Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 02:46 PM JST

PDB ID	:	6A70
EMDB ID	:	EMD-6991
Title	:	Structure of the human PKD1/PKD2 complex
Authors	:	Su, Q.; Hu, F.; Ge, X.; Lei, J.; Yu, S.; Wang, T.; Zhou, Q.; Mei, C.; Shi, Y.
Deposited on	:	2018-06-29
Resolution	:	3.60 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 (i) 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 (i)) were used in the production of this report:

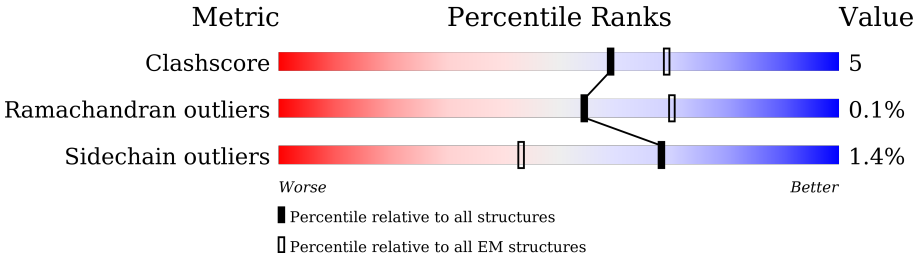
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	577	32% 73% 5% 22%
1	F	577	18% 69% 10% • 20%
1	G	577	22% 69% 12% • 18%
2	B	1153	44% 53% 8% 39%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15142 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 Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	448	2579	1608	472	492	7	0	0
			Total	C	N	O	S		
1	F	463	3762	2476	593	674	19	0	0
			Total	C	N	O	S		
1	G	471	3841	2534	604	684	19	0	0

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MET	-	expression tag	UNP Q13563
A	148	GLY	-	expression tag	UNP Q13563
A	149	SER	-	expression tag	UNP Q13563
A	150	ALA	-	expression tag	UNP Q13563
A	151	GLY	-	expression tag	UNP Q13563
A	152	TRP	-	expression tag	UNP Q13563
A	153	SER	-	expression tag	UNP Q13563
A	154	HIS	-	expression tag	UNP Q13563
A	155	PRO	-	expression tag	UNP Q13563
A	156	GLN	-	expression tag	UNP Q13563
A	157	PHE	-	expression tag	UNP Q13563
A	158	GLU	-	expression tag	UNP Q13563
A	159	LYS	-	expression tag	UNP Q13563
A	160	GLY	-	expression tag	UNP Q13563
A	161	GLY	-	expression tag	UNP Q13563
A	162	GLY	-	expression tag	UNP Q13563
A	163	SER	-	expression tag	UNP Q13563
A	164	GLY	-	expression tag	UNP Q13563
A	165	GLY	-	expression tag	UNP Q13563
A	166	GLY	-	expression tag	UNP Q13563
A	167	SER	-	expression tag	UNP Q13563
A	168	GLY	-	expression tag	UNP Q13563
A	169	GLY	-	expression tag	UNP Q13563
A	170	SER	-	expression tag	UNP Q13563

