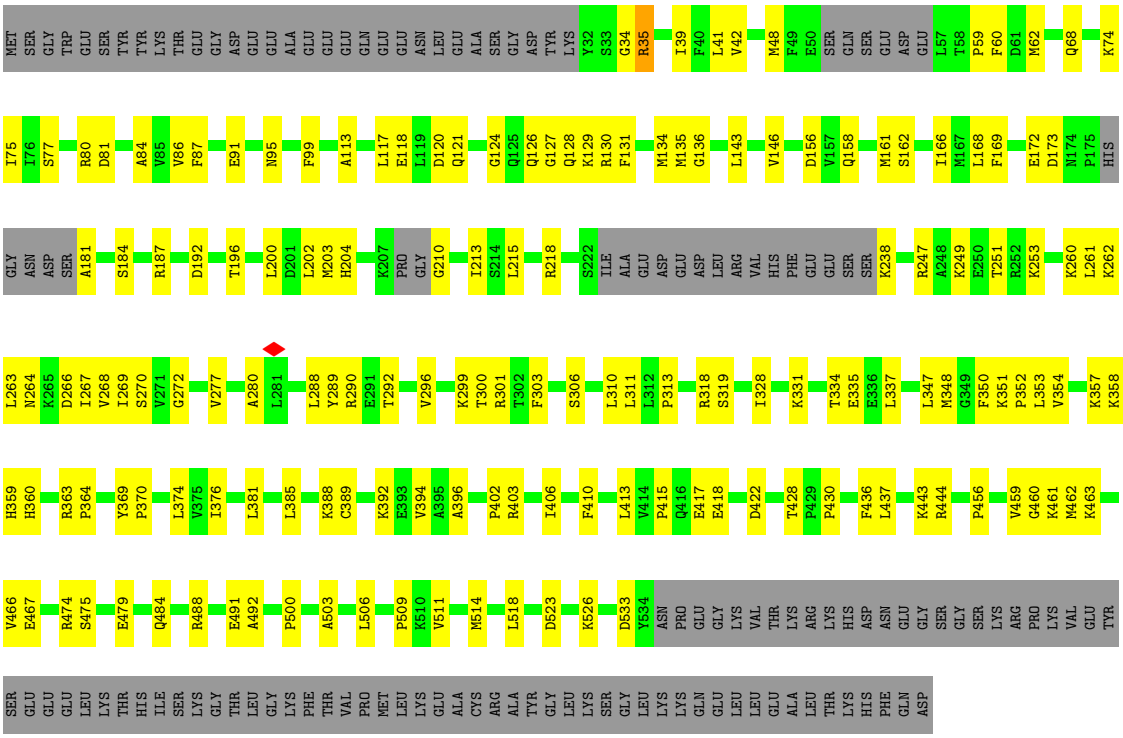



W2479 I2480 Y2484 R2485 D2486 D2492 S2495 K2500 L2501 A2502 K2503 D2504 V2505 Q2508 D2512 E2513 N2514 L2517 H2527 E2528 T2529 R2530 L2531 P2532 D2537 R2538 L2539 L2540 S2544 S2547 P2548 K2549 I2550 H2553 L2557 L2562 L2563 E2564 M2565 T2566 S2567 Y2572 P2573 N2574 P2575
E2578 F2586 Y2589 R2596 PHE ARG SER THR VAL LEU THR PRO MET PHE VAL GLU THR GLN ALA SER GLN GLY THR LEU GLN THR ARG THR GLN GLU GLY SER LEU SER ALA ARG TRP PRO VAL ALA GLY GLN ILE ARG ALA THR GLN GLN GLN HIS ASP PHE THR LEU THR GLN
THR ALA ASP GLY ARG SER SER PHE ASP TRP LEU THR GLY SER SER THR ASP PRO LEU VAL ASP HIS THR SER PRO SER SER ASP SER LEU LEU PHE ALA HIS LYS ARG SER GLU ARG LEU GLN ARG ALA PRO LEU LYS SER VAL GLY PRO ASP PHE GLY LYS LYS ARG LEU GLY LEU PRO
GLY ASP GLU VAL ASP ASN LYS VAL LYS GLY ALA ALA GLY ARG THR THR ASP LEU LEU ARG LEU ARG ARG PHE MET ARG ASP GLN GLU LYS LEU SER LEU MET TYR ALA ARG LYS GLY VAL ALA GLU GLN LYS ARG GLU LYS GLU ILE LYS SER GLU LEU LYS MET LYS GLN ASP A2767 Q2768
V2769 R2773 S2774 Y2775 R2776 H2777 D2782 I2783 Q2784 I2785 K2786 H2787 S2788 S2789 L2790 I2791 T2792 P2793 L2794 Q2795 Q2799 R2800 I2803 K2806 Q2807 L2808 S2814 K2818 E2819 M2820 T2825 K2829 I2832 K2835 D2839 F2840 N2841 R2842 F2843 L2844 V2855 S2856 C2857 I2858 Q2859 D2860 I2861
P2873 C2880 Q2886 R2891 L2892 L2893 E2894 E2895 R2899 LEU LEU PRO ALA GLU LEU PRO ALA LYS ARG VAL ARG GLY LYS ALA ARG LEU PRO P2918 R2922 W2923 E2946 T2953 L2957 R2962 E2967 K2970 E2990 F2993 W2994 E2995 L2999 K3009 C3014
S3015 S3018 N3023 D3026 L3027 N3028 K3029 I3030 W3031 Q3037 L3041 Q3054 GLY GLU ALA ASP Q3059 S3060 L3061 F3064 I3065 Y3082 S3083 L3086 D3097 K3100 Y3101 Y3102 I3103 Q3104 N3105 N3113 I3117 D3118 L3121 L3129 Q3130 S3131 V3132 Q3133 A3134 L3135 T3136 Q3139
E3140 V3155 P3156 R3159 L3160 L3161 N3162 T3163 W3164 T3165 N3166 R3167 Y3168 P3169 D3170 D3174 P3175 M3176 N3177 I3178 W3179 I3182 I3183 R3186 L3190 L3197 THR PRO LEU PRO GLU ASP ASN SER MET ASN VAL ASP GLN ASP GLY ASP PRO SER ASP ARG MET GLU VAL GLN GLU GLN GLU
GLU D3226 S3229 R3232 S3233 C3234 K3235 M3238 K3239 M3240 S3253 M3256 L3259 S3266 K3267 T3268 W3272 L3273 V3274 S3275 W3276 S3284 L3298 L3301 K3302 T3303 V3304 S3305 L3306 LEU ASP GLU ASN ASN V3312 Y3315 R3324 N3327 I3328 L3329 L3330 T3333 I3336 I3337
C3347 L3348 A3349 E3350 E3353 A3356 I3359 L3360 E3361 L3362 S3363 G3364 S3365 S3366 S3367 E3368 D3369 K3372 V3373 G3376 L3377 R3380 H3384 L3385 S3386 E3387 A3388 V3389 Q3390 A3391 A3392 E3393 A3396 GLN PRO PRO SER TRP SER CYS GLY PRO A3406 A3407 I3410 D3411 A3412 L3416
E3429 ASN ALA SER VAL ILE ASP SER ALA GLU L3439 L3445 K3449 M3450 L3451 K3455 N3459 E3460 L3463 P3466 R3474 L3480 M3483 E3486 S3489 V3490 P3491 C3492 W3493 Q3494 F3495 I3499 M3502 Q3510 A3513 E3520 S3537 Y3540 D3544 T3547
G3548 D3563 I3568 Q3569 D3570 F3571 I3572 N3573 A3574 L3575 D3576 Q3577 L3578 L3583 W3588 R3593 K3598 THR PRO VAL ASN K3603 K3604 N3605 K3608 M3609 Y3610 E3611 R3612 M3613 A3616 L3617 L3625 G3626 A3627 F3628 R3629 R3630 K3631 F3632 I3633 F3636 G3637 K3638 E3639 F3640 D3641 K3642 H3643 F3644
G3648 SER LYS LEU LEU ARG MET LYS LEU S3657 D3658 F3659 N3660 D3661 N3664 K3669 K3672 E3682 W3686 F3694 L3695 R3696 E3700 G3709 K3710 P3711 R3718 F3722 R3725 V3726 T3727 V3728 R3733 R3734 P3735 K3736 R3737 I3740 D3744 E3745 R3746 L3751 V3752 K3753
G3754 G3755 E3756 D3757 L3758 R3759 Q3760 D3761 Q3762 R3763 Q3766 Q3769 V3770 M3771 N3772 G3773 I3774 C3781 R3784 A3785 L3786 Q3787 L3788 R3789 V3793 M3796 T3797 S3798 R3799 L3800 G3801 L3802 I3803 T3809 K3813 L3817 N3818 T3819 M3820 S3821 Q3822 E3823 E3824 K3825 Y3828 LEU SER ASP PRO ARG
A3834 P3835 E3838 Y3839 K3845 M3846 SER GLY LYS HIS D3851 A3854 Y3855 M3856 L3857 M3858 Y3859 K3860 N3863 E3866 T3867 V3868 K3877 V3878 P3879 A3880 D3881 L3882 L3883 K3884 R3885 A3886 F3887 V3888 R3889 M3890 S3891 P3894 E3895 A3896 F3897 R3901 S3902 H3903 A3909 C3912 I3913 W3916



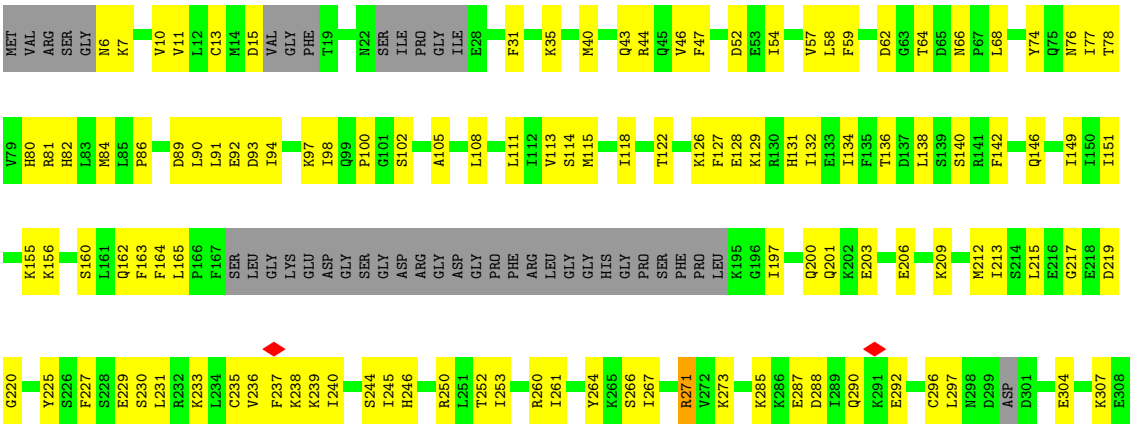
• Molecule 2: X-ray repair cross-complementing protein 6

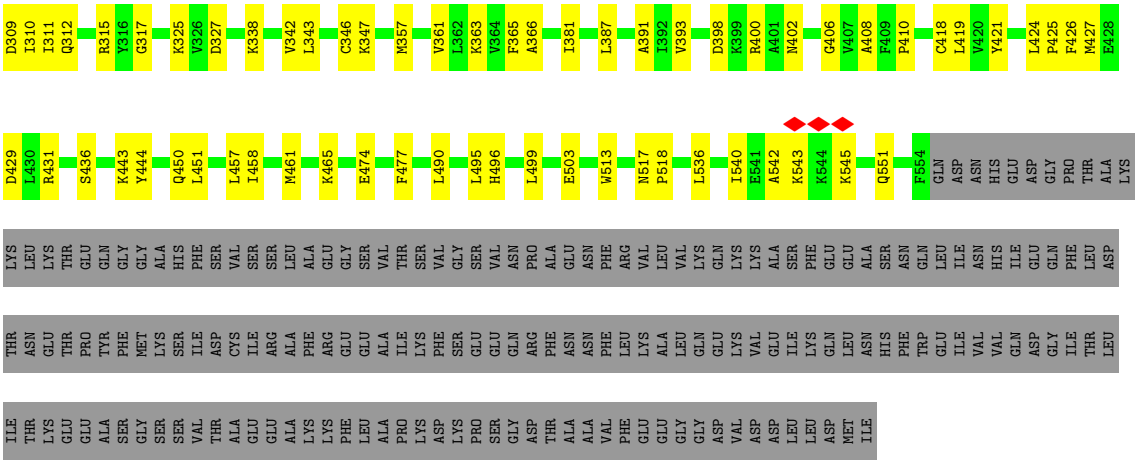
Chain B:



• Molecule 3: X-ray repair cross-complementing protein 5

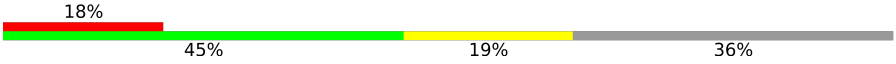
Chain C:

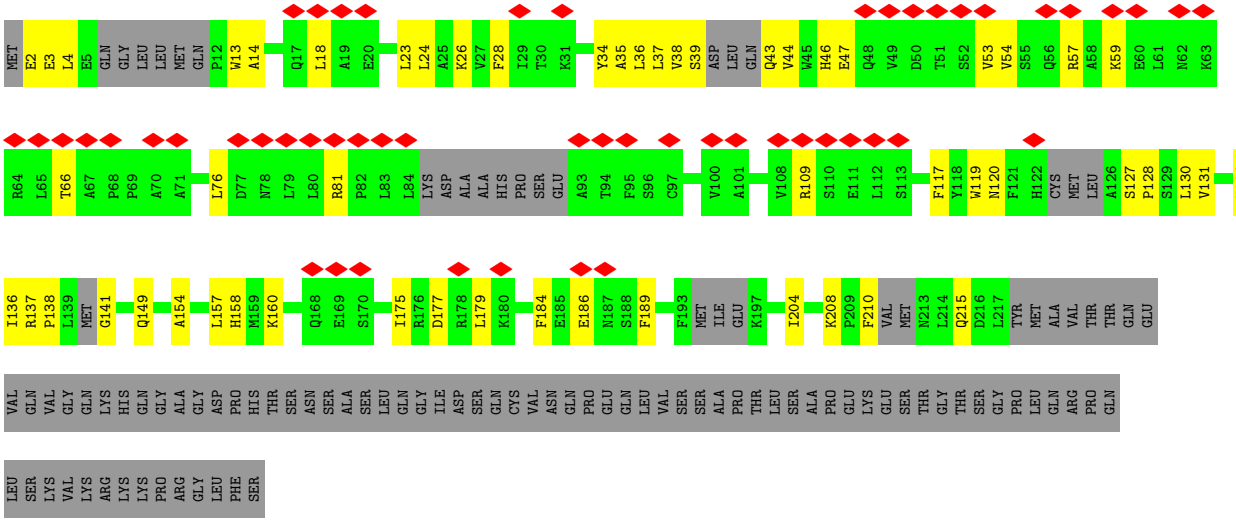




• Molecule 4: Non-homologous end-joining factor 1

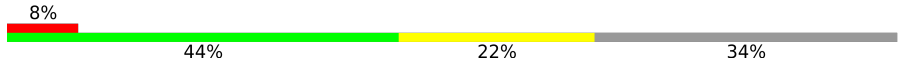
Chain F:

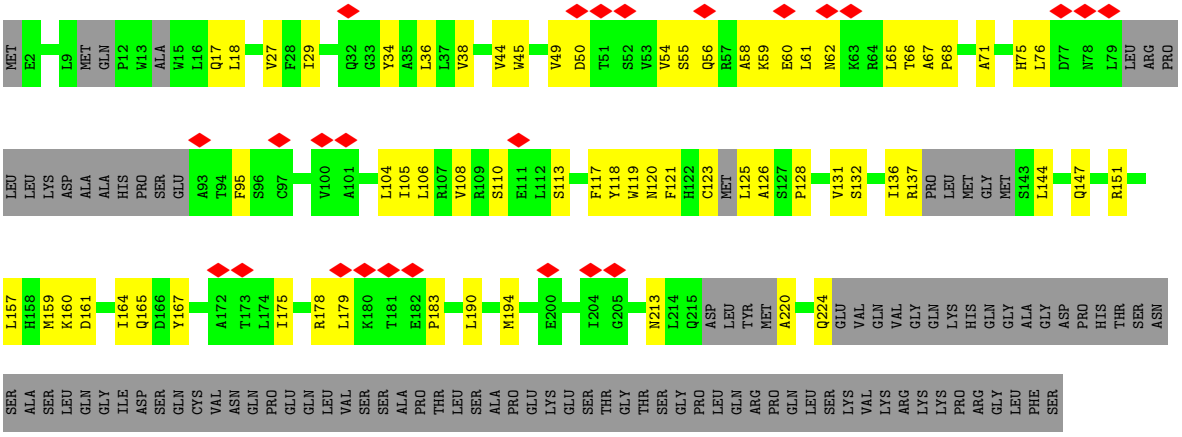




• Molecule 4: Non-homologous end-joining factor 1

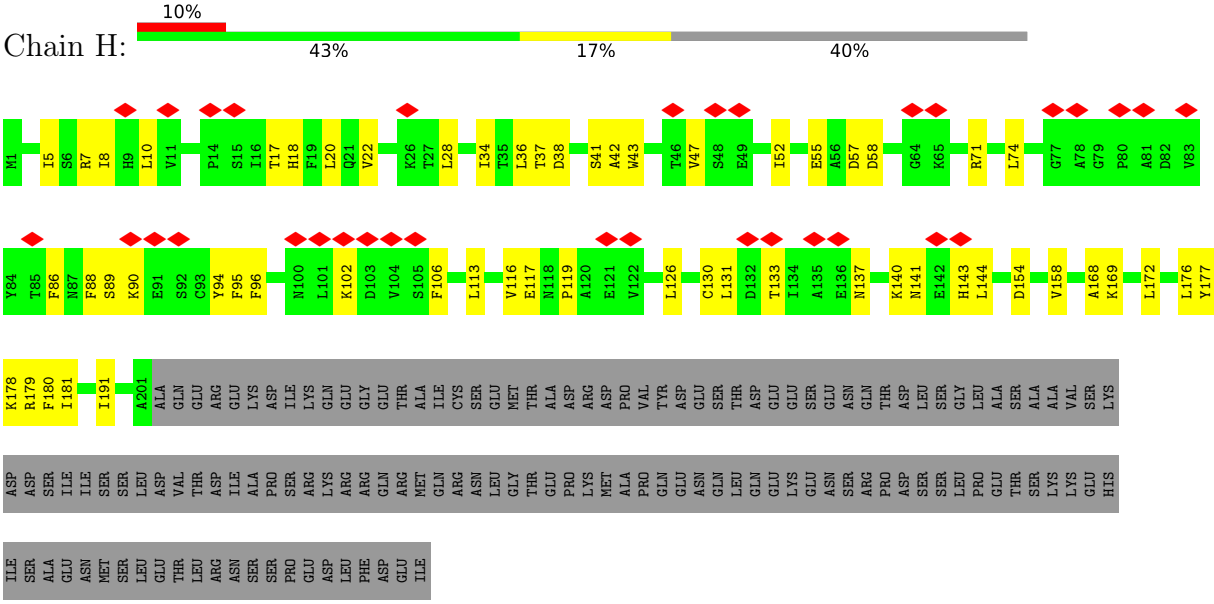
Chain G:





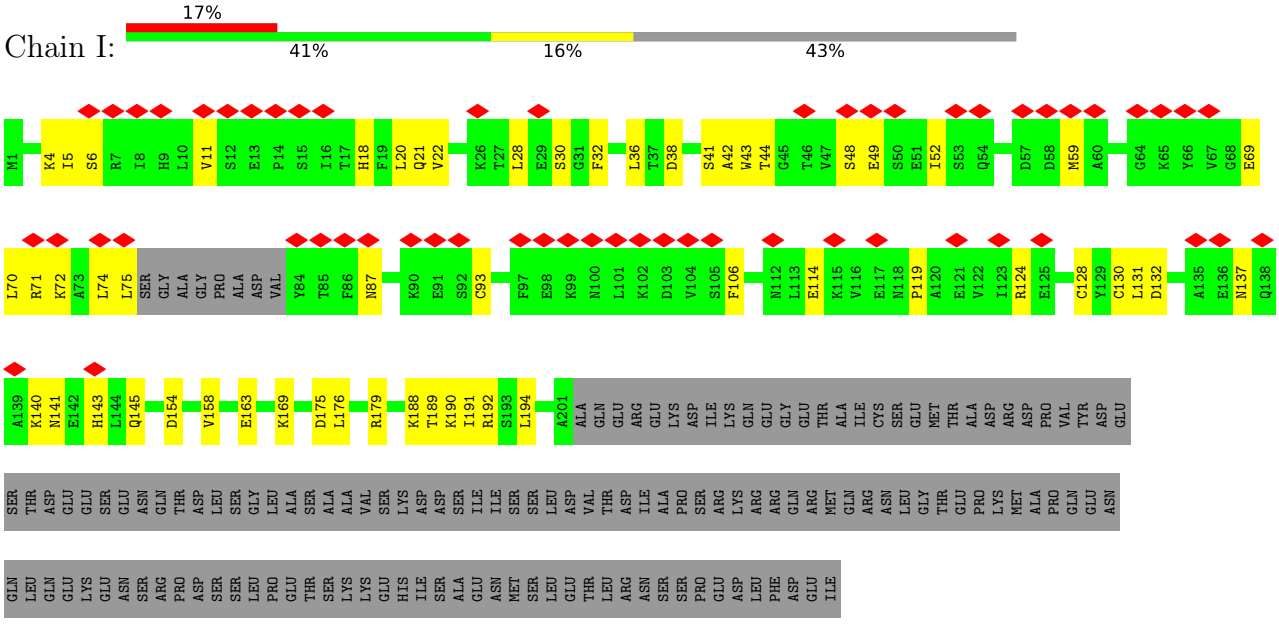
• Molecule 5: DNA repair protein XRCC4

Chain H:



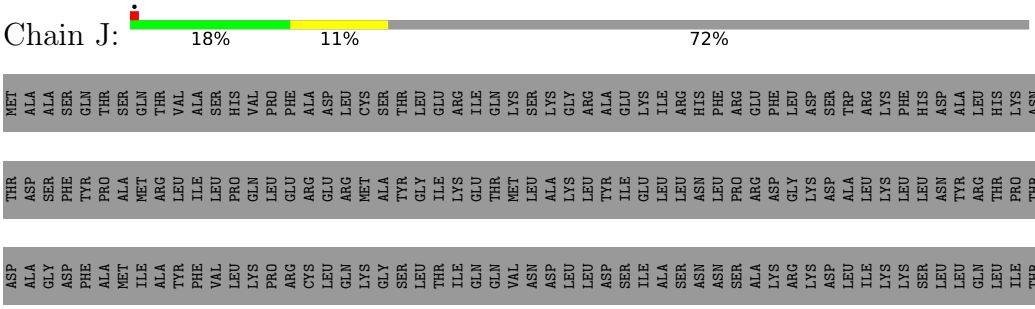
• Molecule 5: DNA repair protein XRCC4

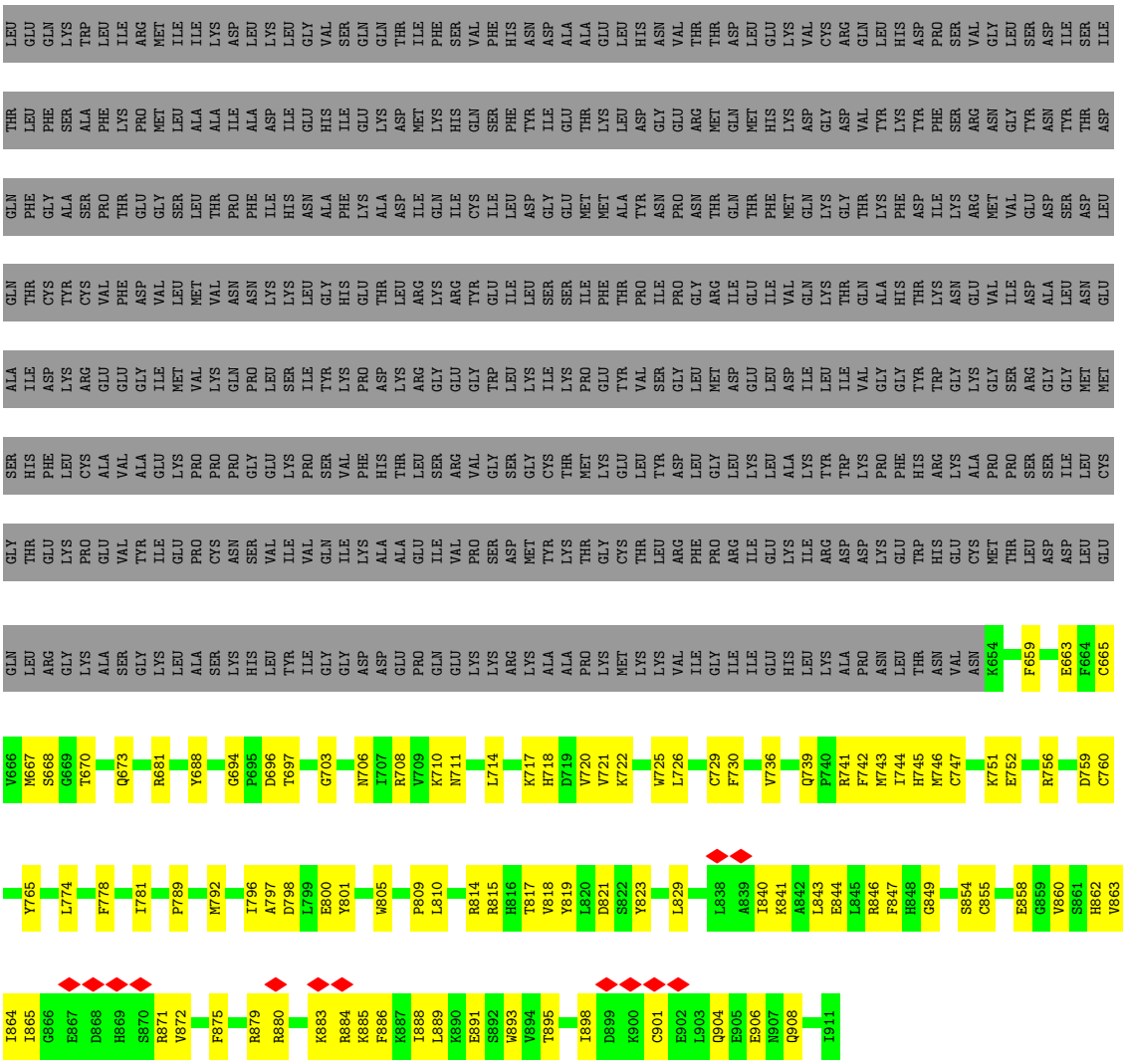
Chain I:



• Molecule 6: DNA ligase 4

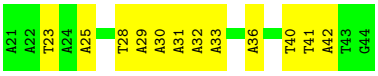
Chain J:





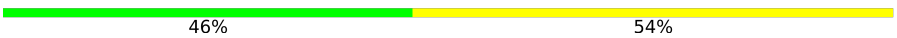
• Molecule 7: DNA (5'-D(P*AP*AP*TP*AP*AP*AP*CP*TP*AP*AP*AP*AP*AP*CP*TP*AP*TP*TP*AP*TP*TP*AP*TP*G)-3')

Chain D:



• Molecule 8: DNA (5'-D(P*TP*AP*AP*TP*AP*AP*TP*AP*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*TP*AP*G)-3')

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45943	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 ($e^-/Å^2$)	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.753	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	704.16003, 704.16003, 704.16003	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

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	0.25	0/28219	0.46	1/38230 (0.0%)
2	B	0.25	0/3740	0.48	0/5053
3	C	0.25	0/4075	0.47	0/5509
4	F	0.24	0/1488	0.48	0/2015
4	G	0.24	0/1522	0.51	0/2064
5	H	0.24	0/1602	0.47	0/2159
5	I	0.24	0/1546	0.47	0/2082
6	J	0.24	0/2073	0.46	0/2807
7	D	0.43	0/554	0.88	0/852
8	E	0.56	0/552	1.09	0/851
All	All	0.26	0/45371	0.49	1/61622 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2277	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

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	27806	0	27233	715	0
2	B	3673	0	3652	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3999	0	3899	136	0
4	F	1465	0	1432	47	0
4	G	1502	0	1439	61	0
5	H	1575	0	1514	57	0
5	I	1521	0	1440	46	0
6	J	2026	0	1895	72	0
7	D	493	0	273	11	0
8	E	494	0	278	15	0
All	All	44554	0	43055	1205	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 14.