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	-	expression tag	UNP Q13563
A	172	TRP	-	expression tag	UNP Q13563
A	173	SER	-	expression tag	UNP Q13563
A	174	HIS	-	expression tag	UNP Q13563
A	175	PRO	-	expression tag	UNP Q13563
A	176	GLN	-	expression tag	UNP Q13563
A	177	PHE	-	expression tag	UNP Q13563
A	178	GLU	-	expression tag	UNP Q13563
A	179	LYS	-	expression tag	UNP Q13563
A	180	GLY	-	expression tag	UNP Q13563
A	181	SER	-	expression tag	UNP Q13563
A	182	ALA	-	expression tag	UNP Q13563
A	183	ALA	-	expression tag	UNP Q13563
A	184	ALA	-	expression tag	UNP Q13563
F	147	MET	-	expression tag	UNP Q13563
F	148	GLY	-	expression tag	UNP Q13563
F	149	SER	-	expression tag	UNP Q13563
F	150	ALA	-	expression tag	UNP Q13563
F	151	GLY	-	expression tag	UNP Q13563
F	152	TRP	-	expression tag	UNP Q13563
F	153	SER	-	expression tag	UNP Q13563
F	154	HIS	-	expression tag	UNP Q13563
F	155	PRO	-	expression tag	UNP Q13563
F	156	GLN	-	expression tag	UNP Q13563
F	157	PHE	-	expression tag	UNP Q13563
F	158	GLU	-	expression tag	UNP Q13563
F	159	LYS	-	expression tag	UNP Q13563
F	160	GLY	-	expression tag	UNP Q13563
F	161	GLY	-	expression tag	UNP Q13563
F	162	GLY	-	expression tag	UNP Q13563
F	163	SER	-	expression tag	UNP Q13563
F	164	GLY	-	expression tag	UNP Q13563
F	165	GLY	-	expression tag	UNP Q13563
F	166	GLY	-	expression tag	UNP Q13563
F	167	SER	-	expression tag	UNP Q13563
F	168	GLY	-	expression tag	UNP Q13563
F	169	GLY	-	expression tag	UNP Q13563
F	170	SER	-	expression tag	UNP Q13563
F	171	ALA	-	expression tag	UNP Q13563
F	172	TRP	-	expression tag	UNP Q13563
F	173	SER	-	expression tag	UNP Q13563
F	174	HIS	-	expression tag	UNP Q13563

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	175	PRO	-	expression tag	UNP Q13563
F	176	GLN	-	expression tag	UNP Q13563
F	177	PHE	-	expression tag	UNP Q13563
F	178	GLU	-	expression tag	UNP Q13563
F	179	LYS	-	expression tag	UNP Q13563
F	180	GLY	-	expression tag	UNP Q13563
F	181	SER	-	expression tag	UNP Q13563
F	182	ALA	-	expression tag	UNP Q13563
F	183	ALA	-	expression tag	UNP Q13563
F	184	ALA	-	expression tag	UNP Q13563
G	147	MET	-	expression tag	UNP Q13563
G	148	GLY	-	expression tag	UNP Q13563
G	149	SER	-	expression tag	UNP Q13563
G	150	ALA	-	expression tag	UNP Q13563
G	151	GLY	-	expression tag	UNP Q13563
G	152	TRP	-	expression tag	UNP Q13563
G	153	SER	-	expression tag	UNP Q13563
G	154	HIS	-	expression tag	UNP Q13563
G	155	PRO	-	expression tag	UNP Q13563
G	156	GLN	-	expression tag	UNP Q13563
G	157	PHE	-	expression tag	UNP Q13563
G	158	GLU	-	expression tag	UNP Q13563
G	159	LYS	-	expression tag	UNP Q13563
G	160	GLY	-	expression tag	UNP Q13563
G	161	GLY	-	expression tag	UNP Q13563
G	162	GLY	-	expression tag	UNP Q13563
G	163	SER	-	expression tag	UNP Q13563
G	164	GLY	-	expression tag	UNP Q13563
G	165	GLY	-	expression tag	UNP Q13563
G	166	GLY	-	expression tag	UNP Q13563
G	167	SER	-	expression tag	UNP Q13563
G	168	GLY	-	expression tag	UNP Q13563
G	169	GLY	-	expression tag	UNP Q13563
G	170	SER	-	expression tag	UNP Q13563
G	171	ALA	-	expression tag	UNP Q13563
G	172	TRP	-	expression tag	UNP Q13563
G	173	SER	-	expression tag	UNP Q13563
G	174	HIS	-	expression tag	UNP Q13563
G	175	PRO	-	expression tag	UNP Q13563
G	176	GLN	-	expression tag	UNP Q13563
G	177	PHE	-	expression tag	UNP Q13563
G	178	GLU	-	expression tag	UNP Q13563

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	179	LYS	-	expression tag	UNP Q13563
G	180	GLY	-	expression tag	UNP Q13563
G	181	SER	-	expression tag	UNP Q13563
G	182	ALA	-	expression tag	UNP Q13563
G	183	ALA	-	expression tag	UNP Q13563
G	184	ALA	-	expression tag	UNP Q13563

- Molecule 2 is a protein called Polycystin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	704	4960	3194	905	845	16	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3017	MET	-	expression tag	UNP P98161
B	3018	GLY	-	expression tag	UNP P98161
B	3019	SER	-	expression tag	UNP P98161
B	3020	ALA	-	expression tag	UNP P98161
B	3021	GLY	-	expression tag	UNP P98161
B	3022	ASP	-	expression tag	UNP P98161
B	3023	TYR	-	expression tag	UNP P98161
B	3024	LYS	-	expression tag	UNP P98161
B	3025	ASP	-	expression tag	UNP P98161
B	3026	HIS	-	expression tag	UNP P98161
B	3027	ASP	-	expression tag	UNP P98161
B	3028	GLY	-	expression tag	UNP P98161
B	3029	ASP	-	expression tag	UNP P98161
B	3030	TYR	-	expression tag	UNP P98161
B	3031	LYS	-	expression tag	UNP P98161
B	3032	ASP	-	expression tag	UNP P98161
B	3033	HIS	-	expression tag	UNP P98161
B	3034	ASP	-	expression tag	UNP P98161
B	3035	ILE	-	expression tag	UNP P98161
B	3036	ASP	-	expression tag	UNP P98161
B	3037	TYR	-	expression tag	UNP P98161
B	3038	LYS	-	expression tag	UNP P98161
B	3039	ASP	-	expression tag	UNP P98161
B	3040	ASP	-	expression tag	UNP P98161
B	3041	ASP	-	expression tag	UNP P98161
B	3042	ASP	-	expression tag	UNP P98161

Continued on next page...

Continued from previous page...

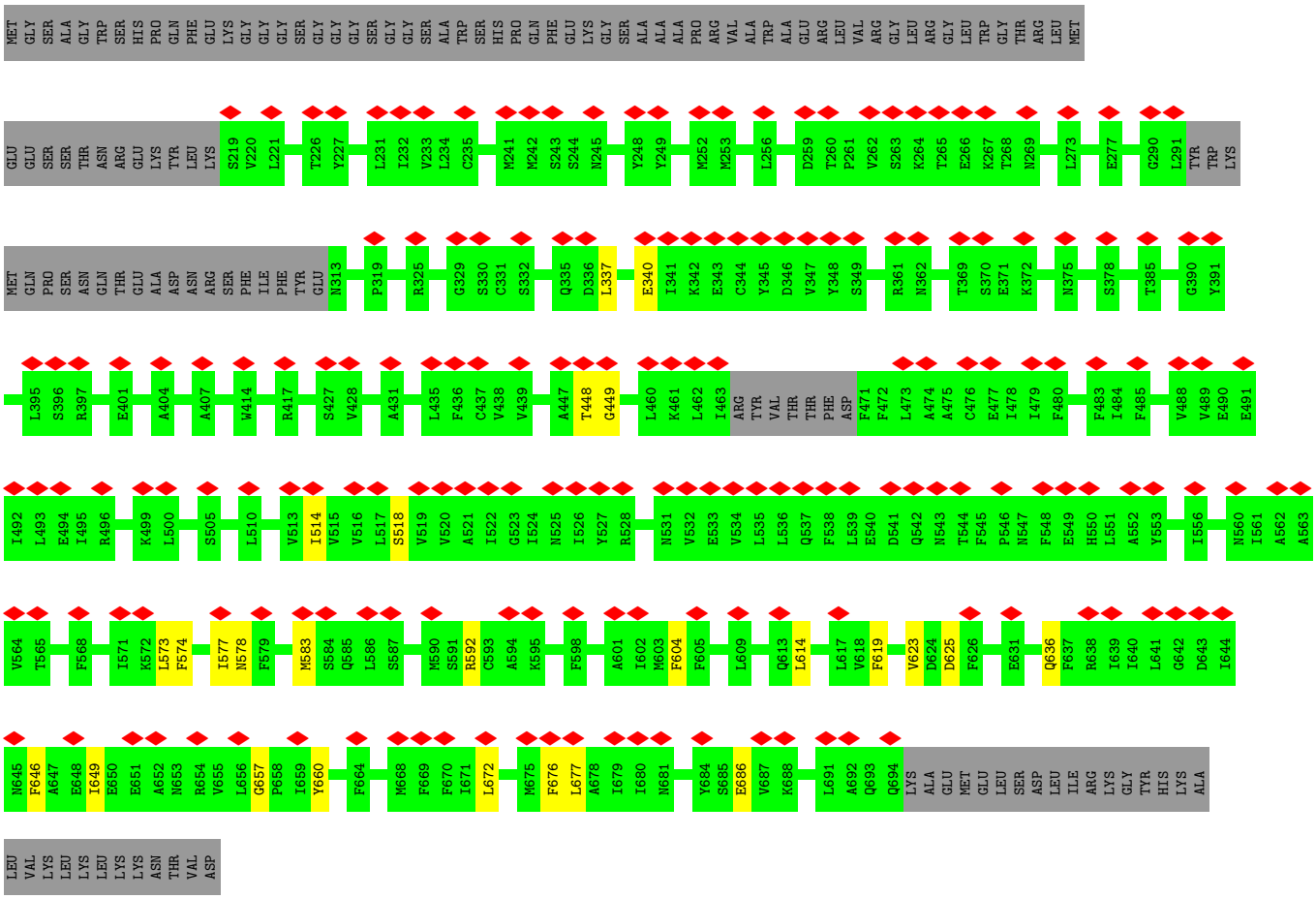
Chain	Residue	Modelled	Actual	Comment	Reference
B	3043	LYS	-	expression tag	UNP P98161
B	3044	GLY	-	expression tag	UNP P98161
B	3045	SER	-	expression tag	UNP P98161
B	3046	ALA	-	expression tag	UNP P98161
B	3047	ALA	-	expression tag	UNP P98161
B	3048	ALA	-	expression tag	UNP P98161