All (1205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3365:SER:HB3	1:A:3376:GLY:HA3	1.61	0.82
2:B:337:LEU:HD11	3:C:490:LEU:HA	1.67	0.77
4:G:128:PRO:O	4:G:132:SER:HB2	1.85	0.77
6:J:814:ARG:HD2	6:J:849:GLY:H	1.50	0.77
4:G:132:SER:HB3	4:G:137:ARG:HH21	1.51	0.76
5:I:5:ILE:HA	5:I:21:GLN:HA	1.68	0.76
1:A:901:MET:HG2	1:A:903:PRO:HD3	1.67	0.75
1:A:3728:VAL:HG22	1:A:3736:LYS:HG2	1.69	0.75
1:A:3727:THR:HB	1:A:3737:ARG:HB3	1.68	0.75
3:C:44:ARG:HD2	3:C:238:LYS:HB3	1.67	0.75
1:A:1184:ARG:NH1	1:A:1265:GLU:OE1	2.20	0.75
1:A:1257:LEU:HA	1:A:1260:LEU:HD12	1.67	0.74
1:A:2480:ILE:O	1:A:2484:TYR:HB2	1.86	0.74
2:B:269:ILE:HD11	2:B:381:LEU:HD23	1.69	0.74
1:A:3361:GLU:HB3	1:A:3366:SER:HA	1.69	0.73
1:A:1724:MET:HG2	1:A:1768:ARG:HD3	1.68	0.73
3:C:77:ILE:HG21	3:C:113:VAL:HG21	1.70	0.73
4:G:44:VAL:HA	4:G:125:LEU:HD23	1.72	0.72
1:A:1098:GLN:HG3	1:A:1151:ARG:HB3	1.71	0.72
1:A:793:LEU:HB3	1:A:870:LEU:HA	1.72	0.71
4:G:106:LEU:HB3	4:G:121:PHE:HB2	1.72	0.71
1:A:2449:VAL:HG23	1:A:2452:ARG:HH12	1.55	0.71
5:H:18:HIS:HD2	5:H:36:LEU:HD21	1.54	0.70
5:I:32:PHE:HE1	5:I:74:LEU:HB3	1.56	0.70
3:C:58:LEU:HB2	3:C:78:THR:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:55:SER:OG	4:G:59:LYS:NZ	2.25	0.69
4:G:147:GLN:HB3	4:G:151:ARG:NH1	2.07	0.69
1:A:2133:LEU:HD11	1:A:2171:LEU:HD22	1.74	0.69
1:A:2428:ASP:HB3	1:A:2431:ARG:HB2	1.74	0.69
1:A:2893:LEU:HD11	1:A:2922:ARG:HB3	1.75	0.69
4:G:126:ALA:HB3	4:G:131:VAL:HG21	1.75	0.69
3:C:10:VAL:HG22	3:C:131:HIS:HB2	1.74	0.69
1:A:1361:LYS:O	1:A:1365:ASN:N	2.23	0.68
4:F:136:ILE:HA	4:G:136:ILE:HG23	1.75	0.68
5:I:141:ASN:O	5:I:145:GLN:NE2	2.26	0.68
3:C:408:ALA:HB1	3:C:419:LEU:HD21	1.76	0.68
1:A:3183:ILE:HD12	1:A:3238:MET:HE2	1.75	0.68
1:A:306:VAL:HA	1:A:309:LYS:HE2	1.75	0.68
3:C:391:ALA:HB3	3:C:408:ALA:HB3	1.76	0.68
4:G:45:TRP:H	4:G:125:LEU:HB3	1.60	0.67
5:I:18:HIS:HB3	5:I:36:LEU:HD11	1.76	0.67
1:A:1624:GLN:O	1:A:1627:LYS:NZ	2.27	0.67
2:B:444:ARG:NH1	3:C:244:SER:OG	2.27	0.67
1:A:3416:LEU:HD23	1:A:3449:LYS:HZ2	1.58	0.67
4:G:161:ASP:O	4:G:165:GLN:NE2	2.28	0.67
5:H:141:ASN:ND2	5:I:141:ASN:OD1	2.27	0.67
2:B:204:HIS:NE2	2:B:210:GLY:O	2.23	0.66
2:B:396:ALA:HB3	2:B:413:LEU:HB2	1.77	0.66
4:G:147:GLN:HB3	4:G:151:ARG:HH12	1.60	0.66
1:A:213:ARG:HD2	2:B:335:GLU:HG2	1.77	0.66
3:C:151:ILE:HD11	3:C:215:LEU:HB2	1.76	0.66
1:A:4041:ARG:HA	1:A:4044:ILE:HG22	1.76	0.66
1:A:1285:GLU:HG3	1:A:1287:GLN:HG2	1.78	0.66
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	1.77	0.66
3:C:44:ARG:NH2	3:C:236:VAL:O	2.22	0.66
5:H:37:THR:HA	5:H:42:ALA:HA	1.78	0.66
1:A:352:VAL:HG11	1:A:1735:ARG:HG2	1.77	0.66
1:A:1379:PRO:HB2	1:A:1384:PHE:HB3	1.78	0.66
5:H:7:ARG:HE	5:I:131:LEU:HB2	1.60	0.66
1:A:1831:CYS:SG	1:A:1832:SER:N	2.70	0.65
1:A:3894:PRO:O	1:A:3895:GLU:HG3	1.96	0.65
1:A:2447:LYS:HG2	1:A:2449:VAL:HG12	1.77	0.65
3:C:44:ARG:HD3	3:C:238:LYS:HE3	1.78	0.65
4:F:18:LEU:HD11	4:F:23:LEU:HD12	1.78	0.65
2:B:523:ASP:HA	2:B:526:LYS:HE2	1.79	0.65
3:C:111:LEU:HB3	3:C:115:MET:HE1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:76:LEU:O	4:F:81:ARG:NH2	2.31	0.64
1:A:3492:CYS:HB3	1:A:3711:PRO:HD3	1.77	0.64
1:A:1453:SER:O	1:A:1457:GLN:NE2	2.30	0.64
2:B:261:LEU:HB3	2:B:269:ILE:HB	1.78	0.64
5:H:43:TRP:HB3	5:H:113:LEU:HB3	1.79	0.64
1:A:566:ASP:OD1	1:A:645:TRP:NE1	2.28	0.64
1:A:3302:LYS:HE2	1:A:3363:SER:HB2	1.80	0.64
4:F:149:GLN:NE2	4:G:194:MET:SD	2.67	0.64
1:A:2894:GLU:HG3	1:A:3973:PRO:HG3	1.80	0.64
3:C:66:ASN:ND2	3:C:74:TYR:O	2.30	0.63
5:H:17:THR:O	5:H:18:HIS:ND1	2.30	0.63
1:A:1180:GLN:HB2	1:A:1183:CYS:HB2	1.80	0.63
1:A:2962:ARG:HA	1:A:3989:ARG:HH12	1.62	0.63
6:J:792:MET:HA	6:J:796:ILE:HB	1.79	0.63
1:A:1437:TYR:HD1	1:A:1503:LEU:HD21	1.63	0.63
1:A:1889:VAL:O	1:A:1909:ASN:N	2.31	0.63
2:B:296:VAL:HG12	3:C:297:LEU:HD23	1.81	0.63
8:E:31:DT:H2"	8:E:32:DT:C4	2.34	0.63
2:B:218:ARG:HB3	4:G:178:ARG:HH12	1.63	0.63
1:A:3766:GLN:OE1	1:A:3769:GLN:NE2	2.32	0.63
3:C:327:ASP:OD1	6:J:711:ASN:ND2	2.31	0.63
1:A:1366:THR:O	1:A:1369:MET:HB3	1.98	0.63
3:C:15:ASP:HB3	3:C:136:THR:HA	1.81	0.62
1:A:1766:LEU:O	1:A:1822:ARG:NH1	2.33	0.62
1:A:2165:LEU:HG	1:A:2169:LEU:HD23	1.80	0.62
1:A:3625:LEU:O	1:A:3630:ARG:NH1	2.32	0.62
3:C:165:LEU:O	3:C:227:PHE:N	2.33	0.62
4:F:128:PRO:HG3	4:G:44:VAL:H	1.62	0.62
1:A:529:ASP:O	1:A:533:HIS:ND1	2.29	0.62
2:B:260:LYS:HZ3	2:B:270:SER:HB3	1.65	0.62
1:A:1789:GLY:O	1:A:1794:GLN:NE2	2.33	0.62
5:H:42:ALA:HB2	5:H:119:PRO:HB3	1.82	0.62
5:I:36:LEU:HB3	5:I:43:TRP:HB2	1.80	0.62
1:A:1769:GLU:O	1:A:1822:ARG:NH1	2.26	0.61
3:C:212:MET:HB3	3:C:220:GLY:HA3	1.81	0.61
5:I:4:LYS:O	5:I:22:VAL:N	2.31	0.61
1:A:2197:THR:HG22	1:A:5009:UNK:HA	1.82	0.61
1:A:3480:LEU:HD21	1:A:3510:GLN:HB3	1.82	0.61
4:F:2:GLU:HG3	4:F:46:HIS:HB2	1.82	0.61
1:A:3445:LEU:O	1:A:3449:LYS:HG2	2.00	0.61
1:A:896:VAL:HB	1:A:903:PRO:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:11:VAL:HG22	5:I:87:ASN:HB3	1.83	0.61
5:I:179:ARG:NH2	6:J:781:ILE:O	2.32	0.61
1:A:65:LEU:O	1:A:69:VAL:N	2.23	0.61
4:F:128:PRO:HB3	4:G:44:VAL:HG23	1.82	0.61
1:A:978:GLN:HE21	1:A:979:VAL:HG13	1.64	0.61
1:A:2574:ASN:O	1:A:2787:HIS:ND1	2.33	0.61
1:A:1389:VAL:HG22	1:A:1390:GLN:H	1.64	0.61
1:A:3327:ASN:HB2	1:A:3388:ALA:HB2	1.82	0.61
4:F:158:HIS:NE2	4:F:184:PHE:O	2.32	0.61
1:A:258:PRO:HG2	3:C:551:GLN:HG2	1.82	0.61
1:A:1475:LEU:HD13	1:A:1527:ARG:HG3	1.83	0.61
3:C:346:CYS:SG	3:C:347:LYS:N	2.74	0.61
1:A:1102:GLU:HG2	1:A:1154:PRO:HA	1.83	0.60
4:G:62:ASN:HB2	4:G:65:LEU:HB2	1.82	0.60
1:A:2563:LEU:HD12	1:A:2795:GLN:HB2	1.83	0.60
1:A:1662:ASN:ND2	1:A:1701:SER:O	2.34	0.60
2:B:181:ALA:N	2:B:184:SER:HG	1.98	0.60
1:A:2529:THR:OG1	1:A:2530:ARG:NH1	2.35	0.60
1:A:3593:ARG:NH1	1:A:3664:ASN:OD1	2.34	0.60
1:A:3657:SER:OG	1:A:3660:ASN:ND2	2.34	0.60
2:B:303:PHE:HA	2:B:311:LEU:H	1.66	0.60
1:A:1741:ASP:O	1:A:1745:LYS:HG2	2.02	0.60
4:G:18:LEU:HA	4:G:95:PHE:HB2	1.82	0.60
1:A:65:LEU:HA	1:A:68:PHE:HB2	1.84	0.60
1:A:672:ILE:O	1:A:676:ASN:ND2	2.34	0.60
1:A:1432:CYS:HB2	1:A:1486:LEU:HD21	1.84	0.60
1:A:1809:ASP:HB3	1:A:1811:ARG:HH12	1.65	0.60
1:A:2538:ARG:HG2	1:A:2565:MET:SD	2.41	0.60
6:J:670:THR:H	6:J:703:GLY:HA3	1.66	0.60
1:A:3796:MET:H	1:A:3801:GLY:HA2	1.67	0.60
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.83	0.59
1:A:3140:GLU:OE2	1:A:3167:ARG:NH1	2.35	0.59
1:A:3480:LEU:HD23	1:A:3513:ALA:HB2	1.82	0.59
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	1.84	0.59
2:B:351:LYS:NZ	3:C:477:PHE:O	2.35	0.59
1:A:419:SER:HA	1:A:422:LEU:HD12	1.85	0.59
1:A:2373:PRO:O	1:A:2377:ARG:NH1	2.35	0.59
1:A:1175:HIS:HB3	1:A:1178:ARG:HE	1.67	0.59
1:A:1724:MET:HA	1:A:1768:ARG:HH11	1.66	0.59
1:A:3134:ALA:HB2	1:A:3182:ILE:HG22	1.83	0.59
2:B:289:TYR:HD2	2:B:292:THR:H	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:VAL:HB	3:C:54:ILE:HG22	1.84	0.59
5:I:140:LYS:HA	5:I:143:HIS:NE2	2.18	0.59
1:A:1899:VAL:HB	1:A:1911:LEU:HD13	1.85	0.59
2:B:263:LEU:HA	2:B:347:LEU:HB3	1.85	0.59
5:H:158:VAL:HG12	5:I:158:VAL:HG12	1.84	0.59
1:A:877:ASP:HA	1:A:880:MET:HG2	1.85	0.59
1:A:928:VAL:HG21	1:A:2769:VAL:HG22	1.84	0.59
1:A:678:LYS:NZ	1:A:775:GLU:OE1	2.35	0.59
1:A:3359:ILE:HA	1:A:3362:LEU:HB2	1.83	0.59
1:A:3755:GLY:N	1:A:3799:ARG:O	2.36	0.59
4:G:17:GLN:NE2	4:G:18:LEU:O	2.35	0.59
4:F:208:LYS:HE2	4:G:144:LEU:HD13	1.83	0.58
5:I:42:ALA:HB2	5:I:119:PRO:HA	1.84	0.58
1:A:1528:LEU:HD11	1:A:1571:LEU:HD21	1.85	0.58
2:B:350:PHE:HE2	3:C:458:ILE:HG12	1.66	0.58
3:C:81:ARG:HG3	3:C:90:LEU:HD11	1.85	0.58
1:A:472:GLY:O	1:A:476:ARG:NH1	2.35	0.58
1:A:1622:ILE:HA	1:A:1625:HIS:CE1	2.39	0.58
2:B:488:ARG:HH12	2:B:503:ALA:H	1.52	0.58
3:C:122:THR:HA	3:C:127:PHE:HE2	1.69	0.58
1:A:1751:GLU:O	1:A:1754:GLN:NE2	2.28	0.58
1:A:3857:LEU:HA	1:A:3860:LYS:HB2	1.85	0.58
2:B:369:TYR:OH	3:C:436:SER:O	2.20	0.58
3:C:496:HIS:NE2	3:C:503:GLU:HB3	2.18	0.58
4:G:61:LEU:HD13	4:G:120:ASN:HD21	1.68	0.58
1:A:111:CYS:HB2	1:A:130:LEU:HD22	1.86	0.58
4:F:137:ARG:O	4:F:141:GLY:N	2.37	0.58
5:I:175:ASP:OD1	5:I:176:LEU:N	2.37	0.58
1:A:1346:THR:HG21	1:A:1401:ASN:HB3	1.86	0.58
1:A:1696:LEU:O	1:A:1699:PHE:N	2.37	0.58
3:C:402:ASN:HD21	7:D:25:DA:H3'	1.67	0.58
1:A:3240:MET:SD	1:A:3275:SER:OG	2.62	0.58
1:A:1820:VAL:O	1:A:1825:LEU:N	2.32	0.57
1:A:3813:LYS:HB2	1:A:3925:LEU:HB3	1.86	0.57
1:A:3863:ASN:HB3	1:A:3866:GLU:HG2	1.86	0.57
4:F:175:ILE:HG22	4:F:177:ASP:H	1.69	0.57
1:A:1181:THR:HG22	1:A:1184:ARG:HH12	1.69	0.57
1:A:3744:ASP:O	1:A:3746:ARG:NH1	2.36	0.57
2:B:288:LEU:O	3:C:311:ILE:N	2.32	0.57
1:A:2277:LEU:HA	1:A:2280:VAL:HG22	1.86	0.57
1:A:3878:VAL:O	1:A:3965:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:410:PRO:HA	3:C:419:LEU:HA	1.86	0.57
6:J:904:GLN:OE1	6:J:908:GLN:NE2	2.37	0.57
1:A:2325:LEU:HD23	1:A:2328:ARG:HH12	1.69	0.57
2:B:48:MET:HB2	2:B:59:PRO:HB2	1.87	0.57
1:A:534:LEU:O	1:A:561:ASN:ND2	2.36	0.57
1:A:1826:THR:O	1:A:1830:HIS:ND1	2.31	0.57
3:C:406:GLY:HA3	3:C:421:TYR:HE1	1.68	0.57
6:J:865:ILE:HG13	6:J:888:ILE:HG23	1.87	0.57
1:A:1844:VAL:O	1:A:1848:ILE:HG12	2.04	0.57
4:G:29:ILE:HG21	4:G:76:LEU:HB3	1.87	0.57
5:I:38:ASP:OD1	5:I:41:SER:N	2.37	0.57
6:J:747:CYS:O	6:J:751:LYS:N	2.36	0.57
1:A:2349:LEU:HB3	1:A:2360:PHE:HE1	1.70	0.57
2:B:187:ARG:HE	4:G:175:ILE:HG21	1.70	0.57
1:A:1179:PRO:HB3	1:A:1259:LEU:HD23	1.86	0.57
1:A:3867:THR:OG1	1:A:4119:ARG:NH2	2.37	0.57
4:F:39:SER:HB2	4:F:44:VAL:HA	1.86	0.57
1:A:163:LYS:H	2:B:301:ARG:HB2	1.69	0.57
2:B:75:ILE:HD11	3:C:317:GLY:HA3	1.86	0.57
2:B:251:THR:HA	3:C:431:ARG:HH12	1.69	0.57
2:B:533:ASP:OD1	3:C:250:ARG:NH2	2.33	0.57
2:B:352:PRO:HA	2:B:394:VAL:HA	1.86	0.56
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.87	0.56
1:A:3868:VAL:HG22	1:A:4114:PRO:HB2	1.85	0.56
1:A:450:SER:O	1:A:454:GLN:N	2.31	0.56
1:A:1769:GLU:HB2	1:A:1772:HIS:CD2	2.39	0.56
6:J:817:THR:OG1	6:J:884:ARG:NH2	2.38	0.56
4:F:14:ALA:H	4:F:26:LYS:HB3	1.70	0.56
4:F:57:ARG:HH22	4:F:120:ASN:HB2	1.70	0.56
4:G:56:GLN:O	4:G:60:GLU:HG3	2.06	0.56
1:A:1733:THR:HG23	1:A:1736:PHE:H	1.70	0.56
1:A:3159:ARG:HA	1:A:3162:ASN:ND2	2.21	0.56
3:C:105:ALA:O	3:C:140:SER:OG	2.24	0.56
6:J:879:ARG:HH21	6:J:880:ARG:HH12	1.54	0.56
2:B:166:ILE:HB	2:B:200:LEU:HD13	1.88	0.56
3:C:64:THR:HG22	3:C:76:ASN:H	1.71	0.56
1:A:4062:ASP:HA	1:A:4065:LEU:HD12	1.88	0.56
5:H:168:ALA:HB3	6:J:810:LEU:HD21	1.87	0.56
5:I:6:SER:O	5:I:20:LEU:N	2.38	0.56
1:A:278:HIS:HB3	1:A:281:GLN:HG3	1.88	0.56
1:A:913:ARG:O	1:A:913:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3627:ALA:N	1:A:3682:GLU:O	2.38	0.56
1:A:2957:LEU:HD21	1:A:2993:PHE:HZ	1.70	0.55
1:A:3751:LEU:N	1:A:3803:ILE:O	2.36	0.55
1:A:862:LEU:O	1:A:3133:GLN:NE2	2.35	0.55
1:A:3757:ASP:OD1	1:A:3759:ARG:NH1	2.39	0.55
2:B:363:ARG:HG3	2:B:364:PRO:HD2	1.87	0.55
3:C:94:ILE:HA	3:C:98:ILE:HD13	1.88	0.55
1:A:321:LYS:O	1:A:324:SER:OG	2.24	0.55
1:A:3798:SER:OG	1:A:3799:ARG:NH1	2.38	0.55
1:A:3855:TYR:O	1:A:3858:MET:HG3	2.06	0.55
2:B:168:LEU:HB3	2:B:202:LEU:HD12	1.88	0.55
1:A:139:ARG:HH21	1:A:182:GLY:H	1.52	0.55
2:B:42:VAL:HG22	2:B:169:PHE:HB2	1.89	0.55
3:C:393:VAL:O	3:C:406:GLY:N	2.39	0.55
1:A:256:ILE:HG22	1:A:258:PRO:HD3	1.89	0.55
1:A:1802:TYR:OH	1:A:1846:ASP:OD2	2.23	0.55
1:A:3014:CYS:HA	1:A:3018:SER:HB2	1.89	0.55
1:A:1813:SER:HB3	1:A:1936:ARG:HH22	1.72	0.55
1:A:2387:PRO:HD3	1:A:2418:LYS:HD2	1.89	0.55
6:J:801:TYR:HB2	6:J:815:ARG:NH2	2.21	0.55
6:J:823:TYR:OH	6:J:854:SER:OG	2.25	0.55
1:A:172:GLU:HG2	1:A:220:LEU:HD12	1.87	0.55
1:A:1483:LEU:O	1:A:1487:VAL:HG22	2.06	0.55
1:A:1709:GLU:HG3	1:A:1712:ARG:HE	1.71	0.55
2:B:59:PRO:HA	2:B:62:MET:SD	2.47	0.54
4:G:160:LYS:O	4:G:164:ILE:HG12	2.08	0.54
1:A:1233:SER:HB3	1:A:3695:LEU:HD23	1.90	0.54
1:A:1942:CYS:O	1:A:1946:ASN:ND2	2.40	0.54
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.39	0.54
3:C:31:PHE:CG	3:C:100:PRO:HG3	2.42	0.54
5:I:30:SER:HA	5:I:52:ILE:HG13	1.89	0.54
6:J:726:LEU:O	6:J:730:PHE:N	2.36	0.54
1:A:3101:TYR:O	1:A:3104:GLN:HG3	2.08	0.54
3:C:450:GLN:HG3	3:C:536:LEU:HD22	1.88	0.54
4:G:59:LYS:HA	4:G:66:THR:HA	1.88	0.54
6:J:844:GLU:HB3	6:J:898:ILE:HD12	1.89	0.54
1:A:2544:SER:HA	1:A:2842:ARG:HH22	1.73	0.54
1:A:3819:THR:HA	1:A:3889:ARG:HH12	1.73	0.54
1:A:1009:LEU:O	1:A:1013:ILE:HG12	2.07	0.54
4:G:27:VAL:HB	4:G:36:LEU:HA	1.89	0.54
4:G:29:ILE:HG23	4:G:34:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:SER:HB2	1:A:69:VAL:HG21	1.90	0.54
1:A:865:GLN:HG3	1:A:866:ILE:HD12	1.89	0.54
1:A:2271:SER:HA	1:A:2274:ILE:HD12	1.89	0.54
2:B:156:ASP:O	2:B:158:GLN:NE2	2.38	0.54
1:A:3226:ASP:OD2	1:A:3229:SER:OG	2.25	0.54
2:B:350:PHE:CE2	3:C:458:ILE:HG12	2.43	0.54
2:B:402:PRO:HD2	2:B:406:ILE:HG21	1.89	0.54
3:C:450:GLN:NE2	3:C:536:LEU:O	2.33	0.54
5:H:36:LEU:HB3	5:H:43:TRP:HB2	1.90	0.54
1:A:3916:TRP:CE2	1:A:4107:LEU:HD21	2.43	0.54
6:J:818:VAL:HG12	6:J:862:HIS:HB2	1.90	0.54
1:A:741:ILE:HG21	1:A:776:TRP:CE2	2.44	0.53
1:A:1607:GLU:HG3	1:A:1611:GLN:HB2	1.90	0.53
1:A:2371:PHE:HD2	1:A:2374:LEU:HG	1.73	0.53
3:C:296:CYS:HA	3:C:304:GLU:HA	1.88	0.53
5:H:36:LEU:O	5:H:43:TRP:N	2.31	0.53
8:E:31:DT:H2"	8:E:32:DT:C5	2.43	0.53
1:A:721:TYR:HB2	1:A:726:LEU:HD13	1.91	0.53
2:B:352:PRO:HB2	2:B:354:VAL:HG22	1.90	0.53
5:H:7:ARG:HG2	5:I:131:LEU:HD12	1.90	0.53
6:J:872:VAL:HA	6:J:875:PHE:HD2	1.73	0.53
1:A:1868:THR:HA	1:A:1871:MET:HE2	1.91	0.53
2:B:303:PHE:H	3:C:290:GLN:HE22	1.57	0.53
1:A:3880:ALA:HA	1:A:3966:GLN:HE22	1.74	0.53
3:C:240:ILE:HD12	3:C:273:LYS:HZ3	1.72	0.53
6:J:710:LYS:O	6:J:714:LEU:N	2.37	0.53
1:A:754:MET:HA	1:A:757:LYS:HG2	1.90	0.53
1:A:767:GLU:O	1:A:771:ASN:ND2	2.41	0.53
1:A:2225:HIS:ND1	1:A:2226:PRO:O	2.42	0.53
1:A:2540:LEU:HD13	1:A:2835:LYS:HD3	1.89	0.53
1:A:583:LEU:HB3	1:A:612:LEU:HD22	1.90	0.53
1:A:1175:HIS:HA	1:A:1228:GLY:HA2	1.89	0.53
1:A:1697:PRO:HG2	1:A:1749:ALA:HB1	1.91	0.53
1:A:3883:LEU:HD23	1:A:3970:LEU:HB2	1.91	0.53
2:B:410:PHE:HB3	2:B:437:LEU:HD12	1.90	0.53
5:H:38:ASP:OD1	5:H:41:SER:N	2.41	0.53
5:H:140:LYS:HA	5:H:143:HIS:CE1	2.44	0.53
7:D:41:DT:H1'	7:D:42:DA:C8	2.43	0.53
1:A:1151:ARG:NH2	1:A:1163:LEU:O	2.28	0.53
1:A:2260:PHE:HB2	1:A:2306:ASN:HD21	1.74	0.53
1:A:3858:MET:SD	1:A:4119:ARG:HB2	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:809:PRO:HB2	6:J:901:CYS:HB3	1.91	0.53
1:A:935:HIS:ND1	1:A:987:LEU:HD22	2.23	0.53
1:A:567:GLU:HA	1:A:570:LYS:HG2	1.90	0.53
1:A:1549:SER:OG	1:A:1550:VAL:N	2.42	0.53
6:J:823:TYR:O	6:J:871:ARG:NH2	2.39	0.53
1:A:1191:PHE:O	1:A:1195:VAL:HG23	2.09	0.52
1:A:3660:ASN:OD1	1:A:3661:ASP:N	2.42	0.52
3:C:7:LYS:HB3	3:C:128:GLU:H	1.74	0.52
6:J:722:LYS:HE2	6:J:742:PHE:HA	1.90	0.52
1:A:860:GLY:HA3	1:A:3136:THR:HG21	1.91	0.52
3:C:513:TRP:O	3:C:517:ASN:ND2	2.37	0.52
1:A:169:THR:HG21	8:E:21:DA:H5'	1.90	0.52
1:A:380:ASP:O	1:A:384:MET:HG2	2.09	0.52
1:A:1825:LEU:HD21	1:A:1875:LYS:HB3	1.92	0.52
1:A:3616:ALA:O	1:A:3629:ARG:NH2	2.42	0.52
2:B:303:PHE:HB2	2:B:310:LEU:HA	1.91	0.52
1:A:349:ILE:O	1:A:391:ARG:NH2	2.42	0.52
1:A:1098:GLN:HG2	1:A:1152:ARG:HG3	1.90	0.52
1:A:1264:LEU:HD21	1:A:1341:ILE:HA	1.91	0.52
1:A:1829:TRP:O	1:A:1883:ARG:NH2	2.43	0.52
1:A:3328:ILE:HD11	1:A:3412:ALA:HB2	1.90	0.52
1:A:3781:CYS:HB2	1:A:3786:LEU:HD12	1.91	0.52
1:A:4082:ARG:HH21	1:A:4091:ALA:HA	1.75	0.52
4:F:57:ARG:NH2	4:F:120:ASN:HB2	2.24	0.52
1:A:1281:VAL:HG13	1:A:1282:LEU:HG	1.92	0.52
2:B:331:LYS:O	2:B:334:THR:N	2.43	0.52
4:F:186:GLU:HA	4:F:189:PHE:HB3	1.91	0.52
8:E:17:DT:H2"	8:E:18:DA:C4	2.45	0.52
1:A:3813:LYS:HE2	1:A:3817:LEU:HD11	1.92	0.52
4:G:36:LEU:HG	4:G:38:VAL:HG13	1.92	0.52
1:A:295:GLU:HB3	1:A:299:LYS:NZ	2.25	0.52
1:A:1039:TRP:O	1:A:1043:GLN:N	2.42	0.52
1:A:3266:SER:HA	1:A:3272:TRP:HB3	1.92	0.52
4:G:110:SER:H	4:G:117:PHE:HB3	1.74	0.52
5:H:8:ILE:HB	5:H:86:PHE:CG	2.44	0.52
5:I:163:GLU:O	6:J:846:ARG:NH2	2.43	0.52
6:J:720:VAL:HB	6:J:745:HIS:HB3	1.92	0.52
1:A:1926:ASN:HB2	1:A:1974:ASN:HD21	1.75	0.52
5:H:130:CYS:O	5:H:133:THR:OG1	2.25	0.52
5:H:180:PHE:HB2	6:J:774:LEU:HD21	1.91	0.52
5:I:48:SER:OG	5:I:49:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2773:ARG:HG3	1:A:2775:TYR:H	1.74	0.52
1:A:3897:PHE:CE2	1:A:3901:ARG:HD2	2.45	0.52
2:B:91:GLU:H	2:B:136:GLY:HA3	1.75	0.52
5:H:28:LEU:HA	5:H:71:ARG:HH21	1.75	0.52
1:A:1058:SER:HA	1:A:1061:LYS:HE2	1.91	0.51
1:A:1064:TYR:HA	1:A:1106:ILE:HG21	1.92	0.51
1:A:2395:THR:OG1	1:A:2431:ARG:NH1	2.43	0.51
1:A:1657:SER:OG	1:A:1660:SER:OG	2.22	0.51
1:A:2474:TYR:HD2	1:A:2517:LEU:HD11	1.74	0.51
1:A:19:LEU:HD22	1:A:34:LEU:HA	1.93	0.51
1:A:1667:SER:OG	1:A:1667:SER:O	2.28	0.51
1:A:1772:HIS:CE1	1:A:1773:VAL:HG13	2.45	0.51
2:B:95:ASN:HD21	2:B:99:PHE:H	1.58	0.51
6:J:798:ASP:HA	6:J:801:TYR:HB3	1.92	0.51
1:A:2501:LEU:O	1:A:2505:VAL:HG22	2.11	0.51
1:A:3809:THR:OG1	1:A:3930:VAL:O	2.29	0.51
1:A:3380:ARG:O	1:A:3384:HIS:ND1	2.44	0.51
8:E:30:DT:H2'	8:E:31:DT:H72	1.93	0.51
1:A:269:SER:HB3	1:A:308:LEU:HD23	1.92	0.51
1:A:3819:THR:HG23	1:A:3889:ARG:HH12	1.76	0.51
2:B:456:PRO:HA	2:B:459:VAL:HG22	1.92	0.51
1:A:934:LEU:HA	1:A:937:MET:HG2	1.93	0.51
1:A:2839:ASP:O	1:A:2842:ARG:HG2	2.10	0.51
4:F:2:GLU:N	4:F:47:GLU:O	2.44	0.51
4:F:3:GLU:HG2	4:F:4:LEU:H	1.76	0.51
4:F:204:ILE:O	4:F:208:LYS:NZ	2.43	0.51
3:C:40:MET:O	3:C:43:GLN:HG2	2.11	0.51
3:C:62:ASP:OD1	3:C:102:SER:N	2.41	0.51
5:H:88:PHE:HA	5:H:95:PHE:HA	1.93	0.51
1:A:1097:GLU:HB2	1:A:1151:ARG:HD3	1.92	0.51
1:A:2379:MET:SD	1:A:2379:MET:N	2.83	0.51
1:A:2094:MET:HA	1:A:2097:LEU:HD12	1.92	0.51
1:A:4013:TRP:CE2	1:A:4035:GLU:HB2	2.46	0.51
2:B:350:PHE:HB3	2:B:394:VAL:HB	1.92	0.51
7:D:23:DT:H3	8:E:33:DA:H2	1.59	0.51
7:D:36:DA:N6	8:E:22:DG:H1	2.09	0.51
1:A:1694:THR:HB	1:A:1745:LYS:HB3	1.93	0.50
1:A:3159:ARG:HA	1:A:3162:ASN:HD21	1.76	0.50
3:C:315:ARG:NE	3:C:317:GLY:O	2.44	0.50
6:J:792:MET:SD	6:J:796:ILE:HD12	2.50	0.50
1:A:798:GLY:O	1:A:802:THR:OG1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:ALA:O	1:A:1162:SER:OG	2.29	0.50
1:A:1519:PHE:HB3	1:A:1570:GLU:OE1	2.11	0.50
1:A:1169:VAL:HG21	1:A:1198:LEU:HD21	1.93	0.50
1:A:1675:TYR:CE1	1:A:1696:LEU:HG	2.45	0.50
1:A:1818:SER:HA	1:A:1821:ASP:HB2	1.93	0.50
1:A:4017:GLU:O	1:A:4021:LEU:HG	2.11	0.50
3:C:44:ARG:HG3	3:C:235:CYS:SG	2.52	0.50
6:J:746:MET:O	6:J:751:LYS:NZ	2.42	0.50
1:A:2145:PHE:CZ	1:A:2149:LEU:HD11	2.46	0.50
1:A:3451:LEU:HD13	1:A:3486:GLU:HB2	1.94	0.50
3:C:58:LEU:N	3:C:78:THR:O	2.37	0.50
5:H:43:TRP:HH2	5:H:90:LYS:HE3	1.76	0.50
1:A:2547:SER:HB3	1:A:2550:ILE:HG12	1.94	0.50
1:A:3845:LYS:HD2	1:A:3846:MET:HG2	1.92	0.50
4:F:26:LYS:HD3	4:F:37:LEU:HD12	1.94	0.50
4:G:66:THR:N	5:H:57:ASP:OD2	2.45	0.50
1:A:180:LEU:O	1:A:185:HIS:NE2	2.44	0.50
1:A:752:LEU:HD22	1:A:776:TRP:CZ3	2.46	0.50
1:A:1258:ASP:HA	1:A:1261:LEU:HD12	1.93	0.50
1:A:1338:VAL:O	1:A:1342:MET:HG2	2.12	0.50
1:A:1725:GLN:OE1	1:A:1726:SER:N	2.44	0.50
1:A:2500:LYS:HA	1:A:2503:LYS:HZ2	1.77	0.50
2:B:264:ASN:ND2	2:B:266:ASP:OD1	2.44	0.50
4:F:154:ALA:O	4:F:158:HIS:ND1	2.45	0.50
4:G:104:LEU:HD21	4:G:106:LEU:HD13	1.92	0.50
5:H:140:LYS:HA	5:H:143:HIS:ND1	2.26	0.50
1:A:221:ALA:O	1:A:225:LYS:HG2	2.11	0.50
1:A:1920:TYR:HA	1:A:1923:PHE:CE1	2.47	0.50
1:A:2461:PHE:HA	1:A:2464:HIS:HE2	1.76	0.50
3:C:342:VAL:HG12	3:C:393:VAL:HG13	1.94	0.50
4:G:213:ASN:O	4:G:220:ALA:N	2.45	0.50
6:J:752:GLU:O	6:J:756:ARG:N	2.44	0.50
5:H:176:LEU:HA	5:H:179:ARG:HD2	1.93	0.50
6:J:843:LEU:O	6:J:847:PHE:N	2.45	0.50
1:A:602:MET:O	1:A:1087:ARG:NH1	2.39	0.50
4:F:36:LEU:HG	4:F:38:VAL:H	1.77	0.50
4:G:58:ALA:HB1	4:G:67:ALA:HB3	1.93	0.50
6:J:819:TYR:HB2	6:J:860:VAL:HG13	1.93	0.50
1:A:137:THR:O	1:A:141:SER:N	2.38	0.49
1:A:1700:THR:O	1:A:1703:THR:OG1	2.26	0.49
1:A:2567:SER:HA	1:A:2572:TYR:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2839:ASP:HA	1:A:2842:ARG:HE	1.77	0.49
1:A:3156:PRO:O	1:A:3159:ARG:HG3	2.12	0.49
2:B:126:GLN:HA	2:B:129:LYS:HG2	1.93	0.49
3:C:6:ASN:ND2	3:C:128:GLU:OE1	2.41	0.49
6:J:864:ILE:HD12	6:J:893:TRP:HB3	1.93	0.49
1:A:3658:ASP:OD1	1:A:3658:ASP:N	2.45	0.49
2:B:460:GLY:HA2	2:B:463:LYS:HE3	1.94	0.49
1:A:542:ASP:HA	1:A:545:LEU:HG	1.94	0.49
1:A:684:GLU:OE1	1:A:684:GLU:N	2.43	0.49
1:A:2105:HIS:CE1	1:A:2156:VAL:HA	2.48	0.49
1:A:2859:GLN:NE2	1:A:2880:CYS:SG	2.80	0.49
1:A:1093:GLU:HA	1:A:1096:VAL:HB	1.94	0.49
1:A:1363:LEU:O	1:A:1367:HIS:ND1	2.27	0.49
2:B:348:MET:SD	3:C:518:PRO:HD3	2.53	0.49
4:G:54:VAL:HA	4:G:119:TRP:CZ3	2.47	0.49
5:H:55:GLU:HA	5:H:58:ASP:HB2	1.93	0.49
1:A:2102:LYS:O	1:A:2106:ARG:HG2	2.12	0.49
2:B:290:ARG:HD2	3:C:309:ASP:HA	1.94	0.49
2:B:300:THR:OG1	3:C:292:GLU:O	2.26	0.49
2:B:417:GLU:O	2:B:428:THR:OG1	2.29	0.49
4:F:13:TRP:HB3	4:F:215:GLN:NE2	2.27	0.49
5:I:18:HIS:NE2	5:I:38:ASP:HB3	2.28	0.49
1:A:373:CYS:SG	1:A:381:VAL:HG22	2.52	0.49
1:A:713:GLU:HB2	1:A:717:LYS:HE3	1.95	0.49
1:A:774:GLU:HG2	1:A:858:MET:SD	2.53	0.49
1:A:3490:VAL:HG21	1:A:3493:TRP:CE3	2.48	0.49
2:B:488:ARG:HH12	2:B:503:ALA:N	2.10	0.49
3:C:13:CYS:HB3	3:C:59:PHE:HE2	1.78	0.49
3:C:93:ASP:HB3	3:C:97:LYS:HD2	1.94	0.49
6:J:720:VAL:HG12	6:J:744:ILE:HD12	1.95	0.49
1:A:141:SER:O	1:A:141:SER:OG	2.28	0.49
1:A:3455:LYS:HA	1:A:3491:PRO:HB3	1.94	0.49
1:A:3640:PHE:O	1:A:3644:PHE:HB3	2.13	0.49
2:B:124:GLY:O	2:B:128:GLN:N	2.45	0.49
3:C:219:ASP:OD1	3:C:219:ASP:N	2.45	0.49
4:F:43:GLN:HG2	4:G:128:PRO:HB2	1.93	0.49
6:J:694:GLY:O	6:J:718:HIS:NE2	2.45	0.49
1:A:2269:ASP:CG	1:A:2270:ASN:H	2.16	0.49
1:A:3617:LEU:HB2	1:A:3632:PHE:HE2	1.78	0.49
2:B:261:LEU:HD23	2:B:269:ILE:HD12	1.95	0.49
2:B:422:ASP:OD1	2:B:422:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:TYR:HD2	1:A:765:LEU:HG	1.78	0.49
1:A:1014:LEU:O	1:A:1018:VAL:HG12	2.13	0.49
1:A:2219:LEU:O	1:A:2223:VAL:N	2.45	0.49
1:A:3183:ILE:HG23	1:A:3238:MET:CE	2.43	0.49
5:H:172:LEU:O	5:H:176:LEU:HG	2.13	0.49
6:J:841:LYS:HD3	6:J:864:ILE:HB	1.95	0.49
1:A:176:GLU:HA	1:A:227:LEU:HB2	1.95	0.48
1:A:2365:ASN:HA	1:A:2368:THR:HG22	1.94	0.48
1:A:3980:MET:SD	1:A:3980:MET:N	2.86	0.48
6:J:725:TRP:NE1	6:J:736:VAL:O	2.32	0.48
1:A:27:ALA:HB1	1:A:77:GLU:HG3	1.95	0.48
1:A:3161:LEU:O	1:A:3165:THR:HG23	2.13	0.48
3:C:285:LYS:HB2	3:C:287:GLU:OE1	2.13	0.48
4:F:4:LEU:HD12	4:F:28:PHE:HB3	1.93	0.48
5:H:18:HIS:HB3	5:H:36:LEU:HD11	1.94	0.48
7:D:40:DT:H5"	7:D:41:DT:C4	2.48	0.48
1:A:2443:MET:SD	1:A:2476:ILE:HG23	2.53	0.48
1:A:3759:ARG:HH21	1:A:4010:SER:HA	1.78	0.48
1:A:3835:PRO:HG3	1:A:3877:LYS:HB3	1.94	0.48
6:J:829:LEU:HD11	6:J:855:CYS:HB3	1.95	0.48
1:A:139:ARG:NH2	1:A:182:GLY:H	2.10	0.48
1:A:1377:CYS:SG	1:A:1378:GLU:N	2.86	0.48
1:A:3367:SER:HB2	1:A:3372:LYS:HE3	1.94	0.48
1:A:3964:THR:H	1:A:3967:PHE:HD2	1.62	0.48
3:C:13:CYS:HB3	3:C:59:PHE:CE2	2.49	0.48
3:C:131:HIS:ND1	3:C:160:SER:OG	2.46	0.48
3:C:250:ARG:HG2	3:C:260:ARG:HD3	1.95	0.48
4:F:28:PHE:HB2	4:F:35:ALA:HB3	1.96	0.48
6:J:759:ASP:HB3	6:J:765:TYR:CZ	2.48	0.48
1:A:1933:LEU:O	1:A:1937:ARG:N	2.43	0.48
3:C:44:ARG:CD	3:C:238:LYS:HE3	2.44	0.48
1:A:1069:HIS:CG	1:A:1074:LYS:HD2	2.48	0.48
1:A:1949:ILE:HG23	1:A:2100:LEU:HD22	1.94	0.48
2:B:203:MET:HB2	2:B:238:LYS:HZ2	1.79	0.48
2:B:357:LYS:HG3	2:B:360:HIS:CE1	2.49	0.48
3:C:457:LEU:O	3:C:461:MET:HG2	2.14	0.48
4:G:178:ARG:HH21	4:G:179:LEU:HD11	1.79	0.48
1:A:363:ILE:HD12	1:A:413:PHE:HA	1.96	0.48
1:A:1052:SER:O	1:A:1056:THR:N	2.47	0.48
1:A:1132:ASP:HB3	1:A:1136:ARG:HH21	1.78	0.48
1:A:1765:VAL:HA	1:A:1768:ARG:NE	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3284:SER:HB2	1:A:3301:LEU:HD21	1.94	0.48
1:A:3821:SER:OG	1:A:3823:GLU:OE1	2.29	0.48
6:J:739:GLN:OE1	6:J:741:ARG:NH2	2.47	0.48
1:A:84:GLU:O	1:A:87:LYS:HG3	2.14	0.48
1:A:232:CYS:HB3	1:A:278:HIS:CE1	2.49	0.48
1:A:1112:ALA:O	1:A:1180:GLN:NE2	2.47	0.48
1:A:1568:ASN:OD1	1:A:1569:THR:N	2.46	0.48
1:A:1616:LEU:O	1:A:1620:THR:HG23	2.14	0.48
1:A:1766:LEU:HD13	1:A:1778:PHE:CD2	2.49	0.48
1:A:3583:LEU:HB3	1:A:3733:ARG:HH11	1.79	0.48
1:A:3759:ARG:O	1:A:3763:ARG:HG2	2.14	0.48
5:H:178:LYS:HA	5:H:181:ILE:HD12	1.95	0.48
1:A:3082:TYR:O	1:A:3086:LEU:HG	2.14	0.48
4:F:59:LYS:HG2	4:F:66:THR:HB	1.96	0.48
1:A:885:ALA:O	1:A:888:ARG:NH2	2.47	0.48
1:A:2562:LEU:O	1:A:2566:THR:HG23	2.14	0.48
1:A:2814:SER:O	1:A:2818:LYS:HG2	2.14	0.48
2:B:357:LYS:O	2:B:358:LYS:HG2	2.14	0.48
1:A:237:SER:OG	1:A:280:SER:O	2.29	0.47
1:A:483:VAL:HG21	1:A:567:GLU:HG2	1.96	0.47
1:A:2461:PHE:HA	1:A:2464:HIS:NE2	2.29	0.47
1:A:542:ASP:N	1:A:542:ASP:OD1	2.44	0.47
1:A:566:ASP:OD2	1:A:570:LYS:NZ	2.42	0.47
1:A:631:ARG:HD3	1:A:668:LYS:HB3	1.96	0.47
1:A:2425:ARG:HH11	1:A:2457:PRO:HB2	1.79	0.47
3:C:338:LYS:HB3	3:C:398:ASP:HA	1.95	0.47
4:F:43:GLN:HB3	4:F:131:VAL:HG21	1.96	0.47
1:A:399:GLN:OE1	1:A:1744:LYS:NZ	2.48	0.47
1:A:2429:ASP:OD1	1:A:2429:ASP:N	2.48	0.47
6:J:659:PHE:CZ	6:J:729:CYS:HB3	2.49	0.47
1:A:1586:SER:HA	1:A:1593:VAL:HG21	1.96	0.47
1:A:1603:GLN:HE22	1:A:1606:ARG:HH22	1.61	0.47
1:A:2415:LEU:HB3	1:A:2420:PHE:HB3	1.96	0.47
1:A:2773:ARG:HD2	1:A:2789:SER:HB2	1.96	0.47
1:A:3175:PRO:HG2	1:A:3178:ILE:HG12	1.95	0.47
1:A:3784:ARG:HH12	1:A:3986:HIS:CD2	2.32	0.47
3:C:200:GLN:O	3:C:203:GLU:HG2	2.13	0.47
5:H:144:LEU:HD11	5:I:145:GLN:OE1	2.15	0.47
1:A:896:VAL:N	1:A:903:PRO:O	2.40	0.47
1:A:1225:GLU:HB3	1:A:1236:LEU:HB2	1.95	0.47
1:A:2425:ARG:NH1	1:A:2457:PRO:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:ALA:HB2	2:B:500:PRO:HD3	1.95	0.47
4:F:53:VAL:O	4:F:57:ARG:HB2	2.14	0.47
1:A:254:LYS:O	1:A:300:TRP:NE1	2.42	0.47
1:A:645:TRP:CZ3	1:A:1505:LEU:HD13	2.50	0.47
1:A:651:TYR:CZ	1:A:655:LEU:HD11	2.49	0.47
1:A:770:LEU:HD11	1:A:858:MET:HG3	1.96	0.47
1:A:982:GLN:OE1	1:A:2589:TYR:OH	2.20	0.47
1:A:1568:ASN:HA	1:A:1600:MET:HE1	1.97	0.47
1:A:1783:ARG:HG2	1:A:1830:HIS:CD2	2.49	0.47
1:A:2320:ALA:HB1	1:A:2367:VAL:HB	1.95	0.47
1:A:2589:TYR:HD1	1:A:2777:HIS:CE1	2.33	0.47
1:A:3298:LEU:HD11	1:A:3336:ILE:HG22	1.97	0.47
1:A:3389:VAL:O	1:A:3393:GLU:HG2	2.14	0.47
2:B:74:LYS:HD2	2:B:81:ASP:HB2	1.96	0.47
2:B:202:LEU:O	2:B:238:LYS:NZ	2.45	0.47
2:B:262:LYS:HA	2:B:268:VAL:HG12	1.95	0.47
2:B:523:ASP:OD1	2:B:523:ASP:N	2.48	0.47
3:C:292:GLU:N	3:C:292:GLU:OE1	2.47	0.47
3:C:400:ARG:NH2	8:E:33:DA:O4'	2.48	0.47
4:F:136:ILE:HG12	4:G:136:ILE:HD13	1.97	0.47
6:J:893:TRP:HA	6:J:904:GLN:HB2	1.96	0.47
1:A:453:MET:HA	1:A:456:VAL:HG22	1.96	0.47
1:A:1675:TYR:CD1	1:A:1696:LEU:HG	2.50	0.47
1:A:1834:ASP:OD1	1:A:1834:ASP:N	2.47	0.47
1:A:2527:HIS:HD2	1:A:2529:THR:H	1.63	0.47
2:B:272:GLY:N	2:B:369:TYR:O	2.38	0.47
3:C:52:ASP:N	3:C:52:ASP:OD1	2.48	0.47
3:C:266:SER:OG	3:C:363:LYS:HG2	2.15	0.47
5:I:188:LYS:HD2	5:I:191:ILE:HD12	1.96	0.47
1:A:75:SER:O	1:A:79:ARG:N	2.48	0.47
1:A:1560:TYR:O	1:A:1564:SER:OG	2.22	0.47
1:A:1748:ASP:OD1	1:A:1749:ALA:N	2.48	0.47
1:A:2792:THR:OG1	1:A:2793:PRO:HD3	2.15	0.47
1:A:3113:ASN:O	1:A:3117:ILE:HG13	2.15	0.47
2:B:42:VAL:HB	2:B:87:PHE:CE1	2.49	0.47
1:A:90:CYS:HA	1:A:93:LEU:HG	1.96	0.47
3:C:54:ILE:HG12	3:C:86:PRO:HG3	1.97	0.47
3:C:108:LEU:HD22	3:C:146:GLN:HB2	1.96	0.47
6:J:800:GLU:O	6:J:805:TRP:N	2.46	0.47
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	1.97	0.46
1:A:3772:ASN:ND2	1:A:3788:LEU:O	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4039:TYR:HB3	1:A:4041:ARG:HD3	1.98	0.46
5:H:130:CYS:HB3	5:I:130:CYS:HB3	1.97	0.46
1:A:998:ASN:HB3	1:A:1044:ILE:HG13	1.96	0.46
1:A:3118:ASP:HB3	1:A:3121:LEU:HG	1.97	0.46
2:B:280:ALA:N	3:C:429:ASP:OD1	2.48	0.46
2:B:369:TYR:CD1	2:B:370:PRO:HD2	2.51	0.46
3:C:13:CYS:HA	3:C:57:VAL:O	2.15	0.46
3:C:132:ILE:O	3:C:162:GLN:N	2.34	0.46
1:A:3700:GLU:OE1	1:A:3700:GLU:N	2.48	0.46
1:A:571:SER:HA	1:A:574:LYS:HE2	1.97	0.46
1:A:1614:GLN:OE1	1:A:1614:GLN:N	2.48	0.46
1:A:3459:ASN:O	1:A:3463:LEU:HG	2.15	0.46
3:C:246:HIS:HB3	3:C:264:TYR:CZ	2.51	0.46
6:J:667:MET:SD	6:J:668:SER:N	2.89	0.46
1:A:3761:ASP:HB2	1:A:3793:VAL:HG11	1.96	0.46
2:B:34:GLY:O	2:B:253:LYS:NZ	2.49	0.46
3:C:7:LYS:HG2	3:C:126:LYS:O	2.16	0.46
1:A:385:TYR:O	1:A:389:ILE:HG12	2.16	0.46
1:A:2967:GLU:OE1	1:A:2967:GLU:N	2.45	0.46
1:A:3735:PRO:HB3	1:A:3753:LYS:HD3	1.97	0.46
2:B:48:MET:HG2	2:B:60:PHE:HB2	1.97	0.46
3:C:43:GLN:HA	3:C:46:VAL:HG22	1.96	0.46
6:J:792:MET:O	6:J:797:ALA:N	2.46	0.46
1:A:100:ILE:HD12	1:A:141:SER:HA	1.98	0.46
1:A:629:PHE:O	1:A:633:ILE:HG12	2.16	0.46
1:A:3571:PHE:CE2	1:A:3575:LEU:HD11	2.51	0.46
3:C:342:VAL:HG12	3:C:393:VAL:HG22	1.97	0.46
1:A:430:VAL:HG11	1:A:1640:GLU:HB2	1.97	0.46
1:A:565:TYR:HE1	1:A:642:PHE:HB2	1.81	0.46
2:B:35:ARG:N	2:B:162:SER:H	2.14	0.46
3:C:164:PHE:CD2	3:C:225:TYR:HB2	2.51	0.46
3:C:213:ILE:HA	3:C:217:GLY:HA2	1.97	0.46
4:G:220:ALA:O	4:G:224:GLN:HG2	2.16	0.46
1:A:1111:LEU:HB2	1:A:1127:CYS:SG	2.56	0.46
1:A:1285:GLU:OE2	1:A:1286:ALA:N	2.45	0.46
1:A:2891:ARG:O	1:A:2895:GLU:HG2	2.15	0.46
1:A:2893:LEU:HD21	1:A:2922:ARG:O	2.16	0.46
1:A:3083:SER:OG	1:A:3102:TYR:O	2.34	0.46
3:C:542:ALA:O	3:C:545:LYS:NZ	2.49	0.46
5:H:89:SER:OG	5:H:94:TYR:O	2.33	0.46
6:J:759:ASP:OD1	6:J:760:CYS:N	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:VAL:O	1:A:753:GLN:HG3	2.16	0.46
1:A:3495:PHE:HB3	1:A:3502:MET:CE	2.45	0.46
4:G:54:VAL:HA	4:G:119:TRP:HZ3	1.79	0.46
5:I:190:LYS:HE3	5:I:194:LEU:HD11	1.98	0.46
8:E:30:DT:C6	8:E:31:DT:H72	2.51	0.46
1:A:87:LYS:O	1:A:91:ILE:HG12	2.16	0.45
1:A:305:ASN:O	1:A:309:LYS:HG3	2.16	0.45
1:A:1260:LEU:HD13	1:A:1297:PHE:CE1	2.51	0.45
1:A:1297:PHE:HA	1:A:1301:ILE:HG12	1.98	0.45
1:A:1475:LEU:HD23	1:A:1475:LEU:H	1.81	0.45
1:A:3131:SER:O	1:A:3135:LEU:HG	2.17	0.45
1:A:3854:ALA:O	1:A:3858:MET:N	2.49	0.45
1:A:4115:ASN:OD1	1:A:4119:ARG:NE	2.36	0.45
2:B:35:ARG:O	2:B:162:SER:N	2.49	0.45
2:B:77:SER:HA	2:B:249:LYS:O	2.17	0.45
3:C:156:LYS:HA	3:C:156:LYS:HD3	1.66	0.45
3:C:271:ARG:H	3:C:271:ARG:HD3	1.81	0.45
4:G:34:TYR:H	4:G:49:VAL:HG21	1.81	0.45
5:I:140:LYS:HA	5:I:143:HIS:CD2	2.51	0.45
1:A:99:LYS:HD2	1:A:99:LYS:HA	1.75	0.45
1:A:2531:LEU:HG	1:A:2538:ARG:NE	2.31	0.45
1:A:2575:PRO:HA	1:A:2786:LYS:HA	1.97	0.45
1:A:2860:ASP:OD1	1:A:2861:ILE:N	2.49	0.45
1:A:2923:TRP:CD2	1:A:2946:GLU:HG3	2.51	0.45
2:B:403:ARG:NH1	7:D:31:DA:O3'	2.49	0.45
3:C:47:PHE:HZ	3:C:495:LEU:HB2	1.81	0.45
3:C:357:MET:HE2	3:C:425:PRO:HB3	1.98	0.45
4:F:160:LYS:NZ	4:G:183:PRO:HA	2.32	0.45
5:H:179:ARG:HB3	6:J:805:TRP:CZ2	2.51	0.45
7:D:29:DA:H2"	7:D:30:DA:C8	2.51	0.45
1:A:468:LEU:HB3	1:A:479:ILE:HD11	1.99	0.45
1:A:491:CYS:HA	1:A:625:ASN:HD22	1.81	0.45
1:A:1454:ALA:O	1:A:1458:LEU:HG	2.17	0.45
1:A:3839:TYR:OH	1:A:4120:THR:O	2.33	0.45
1:A:4013:TRP:NE1	1:A:4017:GLU:OE2	2.50	0.45
3:C:89:ASP:O	3:C:92:GLU:HG2	2.16	0.45
3:C:151:ILE:O	3:C:155:LYS:HG2	2.16	0.45
5:H:36:LEU:N	5:H:43:TRP:O	2.44	0.45
5:I:22:VAL:HG11	5:I:75:LEU:HA	1.99	0.45
6:J:863:VAL:HG23	6:J:886:PHE:HB2	1.98	0.45
8:E:33:DA:H2'	8:E:34:DT:C5	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:LEU:HD13	1:A:1297:PHE:CZ	2.51	0.45
1:A:1760:GLU:O	1:A:1764:GLU:HG2	2.16	0.45
1:A:3588:TRP:HE1	1:A:3610:TYR:HA	1.82	0.45
1:A:3886:ALA:O	1:A:3890:MET:HG2	2.16	0.45
1:A:4055:ASN:ND2	1:A:4057:ALA:HB3	2.31	0.45
3:C:146:GLN:HB3	3:C:149:ILE:HD11	1.97	0.45
1:A:697:ASP:HB2	1:A:700:LYS:HG3	1.97	0.45
1:A:2424:MET:HG2	1:A:2461:PHE:CZ	2.52	0.45
1:A:2532:PRO:HB2	1:A:2537:ASP:OD1	2.16	0.45
1:A:3490:VAL:HG21	1:A:3493:TRP:CD2	2.52	0.45
4:G:117:PHE:CZ	4:G:119:TRP:HB2	2.51	0.45
1:A:977:ASP:O	1:A:981:ARG:HG2	2.17	0.45
1:A:1400:VAL:HG12	1:A:1404:LYS:HZ3	1.80	0.45
1:A:1896:ILE:HG22	1:A:1899:VAL:HG13	1.99	0.45
1:A:2412:TYR:O	1:A:2416:LYS:HG2	2.16	0.45
1:A:3097:ASP:N	1:A:3097:ASP:OD1	2.49	0.45
2:B:247:ARG:NH1	2:B:491:GLU:OE1	2.49	0.45
2:B:318:ARG:NH2	2:B:331:LYS:HE3	2.32	0.45
2:B:385:LEU:O	2:B:389:CYS:N	2.46	0.45
3:C:206:GLU:HA	3:C:209:LYS:HG2	1.98	0.45
5:I:36:LEU:N	5:I:43:TRP:O	2.46	0.45
8:E:25:DT:H2”	8:E:26:DT:H5”	1.99	0.45
1:A:1101:PHE:HD2	1:A:1163:LEU:HD12	1.82	0.45
1:A:1215:GLU:HB2	1:A:1219:PHE:CD2	2.52	0.45
1:A:2130:HIS:HE1	1:A:2164:TRP:HA	1.82	0.45
1:A:2880:CYS:HB3	1:A:2886:GLN:HA	1.99	0.45
1:A:3949:ALA:HB1	1:A:3953:LEU:HD12	1.99	0.45
2:B:134:MET:HG3	2:B:135:MET:HE2	1.99	0.45
3:C:35:LYS:NZ	3:C:98:ILE:O	2.48	0.45
4:G:68:PRO:HG2	5:H:106:PHE:HE1	1.81	0.45
6:J:665:CYS:HB2	6:J:697:THR:HG21	1.98	0.45
1:A:639:ALA:HB1	1:A:642:PHE:HB3	1.99	0.45
1:A:1095:LEU:HB3	1:A:1099:PHE:CE2	2.52	0.45
1:A:2773:ARG:HE	1:A:2774:SER:N	2.14	0.45
1:A:3253:SER:HA	1:A:3256:MET:SD	2.56	0.45
1:A:3860:LYS:HA	1:A:3860:LYS:HD3	1.45	0.45
3:C:206:GLU:HA	3:C:209:LYS:HE3	1.98	0.45
3:C:495:LEU:HD12	3:C:495:LEU:HA	1.74	0.45
5:I:59:MET:O	5:I:59:MET:HG2	2.17	0.45
1:A:478:CYS:O	1:A:482:VAL:HG23	2.17	0.45
1:A:770:LEU:O	1:A:774:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:GLU:N	1:A:900:GLU:OE1	2.49	0.45
1:A:1239:PRO:HG2	1:A:1243:TYR:HE2	1.81	0.45
1:A:1457:GLN:HA	1:A:1460:ARG:HD3	1.98	0.45
1:A:1763:THR:HA	1:A:1766:LEU:HB3	1.99	0.45
1:A:3298:LEU:HD22	1:A:3333:THR:HG23	1.99	0.45
1:A:3455:LYS:NZ	1:A:3489:SER:O	2.24	0.45
1:A:4115:ASN:O	1:A:4119:ARG:HG2	2.17	0.45
1:A:52:ALA:HA	1:A:55:THR:HG22	1.98	0.45
1:A:345:PHE:HA	1:A:348:ILE:HG12	1.99	0.45
1:A:1102:GLU:OE1	1:A:1152:ARG:NH2	2.50	0.45
1:A:1324:PRO:HB2	1:A:1325:GLN:H	1.62	0.45
1:A:2098:THR:C	1:A:2102:LYS:HZ2	2.20	0.45
1:A:3389:VAL:O	1:A:3393:GLU:N	2.50	0.45
3:C:40:MET:O	3:C:44:ARG:HG2	2.17	0.45
5:H:179:ARG:NH1	6:J:805:TRP:HB3	2.32	0.45
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.99	0.44
1:A:1399:CYS:O	1:A:1403:MET:HG2	2.17	0.44
1:A:1776:GLU:HA	1:A:1779:GLN:HG2	1.99	0.44
1:A:2321:GLU:O	1:A:2325:LEU:HG	2.17	0.44
2:B:289:TYR:CE1	3:C:309:ASP:HB3	2.53	0.44
3:C:363:LYS:HD2	3:C:418:CYS:SG	2.57	0.44
3:C:543:LYS:HD3	3:C:545:LYS:HZ3	1.82	0.44
5:H:47:VAL:HG11	5:H:52:ILE:HD12	1.99	0.44
5:H:94:TYR:CE2	5:H:96:PHE:HB3	2.52	0.44
5:H:158:VAL:HG22	6:J:840:ILE:HD11	2.00	0.44
1:A:467:ALA:O	1:A:471:LYS:NZ	2.40	0.44
1:A:624:ILE:O	1:A:628:GLU:HG2	2.17	0.44
1:A:2820:MET:SD	1:A:2829:LYS:HG2	2.57	0.44
2:B:374:LEU:O	3:C:540:ILE:HG13	2.18	0.44
5:H:131:LEU:HD23	5:H:131:LEU:HA	1.79	0.44
1:A:475:LEU:O	1:A:479:ILE:HD13	2.17	0.44
1:A:1115:HIS:CE1	1:A:1181:THR:H	2.35	0.44
1:A:1871:MET:HG2	1:A:1940:TYR:HA	2.00	0.44
1:A:3174:ASP:HB3	1:A:3179:TRP:HE1	1.82	0.44
4:F:158:HIS:CE1	4:F:184:PHE:HB3	2.52	0.44
4:G:105:ILE:HD11	4:G:120:ASN:ND2	2.33	0.44
1:A:1215:GLU:HB2	1:A:1219:PHE:HD2	1.81	0.44
1:A:2424:MET:HG2	1:A:2461:PHE:HZ	1.82	0.44
1:A:2486:ASP:N	1:A:2486:ASP:OD1	2.50	0.44
1:A:2787:HIS:O	1:A:2791:ILE:HG12	2.18	0.44
1:A:3499:ILE:HA	1:A:3502:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3570:ASP:OD2	1:A:3686:TRP:NE1	2.50	0.44
1:A:3880:ALA:HB2	1:A:3965:ARG:CZ	2.48	0.44
2:B:131:PHE:CE1	2:B:135:MET:HG3	2.52	0.44
5:H:22:VAL:HG23	5:H:34:ILE:HA	2.00	0.44
5:I:18:HIS:HE2	5:I:38:ASP:HB3	1.83	0.44
1:A:535:LEU:HD13	1:A:565:TYR:HD2	1.82	0.44
1:A:3923:ARG:HB3	1:A:3928:PHE:HE1	1.83	0.44
3:C:118:ILE:O	3:C:122:THR:HG23	2.17	0.44
6:J:696:ASP:OD1	6:J:696:ASP:N	2.50	0.44
6:J:721:VAL:HG22	6:J:743:MET:SD	2.57	0.44
1:A:849:GLU:HA	1:A:852:ARG:HD3	1.99	0.44
1:A:851:ILE:O	1:A:855:VAL:HG23	2.17	0.44
1:A:2454:LEU:O	1:A:2458:VAL:HG23	2.18	0.44
1:A:2799:GLN:OE1	1:A:2800:ARG:NH1	2.50	0.44
6:J:663:GLU:OE2	6:J:697:THR:OG1	2.30	0.44
1:A:162:LEU:HD21	2:B:299:LYS:HB3	2.00	0.44
1:A:1637:SER:O	1:A:1642:LYS:NZ	2.42	0.44
1:A:2474:TYR:OH	1:A:2512:ASP:OD2	2.24	0.44
1:A:2825:THR:O	1:A:2829:LYS:HG3	2.17	0.44
1:A:3029:LYS:HA	1:A:3064:PHE:HE1	1.82	0.44
1:A:3897:PHE:CZ	1:A:3901:ARG:HD2	2.53	0.44
2:B:118:GLU:O	2:B:121:GLN:HG2	2.18	0.44
3:C:86:PRO:HB3	3:C:90:LEU:HD23	2.00	0.44
4:F:24:LEU:N	4:F:38:VAL:HA	2.33	0.44
1:A:189:MET:SD	1:A:189:MET:N	2.91	0.44
2:B:418:GLU:HB3	2:B:430:PRO:HD3	1.99	0.44
7:D:32:DA:H2"	7:D:33:DA:C8	2.53	0.44
1:A:1403:MET:HB3	1:A:1463:LEU:HD12	1.99	0.44
1:A:1471:GLN:OE1	1:A:1477:HIS:N	2.51	0.44
2:B:68:GLN:HE22	2:B:120:ASP:HA	1.82	0.44
5:I:69:GLU:HG3	5:I:106:PHE:HZ	1.83	0.44
5:I:71:ARG:HE	5:I:75:LEU:HD11	1.83	0.44
1:A:79:ARG:O	1:A:83:GLU:HG2	2.18	0.43
1:A:273:ARG:O	1:A:277:LEU:HG	2.17	0.43
1:A:1009:LEU:HD13	1:A:1036:PHE:CE2	2.53	0.43
1:A:1142:HIS:CG	1:A:1197:LEU:HD12	2.53	0.43
1:A:2125:TRP:O	1:A:2129:LEU:HG	2.18	0.43
1:A:2460:GLU:OE1	1:A:2460:GLU:N	2.50	0.43
1:A:3771:MET:HE2	1:A:3774:ILE:HD12	2.00	0.43
3:C:465:LYS:N	3:C:474:GLU:O	2.47	0.43
5:H:10:LEU:HD21	5:H:18:HIS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:ASP:OD1	1:A:878:GLU:N	2.49	0.43
1:A:907:LEU:HA	1:A:910:PHE:HD2	1.83	0.43
1:A:1857:LYS:NZ	1:A:1860:GLU:HG3	2.32	0.43
1:A:1876:ILE:HA	1:A:1879:VAL:HG22	2.00	0.43
1:A:2466:SER:O	1:A:2467:THR:OG1	2.33	0.43
1:A:2492:ASP:N	1:A:2492:ASP:OD1	2.51	0.43
2:B:35:ARG:HB2	2:B:161:MET:HE1	1.99	0.43
6:J:809:PRO:HG2	6:J:810:LEU:HD12	1.99	0.43