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.

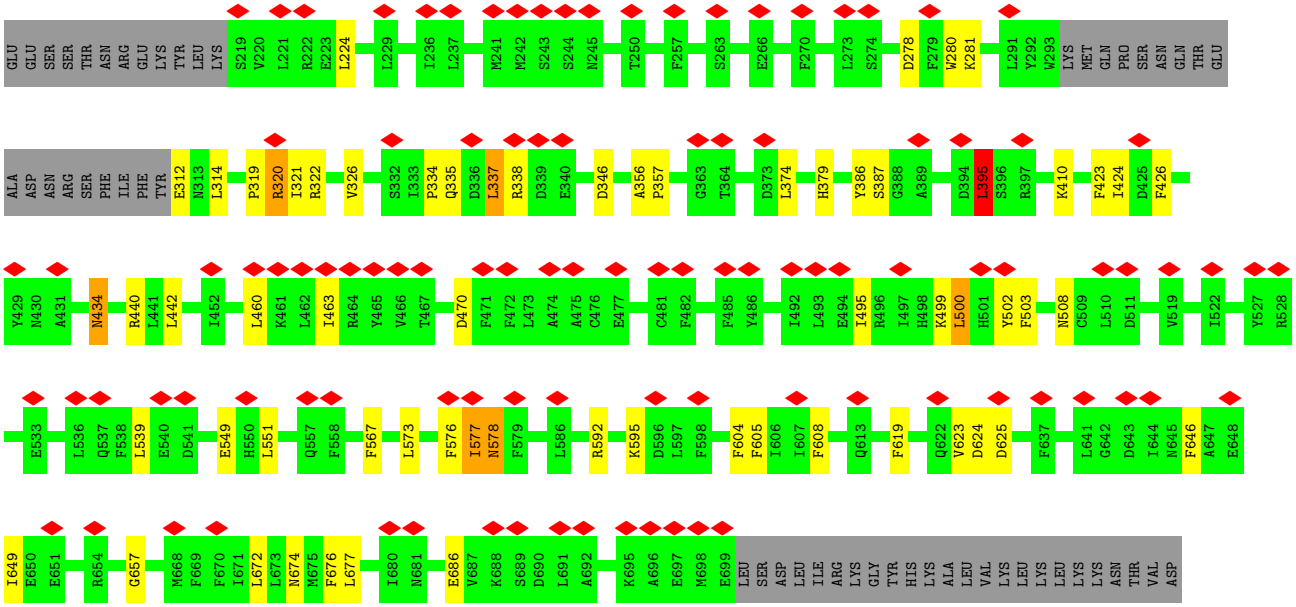
- Molecule 1: Polycystin-2

Chain A:



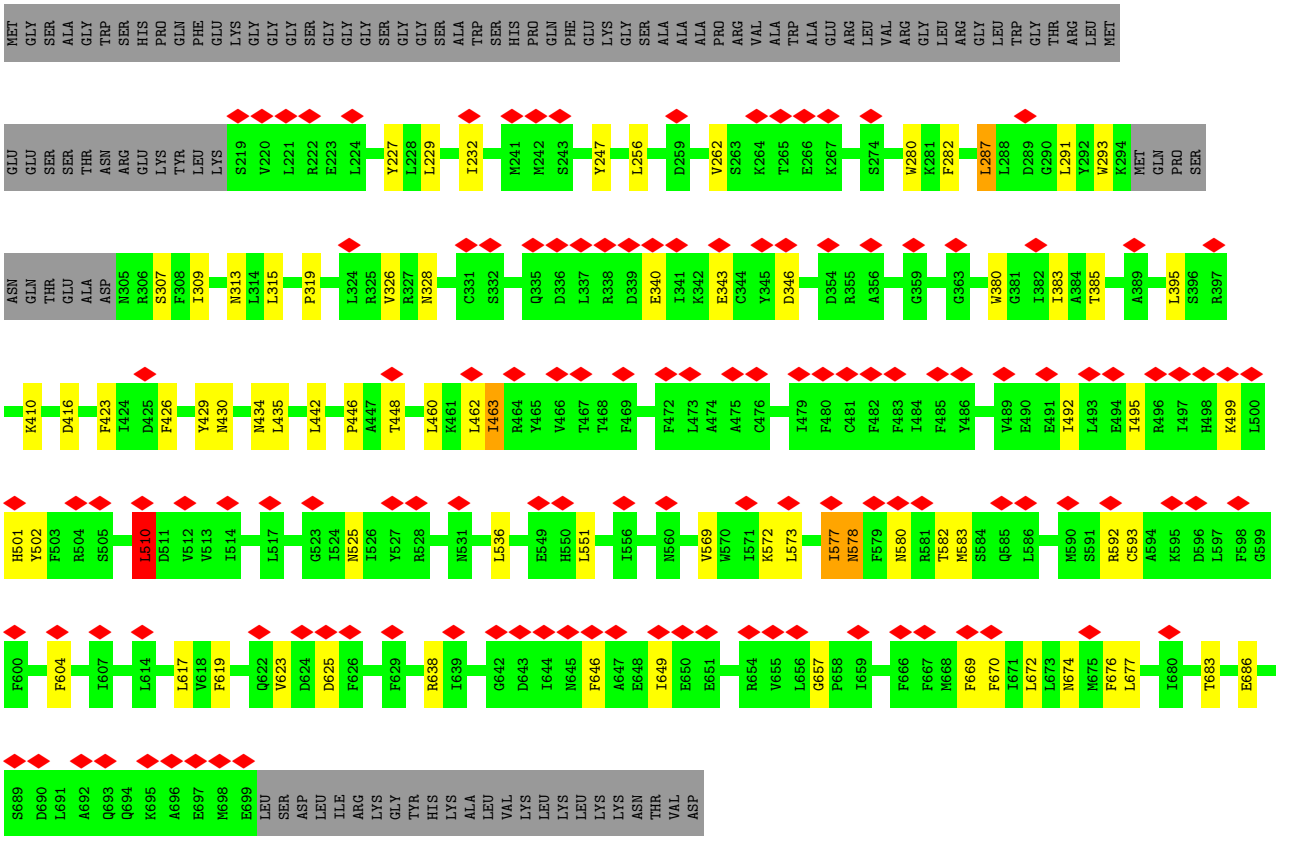
- Molecule 1: Polycystin-2

Chain F:



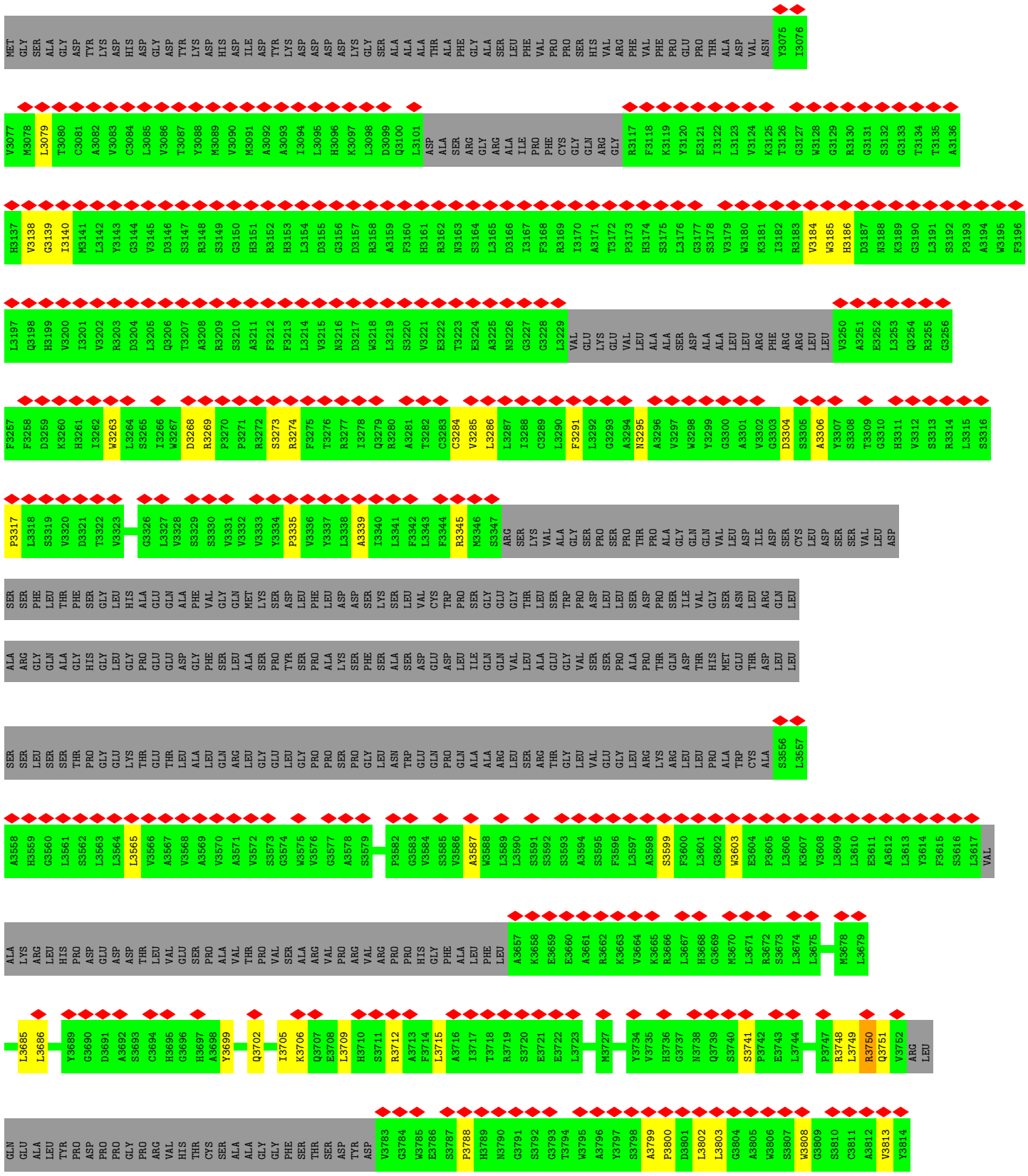
- Molecule 1: Polycystin-2