6:J:821:ASP:OD2	6:J:871:ARG:NH1	2.50	0.43
1:A:484:HIS:CE1	1:A:488:ILE:HD11	2.53	0.43
1:A:913:ARG:HD2	1:A:913:ARG:HA	1.71	0.43
1:A:1413:ASP:OD1	1:A:1414:ILE:N	2.48	0.43
1:A:1824:LEU:O	1:A:1828:LEU:HD23	2.19	0.43
1:A:1860:GLU:OE1	1:A:1861:SER:N	2.52	0.43
1:A:2773:ARG:HH11	1:A:2785:ILE:HB	1.84	0.43
1:A:3588:TRP:CG	1:A:3613:MET:HG3	2.53	0.43
1:A:3828:TYR:HA	1:A:3835:PRO:HD2	2.00	0.43
1:A:3959:MET:HG3	1:A:4124:TRP:CZ2	2.54	0.43
5:H:5:ILE:HG12	5:H:126:LEU:HG	2.00	0.43
5:I:30:SER:OG	5:I:49:GLU:OE1	2.29	0.43
6:J:663:GLU:HA	6:J:688:TYR:HB3	1.99	0.43
1:A:898:PHE:HB2	1:A:901:MET:O	2.18	0.43
1:A:913:ARG:NE	1:A:2803:ILE:HD11	2.32	0.43
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.19	0.43
1:A:1779:GLN:OE1	1:A:1826:THR:HG21	2.18	0.43
1:A:1985:LYS:HD2	1:A:2183:HIS:HB2	2.00	0.43
1:A:2553:HIS:O	1:A:2557:LEU:HG	2.17	0.43
1:A:3129:LEU:O	1:A:3132:VAL:HG12	2.17	0.43
2:B:462:MET:O	2:B:466:VAL:HG12	2.19	0.43
1:A:887:ASP:OD1	1:A:887:ASP:N	2.50	0.43
1:A:1568:ASN:ND2	1:A:1603:GLN:HE21	2.16	0.43
1:A:1627:LYS:HA	1:A:1670:GLU:OE2	2.18	0.43
1:A:2475:ASN:HA	1:A:2478:MET:HG2	1.99	0.43
1:A:3155:VAL:HG22	1:A:3156:PRO:HD3	2.01	0.43
1:A:3544:ASP:OD1	1:A:3548:GLY:N	2.51	0.43
1:A:3722:PHE:HD1	1:A:3740:ILE:HG12	1.83	0.43
1:A:4055:ASN:O	1:A:4058:VAL:HG12	2.18	0.43
2:B:143:LEU:HA	2:B:146:VAL:HG22	2.01	0.43
3:C:203:GLU:HA	3:C:206:GLU:HG3	2.00	0.43
3:C:245:ILE:HD12	3:C:245:ILE:HA	1.90	0.43
3:C:267:ILE:H	3:C:361:VAL:HB	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:GLU:N	1:A:613:HIS:O	2.39	0.43
1:A:1051:LYS:HA	1:A:1054:VAL:HG12	1.99	0.43
1:A:1255:CYS:O	1:A:1259:LEU:HG	2.17	0.43
1:A:1428:ILE:HG12	1:A:1451:VAL:HG11	2.00	0.43
1:A:2500:LYS:HA	1:A:2503:LYS:NZ	2.33	0.43
1:A:3164:TRP:O	1:A:3186:ARG:NH1	2.52	0.43
1:A:3638:LYS:O	1:A:3642:LYS:HG2	2.18	0.43
1:A:3821:SER:O	1:A:3825:LYS:HG3	2.19	0.43
1:A:3879:PRO:HG2	1:A:3882:LEU:HD21	2.01	0.43
3:C:543:LYS:HD3	3:C:543:LYS:HA	1.85	0.43
4:F:44:VAL:H	4:F:131:VAL:HG22	1.83	0.43
6:J:889:LEU:HD11	6:J:906:GLU:HG2	2.00	0.43
1:A:38:LEU:HB3	1:A:84:GLU:HG2	2.01	0.43
1:A:200:PHE:CE1	1:A:227:LEU:HD21	2.53	0.43
1:A:463:LYS:HG3	1:A:544:ILE:HG21	2.01	0.43
1:A:677:ALA:HA	1:A:680:ILE:HG12	2.00	0.43
1:A:2223:VAL:O	1:A:2223:VAL:HG13	2.19	0.43
1:A:3451:LEU:HD11	1:A:3483:MET:HA	2.01	0.43
3:C:80:HIS:O	3:C:81:ARG:HD2	2.18	0.43
1:A:138:PHE:O	1:A:142:ARG:HG2	2.19	0.43
1:A:913:ARG:HE	1:A:2803:ILE:HD11	1.83	0.43
1:A:1849:ASP:HA	1:A:1852:LYS:HG2	1.99	0.43
1:A:2544:SER:HA	1:A:2842:ARG:NH2	2.34	0.43
1:A:3301:LEU:HA	1:A:3304:VAL:HG22	2.00	0.43
1:A:3627:ALA:HA	1:A:3630:ARG:HB2	2.00	0.43
2:B:173:ASP:OD1	2:B:173:ASP:N	2.52	0.43
2:B:266:ASP:OD1	2:B:267:ILE:N	2.52	0.43
2:B:479:GLU:HB3	3:C:427:MET:HG3	2.01	0.43
2:B:509:PRO:HB3	3:C:343:LEU:HA	2.00	0.43
3:C:225:TYR:HB3	3:C:230:SER:OG	2.19	0.43
5:H:117:GLU:OE1	5:H:117:GLU:N	2.51	0.43
1:A:1102:GLU:O	1:A:1106:ILE:HG12	2.19	0.43
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.52	0.43
1:A:1623:LEU:HD13	1:A:1661:PHE:CG	2.52	0.43
1:A:1661:PHE:HA	1:A:1665:HIS:HB2	2.00	0.43
1:A:1780:SER:HB2	1:A:1784:ARG:HH12	1.82	0.43
1:A:3259:LEU:O	1:A:3276:TRP:NE1	2.35	0.43
1:A:3891:SER:O	1:A:3891:SER:OG	2.34	0.43
1:A:3913:ILE:HD13	1:A:3987:ALA:HB3	2.01	0.43
2:B:192:ASP:O	2:B:196:THR:HG23	2.18	0.43
2:B:463:LYS:HG2	3:C:387:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:ARG:HD2	2:B:474:ARG:HA	1.69	0.43
1:A:1055:ASN:O	1:A:1059:LEU:HD23	2.19	0.43
1:A:1960:LYS:C	1:A:1962:TYR:H	2.22	0.43
1:A:2514:ASN:OD1	1:A:2517:LEU:N	2.40	0.43
1:A:2586:PHE:CD1	1:A:2782:ASP:HB2	2.54	0.43
1:A:2832:ILE:O	1:A:2835:LYS:HG3	2.18	0.43
1:A:2962:ARG:HA	1:A:3989:ARG:NH1	2.30	0.43
1:A:2995:GLU:O	1:A:2999:LEU:HG	2.19	0.43
1:A:3139:GLN:O	1:A:3139:GLN:NE2	2.52	0.43
1:A:4002:MET:O	1:A:4005:PHE:HB3	2.18	0.43
2:B:357:LYS:O	2:B:359:HIS:ND1	2.52	0.43
4:F:54:VAL:HG22	4:F:119:TRP:CH2	2.54	0.43
1:A:225:LYS:HE2	1:A:253:LEU:HD22	2.01	0.42
1:A:688:PRO:HG3	1:A:704:PHE:HE2	1.84	0.42
1:A:865:GLN:H	1:A:3169:PRO:HA	1.84	0.42
1:A:1465:HIS:CE1	1:A:1476:HIS:HE1	2.37	0.42
1:A:2452:ARG:NH2	1:A:2453:GLU:OE2	2.52	0.42
1:A:3361:GLU:N	1:A:3361:GLU:OE1	2.52	0.42
1:A:4065:LEU:HA	1:A:4069:GLU:HB2	2.00	0.42
5:I:43:TRP:HD1	5:I:93:CYS:SG	2.42	0.42
6:J:789:PRO:HA	6:J:792:MET:HE2	2.01	0.42
8:E:21:DA:C8	8:E:21:DA:H5"	2.54	0.42
1:A:525:LYS:O	1:A:528:VAL:HG22	2.19	0.42
1:A:1056:THR:O	1:A:1059:LEU:HG	2.19	0.42
1:A:2578:GLU:HA	1:A:2784:GLN:HG3	2.00	0.42
1:A:3014:CYS:SG	1:A:3015:SER:N	2.92	0.42
1:A:3101:TYR:O	1:A:3105:ASN:ND2	2.52	0.42
1:A:3669:LYS:HA	1:A:3672:LYS:HD2	1.99	0.42
2:B:474:ARG:HH11	2:B:475:SER:H	1.67	0.42
4:F:210:PHE:N	4:F:215:GLN:HB3	2.34	0.42
1:A:1178:ARG:HH22	1:A:1183:CYS:HB3	1.84	0.42
1:A:1597:LEU:O	1:A:1601:LEU:HG	2.19	0.42
1:A:1948:ALA:O	1:A:1952:ILE:HG12	2.18	0.42
1:A:2189:ILE:O	1:A:2192:THR:OG1	2.29	0.42
1:A:3636:PHE:CE2	1:A:3640:PHE:HB2	2.54	0.42
1:A:3912:CYS:HB3	1:A:3961:PHE:CG	2.55	0.42
2:B:95:ASN:ND2	2:B:99:PHE:H	2.16	0.42
3:C:7:LYS:O	3:C:129:LYS:N	2.52	0.42
3:C:365:PHE:CE1	3:C:418:CYS:HB3	2.53	0.42
4:G:34:TYR:H	4:G:49:VAL:HG11	1.83	0.42
5:H:168:ALA:HB1	6:J:810:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:673:GLN:HG2	6:J:681:ARG:HH22	1.82	0.42
1:A:2953:THR:HG1	1:A:2994:TRP:HE1	1.66	0.42
1:A:3337:ILE:HG23	1:A:3377:LEU:HD13	2.01	0.42
2:B:127:GLY:HA2	2:B:130:ARG:HG2	2.01	0.42
2:B:277:VAL:HG21	3:C:357:MET:HE3	2.01	0.42
4:F:175:ILE:HG13	4:G:167:TYR:HE1	1.82	0.42
6:J:711:ASN:HA	6:J:714:LEU:HB2	2.00	0.42
8:E:35:DT:H6	8:E:35:DT:H2'	1.63	0.42
1:A:172:GLU:OE1	1:A:172:GLU:N	2.42	0.42
1:A:1261:LEU:HD22	1:A:1340:ARG:HG3	2.01	0.42
1:A:1482:GLU:O	1:A:1486:LEU:HB2	2.19	0.42
1:A:1791:CYS:O	1:A:1795:VAL:HG23	2.18	0.42
1:A:2168:LEU:HD11	1:A:2189:ILE:HG23	2.01	0.42
1:A:2873:PRO:HG3	1:A:2922:ARG:NH1	2.34	0.42
1:A:3176:MET:HE3	1:A:3179:TRP:HB2	2.01	0.42
3:C:381:ILE:HB	3:C:410:PRO:HB3	2.02	0.42
4:F:157:LEU:HD21	4:G:157:LEU:HB2	2.02	0.42
4:F:179:LEU:HD13	4:G:159:MET:SD	2.60	0.42
4:G:45:TRP:HB3	4:G:123:CYS:HB3	2.01	0.42
4:G:132:SER:HA	4:G:136:ILE:HB	2.01	0.42
1:A:1253:THR:O	1:A:1257:LEU:HG	2.18	0.42
1:A:1899:VAL:HB	1:A:1911:LEU:HD22	2.01	0.42
1:A:2215:LEU:O	1:A:2219:LEU:HG	2.20	0.42
1:A:2411:LEU:O	1:A:2415:LEU:HG	2.20	0.42
1:A:2537:ASP:HA	1:A:2540:LEU:HB3	2.02	0.42
1:A:2855:VAL:O	1:A:2859:GLN:HG3	2.20	0.42
1:A:3617:LEU:O	1:A:3633:ILE:HG12	2.19	0.42
1:A:3772:ASN:OD1	1:A:3788:LEU:N	2.53	0.42
1:A:3820:MET:HG3	1:A:3824:GLU:OE1	2.20	0.42
2:B:353:LEU:HD11	2:B:415:PRO:HD2	2.01	0.42
4:F:76:LEU:HD13	4:F:117:PHE:HB2	2.01	0.42
4:G:61:LEU:HD23	4:G:118:TYR:HB3	2.01	0.42
5:H:169:LYS:HB2	5:I:169:LYS:HG3	2.02	0.42
6:J:706:ASN:OD1	6:J:708:ARG:HG2	2.19	0.42
6:J:717:LYS:HG3	6:J:718:HIS:CE1	2.55	0.42
1:A:125:ILE:HB	1:A:126:PRO:HD3	2.02	0.42
1:A:414:LEU:HD11	1:A:464:VAL:HG11	2.02	0.42
1:A:1235:ILE:HD12	1:A:1238:GLN:O	2.20	0.42
1:A:2358:ASP:OD1	1:A:2358:ASP:N	2.53	0.42
1:A:2794:LEU:HD21	1:A:2808:LEU:HD13	2.02	0.42
1:A:3969:ASN:HD22	1:A:3972:LEU:HD13	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:MET:SD	2:B:518:LEU:HD23	2.60	0.42
3:C:406:GLY:HA2	3:C:424:LEU:H	1.85	0.42
5:H:7:ARG:NE	5:I:128:CYS:HA	2.35	0.42
1:A:236:LYS:HE2	1:A:236:LYS:HB2	1.83	0.42
1:A:491:CYS:HA	1:A:625:ASN:ND2	2.34	0.42
1:A:1539:SER:HB2	1:A:1552:HIS:CD2	2.54	0.42
1:A:1920:TYR:O	1:A:1924:THR:OG1	2.31	0.42
1:A:2145:PHE:O	1:A:2149:LEU:HG	2.20	0.42
1:A:2257:PHE:CE1	1:A:2299:TYR:HA	2.54	0.42
1:A:3037:GLN:O	1:A:3041:LEU:HG	2.20	0.42
1:A:3386:SER:O	1:A:3390:GLN:OE1	2.38	0.42
1:A:3537:SER:HA	1:A:3540:TYR:CG	2.54	0.42
2:B:247:ARG:HB3	2:B:484:GLN:HE22	1.85	0.42
2:B:463:LYS:O	2:B:467:GLU:HG2	2.19	0.42
5:H:42:ALA:H	5:H:116:VAL:HG22	1.85	0.42
1:A:131:LEU:HD22	1:A:177:LEU:HG	2.01	0.42
1:A:174:VAL:HA	1:A:177:LEU:HB2	2.02	0.42
1:A:793:LEU:HD22	1:A:869:ASN:HB2	2.01	0.42
1:A:1366:THR:HB	1:A:1370:ARG:HH12	1.83	0.42
1:A:2970:LYS:HE3	1:A:2970:LYS:HB3	1.92	0.42
1:A:3407:ALA:O	1:A:3410:ILE:HG12	2.19	0.42
1:A:3474:ARG:HE	1:A:3474:ARG:HB2	1.67	0.42
1:A:3950:THR:HG23	1:A:3957:GLU:H	1.85	0.42
2:B:113:ALA:O	2:B:117:LEU:HG	2.20	0.42
2:B:215:LEU:HA	2:B:218:ARG:HE	1.85	0.42
3:C:91:LEU:HD21	3:C:499:LEU:HD11	2.00	0.42
5:I:28:LEU:O	5:I:71:ARG:NH1	2.52	0.42
5:I:189:THR:O	5:I:192:ARG:HG3	2.20	0.42
6:J:879:ARG:O	6:J:885:LYS:NZ	2.49	0.42
6:J:889:LEU:HD13	6:J:893:TRP:CD1	2.55	0.42
1:A:1165:LEU:O	1:A:1169:VAL:HG23	2.20	0.42
1:A:3023:ASN:HB2	1:A:3031:TRP:CH2	2.55	0.42
1:A:3100:LYS:HA	1:A:3103:ILE:HG22	2.01	0.42
1:A:3350:GLU:OE1	1:A:3350:GLU:N	2.53	0.42
1:A:3544:ASP:OD1	1:A:3547:THR:N	2.51	0.42
2:B:41:LEU:HD12	2:B:86:VAL:O	2.20	0.42
4:F:130:LEU:O	4:F:134:HIS:HB2	2.20	0.42
4:G:113:SER:O	4:G:113:SER:OG	2.36	0.42
7:D:28:DT:H2"	7:D:29:DA:C8	2.55	0.42
1:A:187:SER:HA	1:A:190:ILE:HB	2.02	0.41
1:A:2325:LEU:HD22	1:A:2328:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ILE:HG22	2:B:84:ALA:HB3	2.02	0.41
2:B:509:PRO:HB2	2:B:511:VAL:HG12	2.02	0.41
5:H:20:LEU:HD23	5:H:74:LEU:HA	2.01	0.41
1:A:82:ARG:O	1:A:86:LEU:HD23	2.20	0.41
1:A:200:PHE:CE2	1:A:227:LEU:HD11	2.55	0.41
1:A:435:LEU:O	1:A:438:LEU:HG	2.20	0.41
1:A:446:PHE:CE2	1:A:530:LEU:HB2	2.54	0.41
1:A:529:ASP:OD1	1:A:529:ASP:N	2.52	0.41
1:A:1092:GLU:OE2	1:A:1094:SER:OG	2.38	0.41
1:A:1101:PHE:CD2	1:A:1163:LEU:HD12	2.55	0.41
1:A:1212:LEU:HD13	1:A:1220:LEU:HD22	2.02	0.41
1:A:1527:ARG:HH12	1:A:1531:LEU:HG	1.86	0.41
1:A:1739:TYR:O	1:A:1743:MET:HG2	2.20	0.41
1:A:2227:LYS:O	1:A:2230:VAL:HG12	2.20	0.41
1:A:2300:PHE:CD1	1:A:2341:LEU:HD21	2.55	0.41
1:A:3588:TRP:CD1	1:A:3613:MET:HB2	2.55	0.41
1:A:3605:ASN:HA	1:A:3608:LYS:HG2	2.02	0.41
4:F:3:GLU:HG2	4:F:4:LEU:N	2.34	0.41
4:F:34:TYR:HD2	4:F:36:LEU:HB3	1.85	0.41
4:G:50:ASP:O	4:G:54:VAL:HG23	2.20	0.41
5:I:140:LYS:HD2	5:I:143:HIS:NE2	2.36	0.41
6:J:670:THR:N	6:J:703:GLY:HA3	2.33	0.41
1:A:71:LYS:HE3	1:A:71:LYS:HB2	1.78	0.41
1:A:778:ILE:HD13	1:A:778:ILE:HA	1.91	0.41
1:A:848:LEU:HA	1:A:851:ILE:HD12	2.01	0.41
1:A:1092:GLU:O	1:A:1096:VAL:HG23	2.20	0.41
1:A:1487:VAL:HG11	1:A:1515:LEU:HD21	2.00	0.41
1:A:3027:LEU:HD13	1:A:3064:PHE:HB2	2.02	0.41
1:A:3903:HIS:HE1	1:A:3936:GLY:HA2	1.86	0.41
2:B:319:SER:HB3	2:B:328:ILE:HA	2.01	0.41
2:B:388:LYS:NZ	3:C:451:LEU:HB3	2.34	0.41
4:G:190:LEU:HA	4:G:194:MET:HG2	2.02	0.41
5:I:69:GLU:HA	5:I:72:LYS:HG2	2.01	0.41
1:A:63:PHE:O	1:A:66:LEU:HB2	2.21	0.41
1:A:1596:VAL:O	1:A:1600:MET:HG2	2.20	0.41
1:A:1862:THR:O	1:A:1866:GLN:OE1	2.39	0.41
1:A:2840:PHE:O	1:A:2844:LEU:HG	2.21	0.41
1:A:3353:GLU:HG2	1:A:3356:ALA:H	1.86	0.41
1:A:3572:ILE:HA	1:A:3575:LEU:HD12	2.03	0.41
1:A:3578:LEU:O	1:A:3736:LYS:HE3	2.19	0.41
1:A:4013:TRP:NE1	1:A:4035:GLU:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ARG:HA	2:B:247:ARG:HD2	1.87	0.41
2:B:360:HIS:CE1	2:B:443:LYS:HE2	2.56	0.41
2:B:479:GLU:HA	3:C:426:PHE:HB3	2.01	0.41
4:F:135:LEU:C	4:F:138:PRO:HD2	2.40	0.41
4:G:71:ALA:HB2	5:H:106:PHE:HZ	1.84	0.41
6:J:858:GLU:OE1	6:J:883:LYS:N	2.49	0.41
1:A:19:LEU:HB3	1:A:34:LEU:HD13	2.03	0.41
1:A:565:TYR:CE1	1:A:642:PHE:HB2	2.56	0.41
1:A:570:LYS:HB3	1:A:645:TRP:CH2	2.55	0.41
1:A:786:GLN:OE1	1:A:786:GLN:N	2.49	0.41
1:A:1089:PHE:HE1	1:A:1099:PHE:HD2	1.68	0.41
1:A:1186:LYS:HD2	1:A:1186:LYS:HA	1.82	0.41
1:A:1212:LEU:HA	1:A:1215:GLU:HG2	2.03	0.41
1:A:2094:MET:HB3	1:A:2145:PHE:HE1	1.84	0.41
1:A:3026:ASP:OD1	1:A:3026:ASP:N	2.53	0.41
1:A:3061:LEU:O	1:A:3065:ILE:HG12	2.19	0.41
1:A:3163:THR:O	1:A:3167:ARG:HG3	2.21	0.41
1:A:3828:TYR:HD1	1:A:3835:PRO:HD2	1.85	0.41
2:B:301:ARG:NH1	2:B:313:PRO:HD3	2.35	0.41
3:C:134:ILE:HB	3:C:163:PHE:HD1	1.85	0.41
3:C:402:ASN:ND2	7:D:25:DA:H3'	2.34	0.41
4:G:108:VAL:O	4:G:108:VAL:HG13	2.21	0.41
5:H:154:ASP:O	5:H:158:VAL:HG23	2.20	0.41
6:J:891:GLU:HB3	6:J:895:THR:HB	2.02	0.41
1:A:574:LYS:HB2	1:A:574:LYS:HE3	1.86	0.41
1:A:1430:GLU:O	1:A:1434:VAL:HG13	2.20	0.41
1:A:2133:LEU:HD23	1:A:2164:TRP:HZ3	1.85	0.41
1:A:2259:LYS:HE2	1:A:2259:LYS:HB2	1.91	0.41
1:A:3232:ARG:NH2	1:A:3268:THR:OG1	2.54	0.41
1:A:3494:GLN:HA	1:A:3709:GLY:HA2	2.01	0.41
1:A:3758:LEU:HD13	1:A:3801:GLY:HA3	2.03	0.41
1:A:570:LYS:O	1:A:574:LYS:HG3	2.20	0.41
1:A:639:ALA:O	1:A:643:GLU:N	2.54	0.41
1:A:865:GLN:HB3	1:A:3170:ASP:HB2	2.02	0.41
1:A:2251:ILE:HD11	1:A:2285:LEU:HD13	2.01	0.41
1:A:3298:LEU:HD13	1:A:3337:ILE:HB	2.02	0.41
1:A:3330:LEU:HD23	1:A:3384:HIS:CD2	2.55	0.41
1:A:3347:CYS:SG	1:A:3348:LEU:N	2.93	0.41
1:A:3856:MET:N	1:A:3856:MET:SD	2.94	0.41
3:C:82:HIS:CE1	3:C:84:MET:HB3	2.55	0.41
5:H:191:ILE:HD13	6:J:765:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HB	1:A:141:SER:HB2	2.01	0.41
1:A:101:ALA:HA	1:A:144:MET:HG3	2.02	0.41
1:A:637:LYS:HD3	1:A:638:GLN:O	2.21	0.41
1:A:664:SER:O	1:A:668:LYS:HG3	2.21	0.41
1:A:3460:GLU:H	1:A:3460:GLU:CD	2.24	0.41
2:B:35:ARG:HD2	2:B:80:ARG:NE	2.36	0.41
3:C:11:VAL:HG21	3:C:114:SER:HB2	2.03	0.41
3:C:197:ILE:HB	3:C:201:GLN:HB2	2.03	0.41
3:C:261:ILE:HA	3:C:366:ALA:HA	2.02	0.41
4:F:46:HIS:NE2	4:F:127:SER:HB2	2.36	0.41
5:I:154:ASP:O	5:I:158:VAL:HG23	2.21	0.41
1:A:86:LEU:HD12	1:A:129:ASP:HB2	2.03	0.41
1:A:174:VAL:O	1:A:178:LEU:HG	2.21	0.41
1:A:295:GLU:HB3	1:A:299:LYS:HZ3	1.86	0.41
1:A:653:LEU:HD11	1:A:669:LEU:HG	2.03	0.41
1:A:712:LYS:O	1:A:716:VAL:HG23	2.21	0.41
1:A:1032:CYS:O	1:A:1035:GLU:HG2	2.21	0.41
1:A:1260:LEU:HD22	1:A:1293:ALA:HB1	2.03	0.41
1:A:1419:LEU:O	1:A:1423:ILE:N	2.49	0.41
1:A:1572:LEU:HA	1:A:1575:LEU:HD21	2.03	0.41
1:A:1608:ARG:HA	1:A:1611:GLN:O	2.21	0.41
1:A:1817:GLN:HG3	1:A:1821:ASP:OD2	2.20	0.41
1:A:2086:ASP:O	1:A:2090:ARG:NE	2.50	0.41
1:A:2368:THR:HG21	1:A:2400:VAL:HG22	2.03	0.41
1:A:2447:LYS:HE2	1:A:2447:LYS:HB2	1.96	0.41
1:A:3324:ARG:HB3	1:A:3391:ALA:HB3	2.02	0.41
1:A:3583:LEU:HD13	1:A:3733:ARG:HD2	2.02	0.41
1:A:3771:MET:CE	1:A:3998:LEU:HD13	2.51	0.41
1:A:3858:MET:HE3	1:A:3858:MET:HB2	1.84	0.41
2:B:363:ARG:HB3	2:B:436:PHE:CD1	2.56	0.41
3:C:138:LEU:HA	3:C:142:PHE:HE2	1.85	0.41
3:C:164:PHE:CD2	3:C:231:LEU:HD22	2.56	0.41
3:C:443:LYS:HG3	3:C:444:TYR:CD2	2.56	0.41
5:H:10:LEU:HD11	5:H:18:HIS:CG	2.55	0.41
6:J:865:ILE:N	6:J:889:LEU:O	2.45	0.41
1:A:204:LEU:O	1:A:207:GLN:N	2.53	0.41
1:A:398:THR:HG23	1:A:399:GLN:HG2	2.03	0.41
1:A:1713:VAL:HA	1:A:1716:GLN:NE2	2.36	0.41
1:A:1923:PHE:HA	1:A:1941:HIS:HD2	1.85	0.41
1:A:2098:THR:HA	1:A:2101:VAL:HG22	2.03	0.41
1:A:2274:ILE:HA	1:A:2277:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3885:ARG:HA	1:A:3888:VAL:HB	2.03	0.41
1:A:4022:LYS:HE2	1:A:4022:LYS:HB2	1.92	0.41
1:A:4055:ASN:HD21	1:A:4057:ALA:HB3	1.86	0.41
5:H:17:THR:HB	5:I:124:ARG:CG	2.50	0.41
1:A:377:ASN:O	1:A:381:VAL:HG23	2.21	0.40
1:A:1793:THR:O	1:A:1797:LEU:HG	2.22	0.40
1:A:3104:GLN:NE2	1:A:3105:ASN:OD1	2.54	0.40
1:A:3233:SER:HA	1:A:3272:TRP:HZ2	1.86	0.40
1:A:3573:ASN:O	1:A:3577:GLN:HG2	2.21	0.40
1:A:3962:ARG:HD2	1:A:3962:ARG:HA	1.93	0.40
1:A:3999:THR:HG23	1:A:4044:ILE:HD11	2.03	0.40
2:B:461:LYS:HE3	2:B:461:LYS:HB3	1.96	0.40
3:C:68:LEU:HD12	3:C:68:LEU:HA	1.96	0.40
6:J:668:SER:O	6:J:670:THR:HG23	2.21	0.40
6:J:879:ARG:HE	6:J:880:ARG:NH1	2.19	0.40
7:D:40:DT:O2	8:E:18:DA:H8	2.04	0.40
1:A:146:GLU:HB2	1:A:184:VAL:H	1.85	0.40
1:A:283:SER:O	1:A:286:LEU:HG	2.21	0.40
1:A:730:LEU:HD13	1:A:755:ALA:HB2	2.03	0.40
1:A:1050:GLU:C	1:A:1053:PRO:HD2	2.42	0.40
1:A:2990:GLU:HG2	1:A:2994:TRP:CE2	2.56	0.40
1:A:3274:VAL:HG13	1:A:3315:TYR:CD1	2.56	0.40
1:A:3909:ALA:HB1	1:A:3984:MET:HE3	2.02	0.40
3:C:236:VAL:HG13	3:C:237:PHE:HD1	1.86	0.40
3:C:307:LYS:O	3:C:310:ILE:HG12	2.21	0.40
4:F:26:LYS:HG2	4:F:37:LEU:HB2	2.04	0.40
4:G:34:TYR:N	4:G:49:VAL:HG11	2.37	0.40
4:G:75:HIS:HB2	5:H:102:LYS:HZ3	1.86	0.40
4:G:128:PRO:O	4:G:132:SER:CB	2.61	0.40
1:A:65:LEU:O	1:A:69:VAL:HG22	2.21	0.40
1:A:2185:MET:O	1:A:2189:ILE:HG12	2.22	0.40
1:A:2367:VAL:O	1:A:2371:PHE:N	2.50	0.40
1:A:2508:GLN:HG2	1:A:2549:LYS:HD2	2.03	0.40
1:A:2818:LYS:HD3	1:A:2818:LYS:HA	1.83	0.40
1:A:3190:LEU:HB2	1:A:3235:LYS:HE3	2.02	0.40
1:A:3771:MET:HE3	1:A:3998:LEU:HD13	2.03	0.40
1:A:3903:HIS:ND1	1:A:3934:THR:O	2.55	0.40
2:B:41:LEU:HD23	2:B:168:LEU:HD13	2.03	0.40
2:B:376:ILE:HG12	3:C:540:ILE:HG12	2.03	0.40
2:B:506:LEU:O	3:C:343:LEU:HD22	2.22	0.40
4:G:54:VAL:HG22	4:G:119:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:7:ARG:NH2	5:I:132:ASP:OD1	2.53	0.40
1:A:1642:LYS:HA	1:A:1645:VAL:HG12	2.03	0.40
1:A:1923:PHE:HA	1:A:1941:HIS:CD2	2.57	0.40
1:A:2231:PHE:O	1:A:2235:LEU:HG	2.21	0.40
1:A:2342:CYS:HB2	1:A:2374:LEU:HD21	2.03	0.40
1:A:2438:ILE:O	1:A:2442:MET:HG3	2.21	0.40
1:A:3369:ASP:O	1:A:3373:VAL:HG23	2.21	0.40
1:A:3493:TRP:HZ3	1:A:3520:GLU:HB3	1.85	0.40
1:A:3834:ALA:O	1:A:3838:GLU:N	2.39	0.40
1:A:4068:HIS:HB3	1:A:4071:ALA:HB3	2.04	0.40
2:B:350:PHE:HD1	2:B:396:ALA:HA	1.86	0.40
4:F:128:PRO:HG3	4:G:44:VAL:N	2.32	0.40
5:H:18:HIS:HA	5:H:37:THR:O	2.22	0.40
5:H:137:ASN:HB3	5:I:137:ASN:HB3	2.02	0.40
5:I:70:LEU:O	5:I:74:LEU:HB2	2.21	0.40
1:A:103:TYR:O	1:A:107:ILE:HG12	2.22	0.40
1:A:1716:GLN:HA	1:A:1719:VAL:HG22	2.03	0.40
1:A:2310:VAL:HB	1:A:2359:LYS:NZ	2.37	0.40
1:A:2492:ASP:O	1:A:2495:SER:N	2.53	0.40
1:A:2773:ARG:HE	1:A:2774:SER:H	1.68	0.40
1:A:2806:LYS:HG3	1:A:2857:CYS:SG	2.61	0.40
1:A:3609:MET:O	1:A:3612:ARG:HG3	2.21	0.40
1:A:3950:THR:HB	1:A:4063:GLU:OE2	2.22	0.40
1:A:4108:MET:O	1:A:4112:THR:HG22	2.22	0.40
1:A:4125:GLU:HB3	1:A:4128:MET:HG2	2.04	0.40
2:B:172:GLU:HG3	2:B:213:ILE:HG21	2.03	0.40
2:B:306:SER:N	3:C:288:ASP:OD1	2.54	0.40
2:B:392:LYS:HB2	2:B:394:VAL:HG22	2.04	0.40
3:C:312:GLN:HG2	3:C:325:LYS:NZ	2.36	0.40
5:H:177:TYR:HE1	6:J:778:PHE:HD2	1.69	0.40
5:I:44:THR:N	5:I:114:GLU:O	2.55	0.40
8:E:22:DG:C5	8:E:23:DT:C4	3.10	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	3483/4156 (84%)	3321 (95%)	160 (5%)	2 (0%)	51 85
2	B	465/609 (76%)	440 (95%)	25 (5%)	0	100 100
3	C	503/732 (69%)	479 (95%)	23 (5%)	1 (0%)	47 81
4	F	174/299 (58%)	159 (91%)	15 (9%)	0	100 100
4	G	183/299 (61%)	164 (90%)	19 (10%)	0	100 100
5	H	199/336 (59%)	192 (96%)	7 (4%)	0	100 100
5	I	189/336 (56%)	178 (94%)	11 (6%)	0	100 100
6	J	256/911 (28%)	237 (93%)	19 (7%)	0	100 100
All	All	5452/7678 (71%)	5170 (95%)	279 (5%)	3 (0%)	54 85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	MET
1	A	3563	ASP
3	C	229	GLU

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	2961/3671 (81%)	2942 (99%)	19 (1%)	86 92
2	B	392/548 (72%)	391 (100%)	1 (0%)	92 95
3	C	428/649 (66%)	423 (99%)	5 (1%)	71 84
4	F	157/262 (60%)	156 (99%)	1 (1%)	86 92
4	G	159/262 (61%)	159 (100%)	0	100 100
5	H	166/303 (55%)	166 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	I	161/303 (53%)	161 (100%)	0	100 100
6	J	212/808 (26%)	212 (100%)	0	100 100
All	All	4636/6806 (68%)	4610 (99%)	26 (1%)	86 92

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	87	LYS
1	A	891	ARG
1	A	1146	ASN
1	A	1537	VAL
1	A	1955	VAL
1	A	2207	LYS
1	A	2835	LYS
1	A	3009	LYS
1	A	3568	ILE
1	A	3696	ARG
1	A	3710	LYS
1	A	3725	ARG
1	A	3784	ARG
1	A	3845	LYS
1	A	3856	MET
1	A	3858	MET
1	A	3860	LYS
1	A	4041	ARG
2	B	35	ARG
3	C	233	LYS
3	C	239	LYS
3	C	252	THR
3	C	253	ILE
3	C	271	ARG
4	F	109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	771	ASN
1	A	978	GLN
1	A	1603	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2130	HIS
1	A	2348	GLN
1	A	2527	HIS
1	A	3104	GLN
1	A	3863	ASN
2	B	360	HIS
3	C	402	ASN
3	C	411	HIS
4	G	165	GLN
5	H	137	ASN
5	H	141	ASN
5	I	137	ASN
5	I	145	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	97.03
1	A	5016:UNK	C	6004:UNK	N	48.85

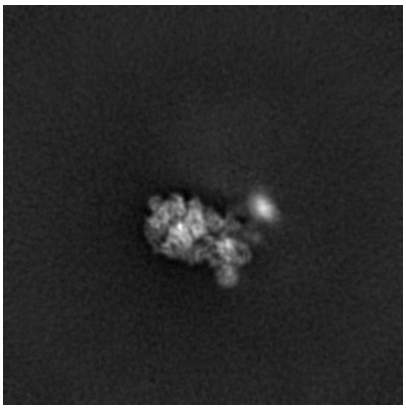
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12301. These allow visual inspection of the internal detail of the map and identification of artifacts.

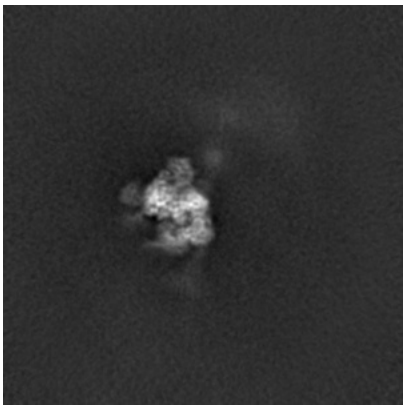
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

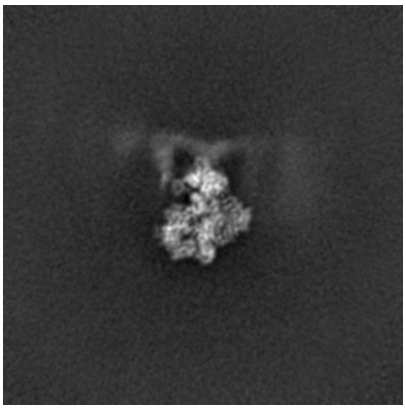
6.1.1 Primary map



X

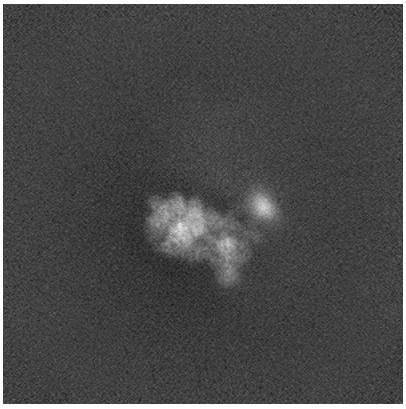


Y

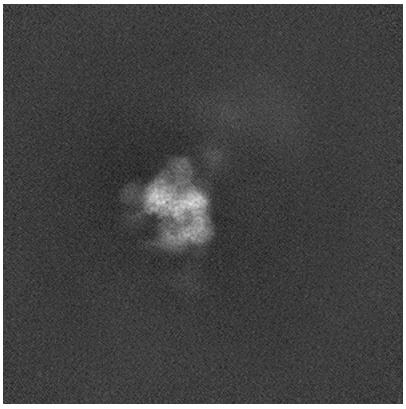


Z

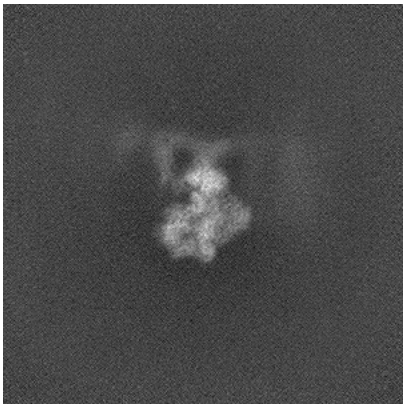
6.1.2 Raw map



X



Y

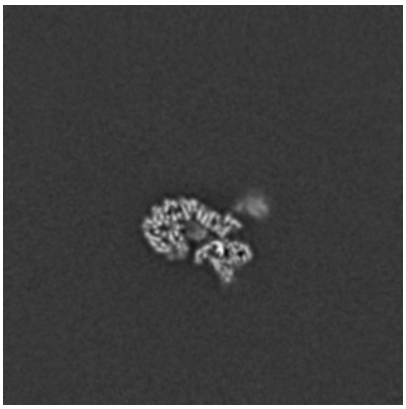


Z

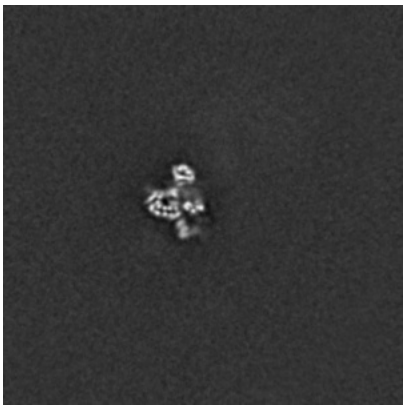
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

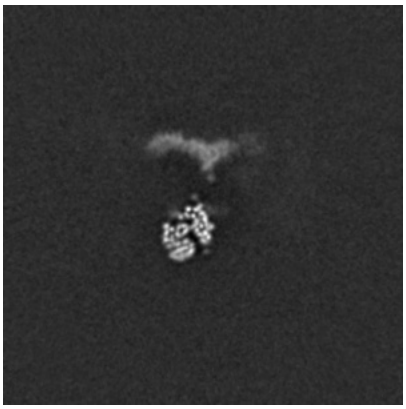
6.2.1 Primary map



X Index: 270

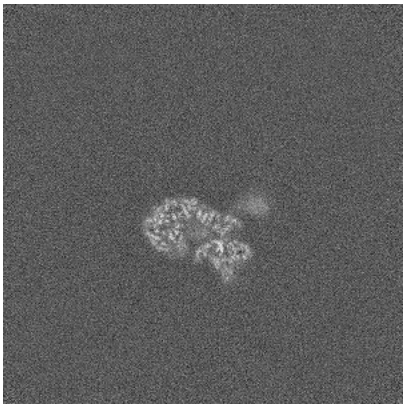


Y Index: 270

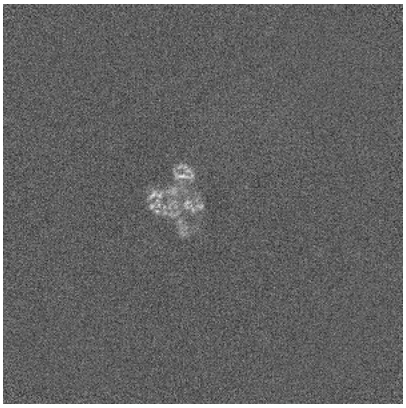


Z Index: 270

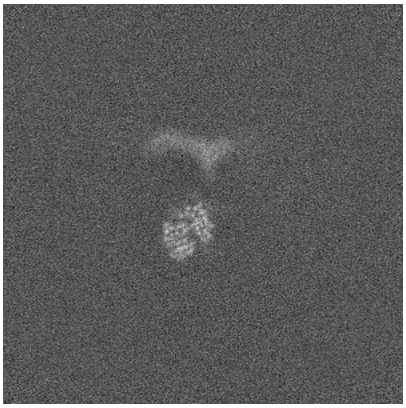
6.2.2 Raw map



X Index: 270



Y Index: 270

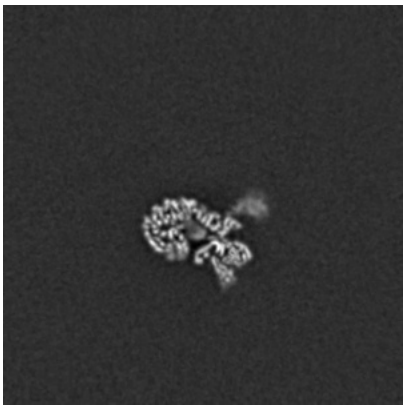


Z Index: 270

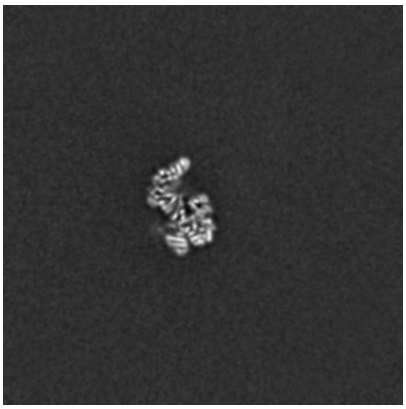
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

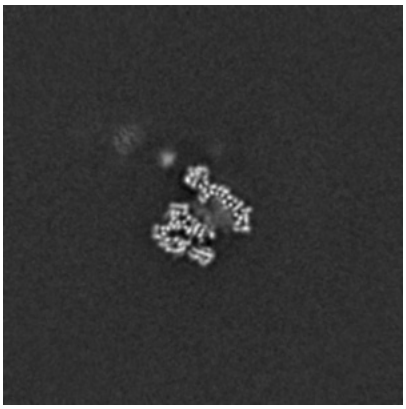
6.3.1 Primary map



X Index: 272

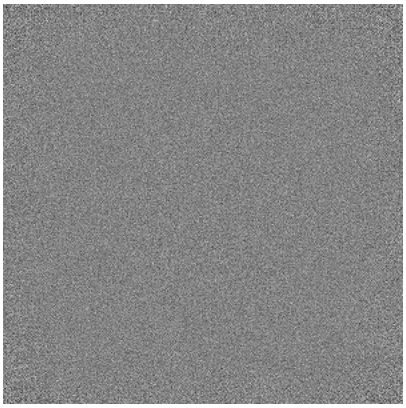


Y Index: 238

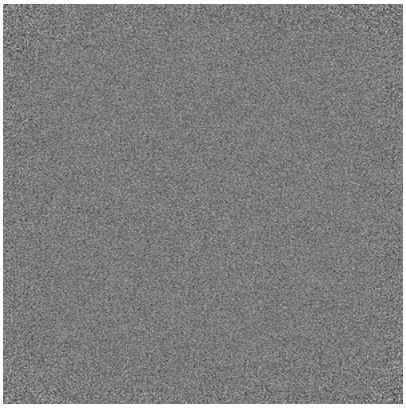


Z Index: 241

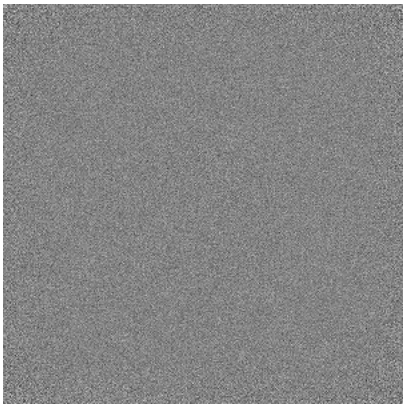
6.3.2 Raw map



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 0.175. 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.

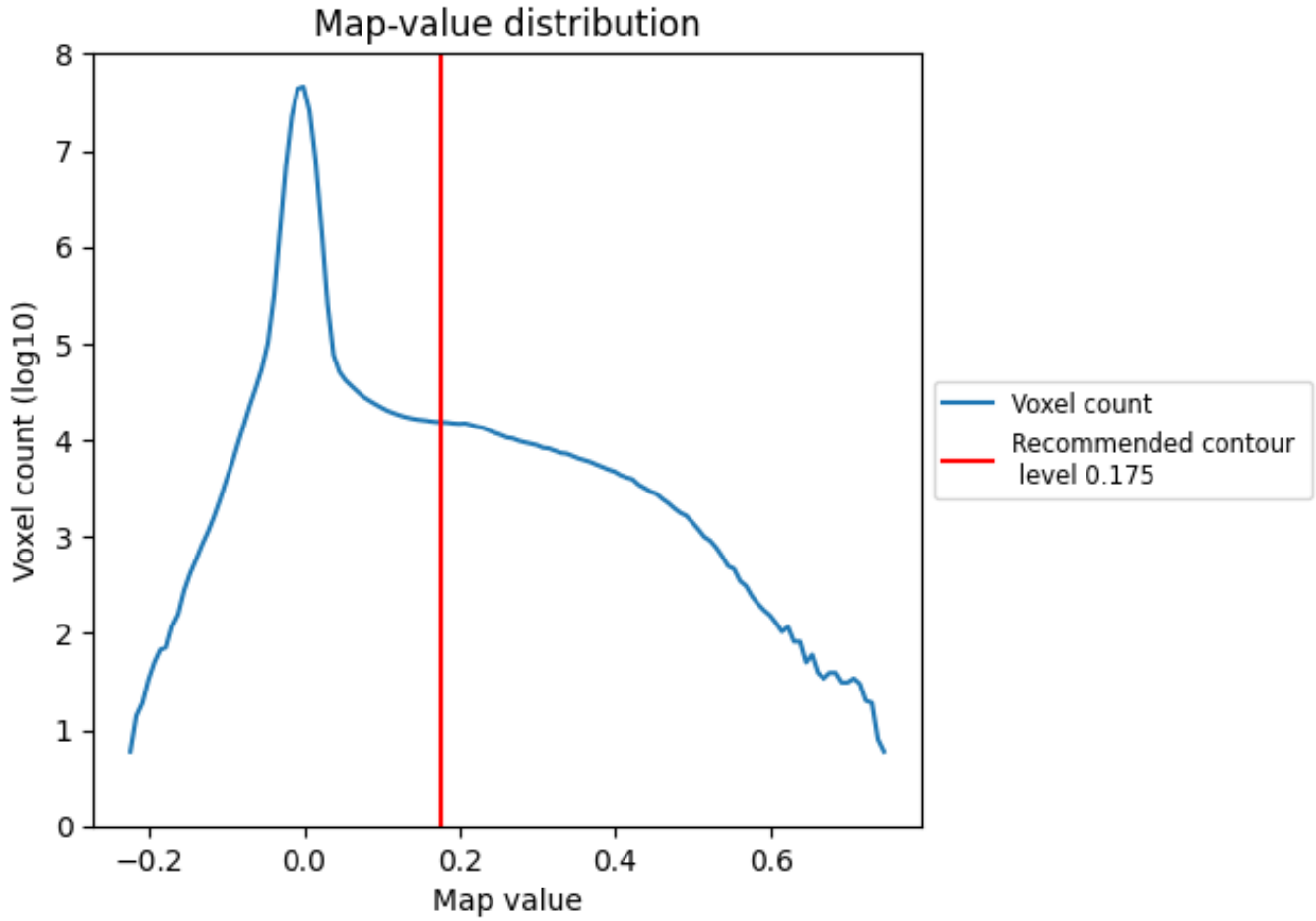
6.5 Mask visualisation (i)

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

7 Map analysis

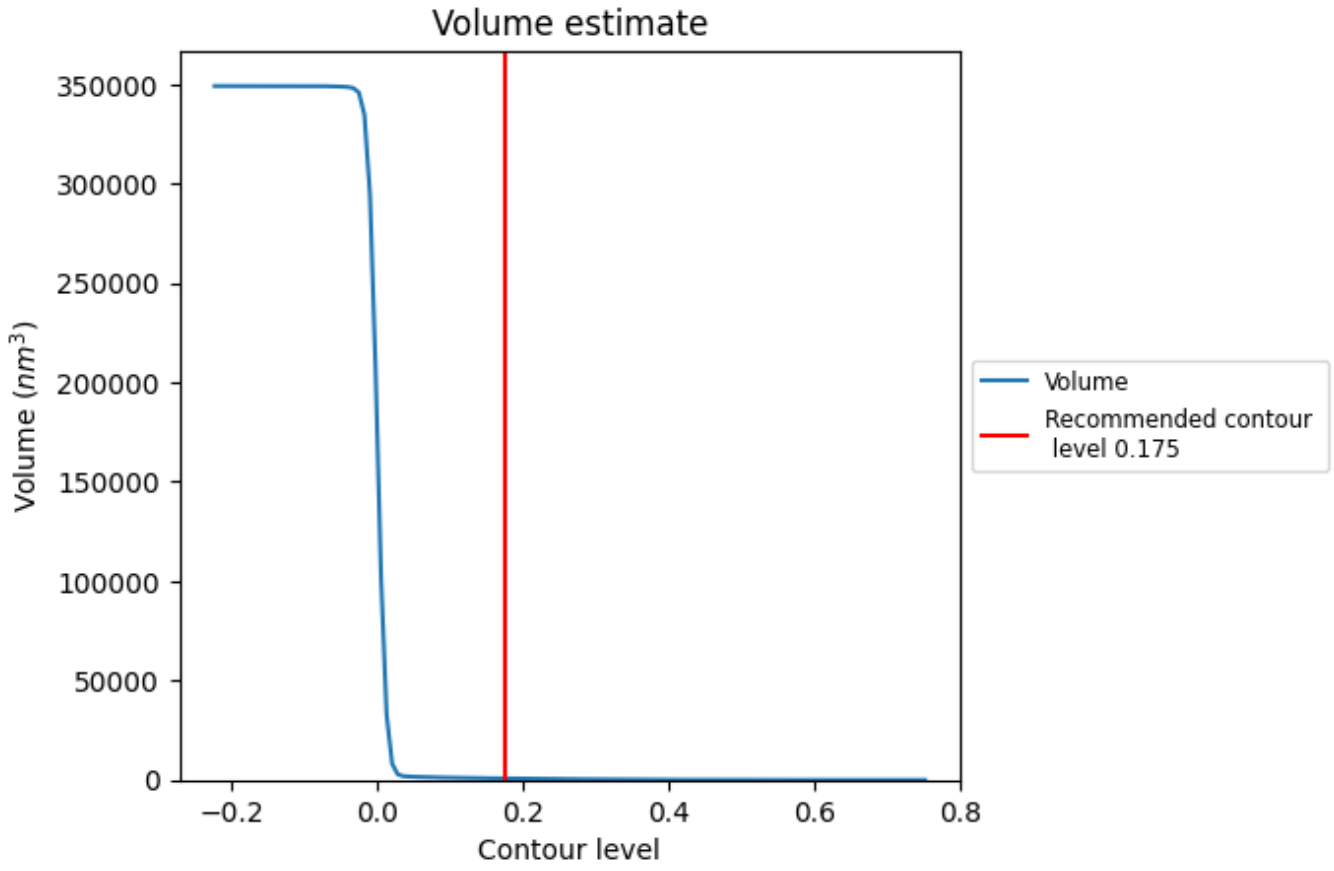
This section contains the results of statistical analysis of the map.

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.

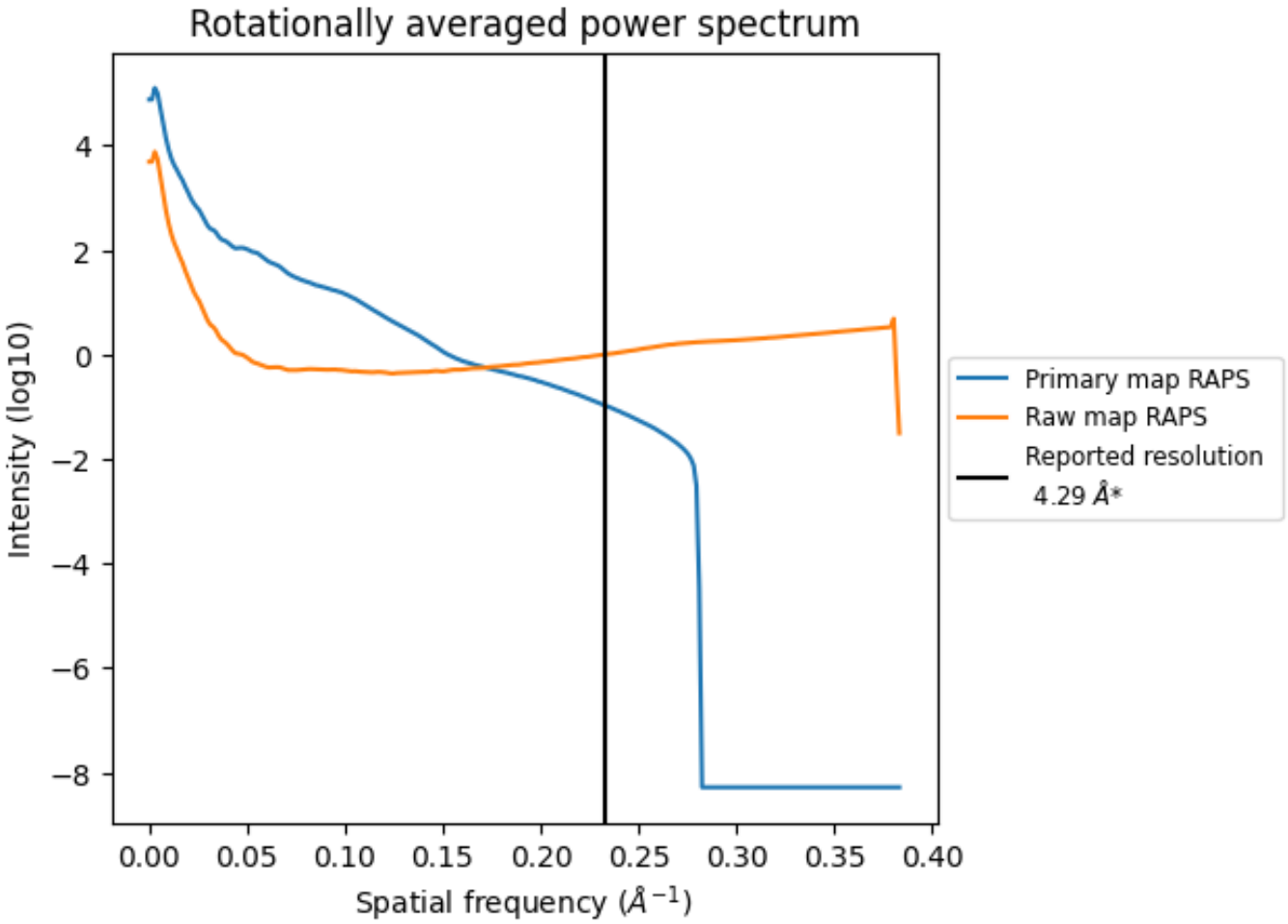
7.2 Volume estimate



The volume at the recommended contour level is 758 nm^3; this corresponds to an approximate mass of 685 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)

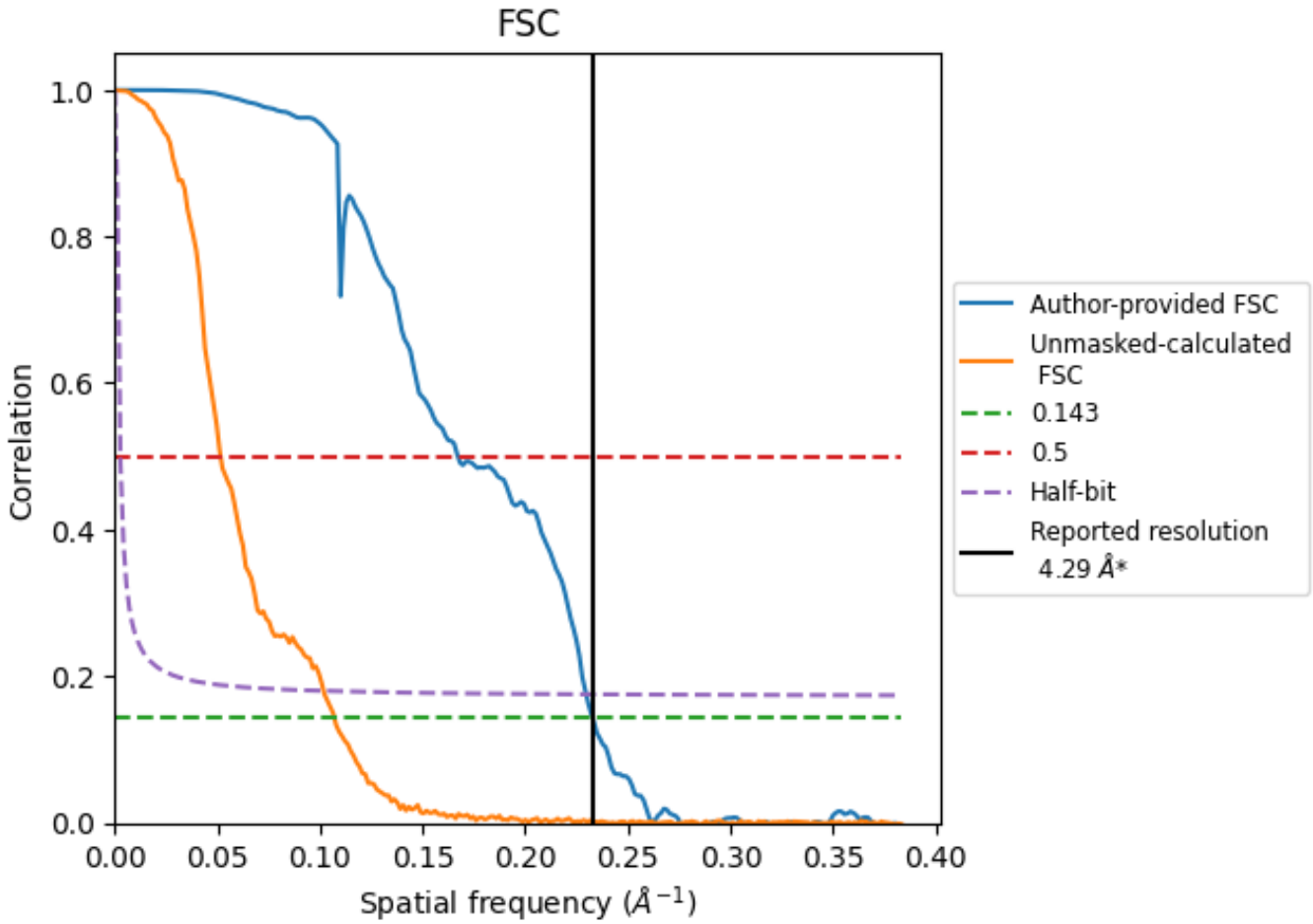


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

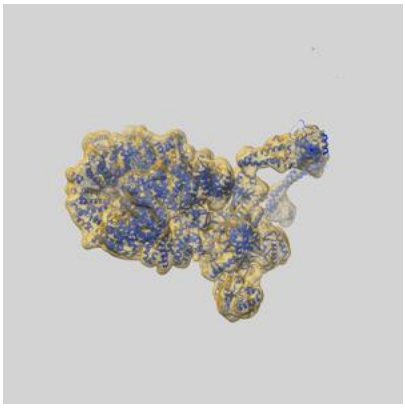
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.29	-	-
Author-provided FSC curve	4.29	5.98	4.35
Unmasked-calculated*	9.34	19.38	9.81

*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 9.34 differs from the reported value 4.29 by more than 10 %

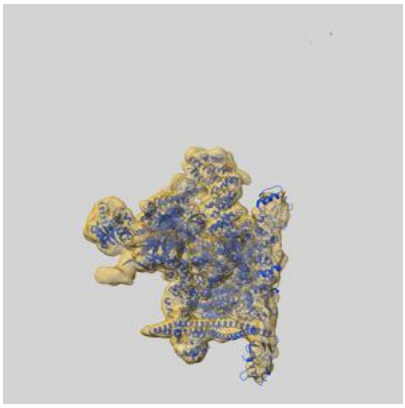
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12301 and PDB model 7NFE. Per-residue inclusion information can be found in section 3 on page 6.

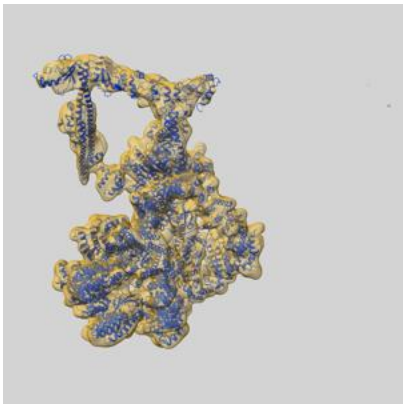
9.1 Map-model overlay



X



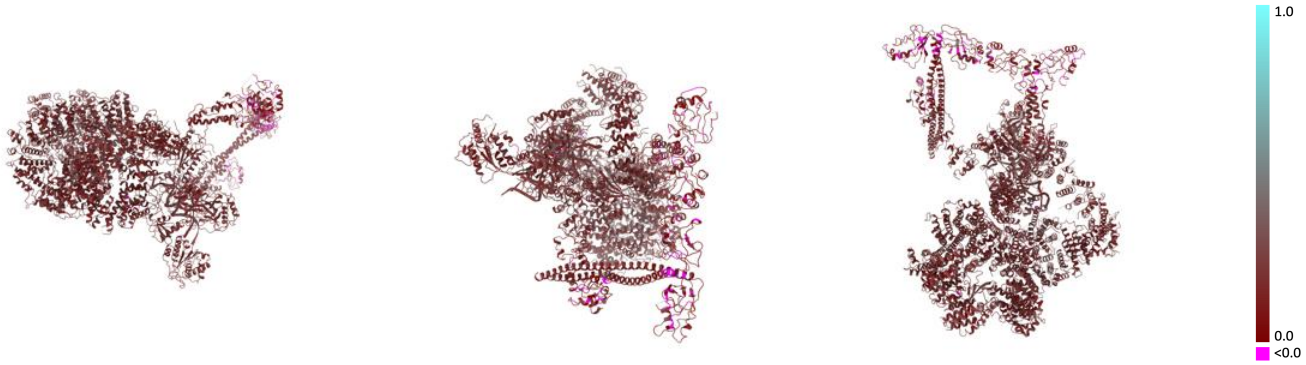
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.175 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.

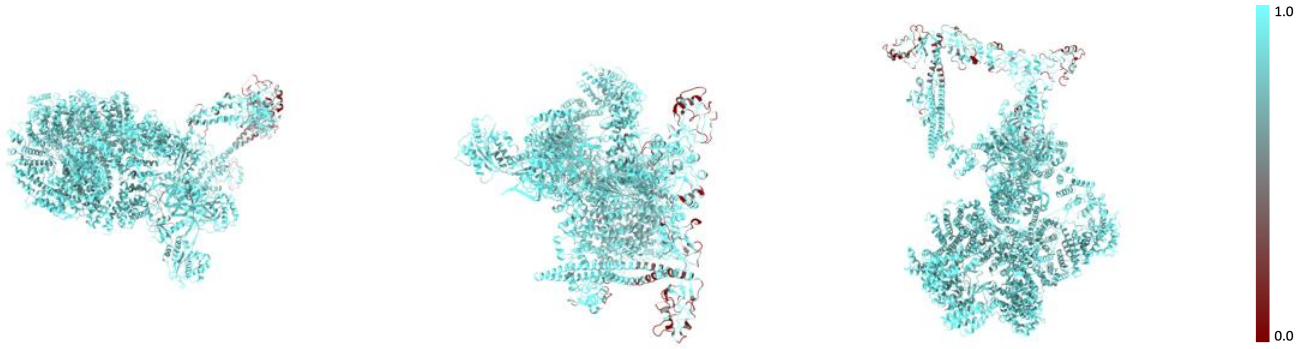
9.2 Q-score mapped to coordinate model (i)



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.

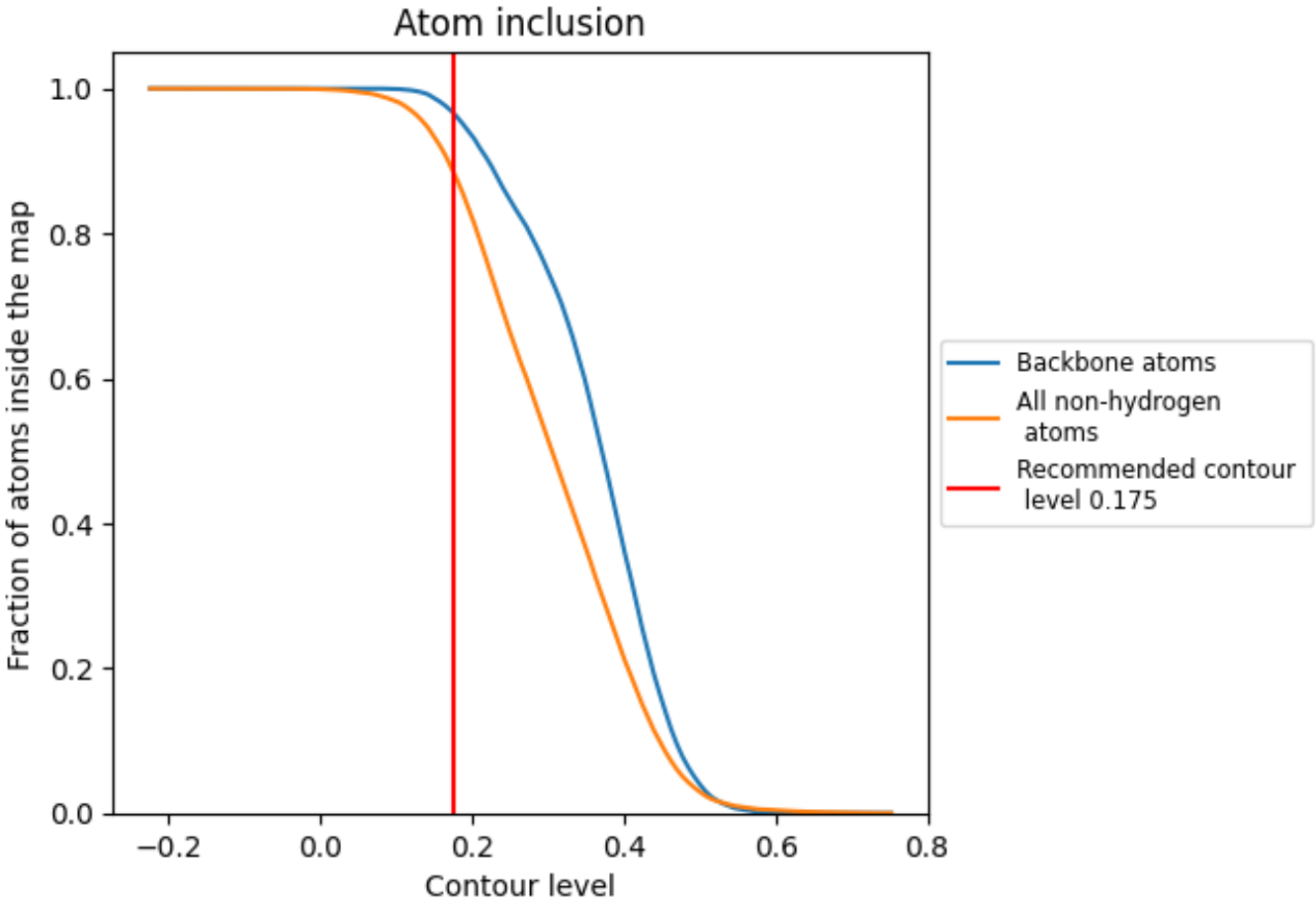
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.175).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8867	0.2030
A	0.9114	0.2140
B	0.9100	0.2270
C	0.9208	0.2180
D	0.9817	0.2580
E	0.9919	0.2600
F	0.6519	0.1300
G	0.8050	0.1390
H	0.7621	0.1350
I	0.6487	0.1360
J	0.8949	0.1560