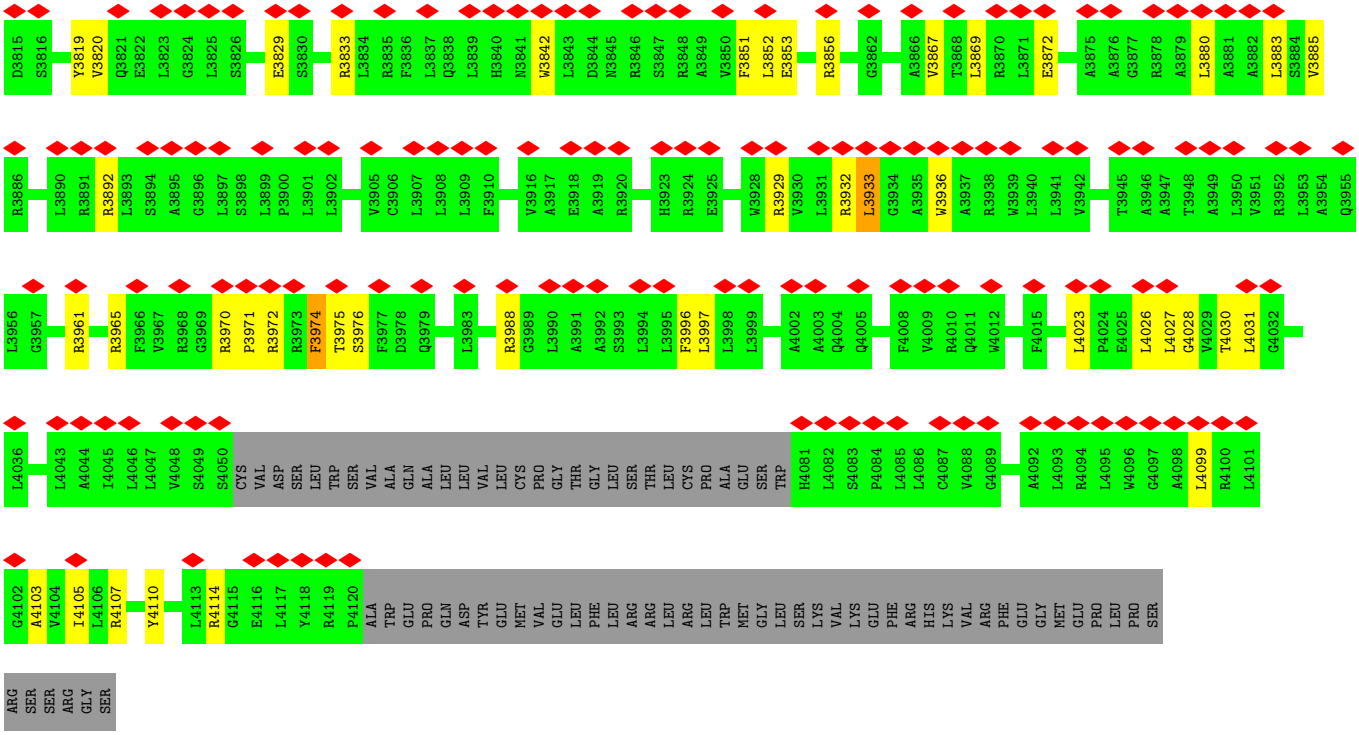
Chain G:



- Molecule 2: Polycystin-1

Chain B:


MET GLY SER ALA GLY ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP ASP ASP LYS GLY SER ALA ALA ALA THR ALA PHE GLY ALA SER LEU PHE VAL PRO PRO SER HIS VAL ARG PHE VAL PHE PRO GLU PRO THR ALA ASP VAL ASN
Y3075 I3076
V3077 M3078 L3079 T3080 C3081 A3082 V3083 C3084 L3085 V3086 T3087 Y3088 M3089 V3090 M3091 A3092 A3093 I3094 L3095 H3096 K3097 L3098 D3099 Q3100 L3101
ASP ALA SER ARG GLY ARG ALA ILE PRO PHE CYS GLY GLN ARG GLY
R3117 F3118 K3119 Y3120 E3121 I3122 L3123 V3124 K3125 T3126 G3127 W3128 G3129 R3130 G3131 S3132 G3133 T3134 T3135 A3136
H3137 V3138 G3139 I3140 M3141 L3142 Y3143 G3144 V3145 D3146 S3147 R3148 S3149 G3150 H3151 R3152 H3153 L3154 D3155 G3156 D3157 R3158 A3159 F3160 H3161 R3162 N3163 S3164 L3165 D3166 I3167 F3168 R3169 I3170 A3171 T3172 P3173 H3174 S3175 L3176 G3177 S3178 V3179 W3180 K3181 I3182 R3183 V3184 W3185 H3186 D3187 N3188 K3189 G3190 L3191 S3192 P3193 A3194 W3195 F3196
L3197 Q3198 H3199 V3200 I3201 V3202 R3203 D3204 L3205 Q3206 T3207 A3208 R3209 S3210 A3211 F3212 F3213 L3214 V3215 N3216 D3217 W3218 L3219 S3220 V3221 E3222 T3223 E3224 A3225 N3226 G3227 G3228 L3229
VAL GLU LYS GLU VAL LEU ALA ALA SER ASP ALA ALA LEU LEU ARG PHE ARG ARG LEU LEU
V3250 A3251 E3252 L3253 Q3254 R3255 G3256
F3257 F3258 D3259 K3260 H3261 I3262 W3263 L3264 S3265 I3266 W3267 D3268 R3269 P3270 P3271 R3272 S3273 R3274 F3275 T3276 R3277 I3278 Q3279 R3280 A3281 T3282 C3283 C3284 V3285 L3286 L3287 I3288 C3289 L3290 F3291 L3292 G3293 A3294 N3295 A3296 V3297 W3298 Y3299 G3300 A3301 V3302 G3303 D3304 S3305 A3306 Y3307 S3308 T3309 G3310 H3311 V3312 S3313 R3314 L3315 S3316
P3317 L3318 S3319 V3320 D3321 T3322 V3323
G3326 L3327 V3328 S3329 S3330 V3331 V3332 V3333 Y3334 P3335 V3336 Y3337 L3338 A3339 I3340 L3341 F3342 L3343 F3344 R3345 M3346 S3347
ARG SER LYS VAL ALA GLY SER PRO SER PRO THR PRO ALA GLY GLN GLN VAL LEU ASP ILE ASP SER CYS LEU ASP SER SER VAL LEU ASP
SER SER PHE LEU THR PHE SER GLY LEU HIS ALA GLU GLN ALA PHE VAL GLY GLN MET LYS SER ASP LEU PHE LEU ASP ASP SER LYS SER LEU VAL CYS TRP PRO SER GLY GLU GLY THR LEU SER TRP PRO ASP LEU LEU SER ASP PRO SER ILE VAL GLY SER ASN LEU ARG GLN LEU
ALA ARG GLY GLN ALA GLY HIS GLY LEU GLY PRO GLU GLU ASP GLY PHE SER SER LEU ALA SER PRO TYR SER PRO ALA LYS SER PHE SER ALA SER ASP GLU ASP LEU ILE GLN GLN VAL LEU ALA GLU GLY VAL SER SER PRO ALA PRO THR GLN ASP THR HIS MET GLU THR ASP LEU LEU
SER SER LEU SER SER THR PRO GLY GLU LYS THR GLU THR LEU ALA LEU GLN ARG LEU GLY GLU LEU GLY GLY PRO PRO SER PRO GLY LEU ASN TRP GLU GLN PRO GLN ALA ALA ARG LEU SER ARG THR GLY LEU VAL GLU GLY LEU ARG LYS ARG LEU LEU PRO ALA TRP CYS ALA
S3556 L3557
A3558 H3559 G3560 L3561 S3562 L3563 L3564 L3565 V3566 A3567 V3568 A3569 V3570 A3571 V3572 S3573 G3574 W3575 V3576 G3577 A3578 S3579
P3582 G3583 V3584 S3585 V3586 A3587 W3588 L3589 L3590 S3591 S3592 S3593 A3594 S3595 F3596 L3597 A3598 S3599 F3600 L3601 G3602 W3603 E3604 P3605 L3606 K3607 V3608 L3609 L3610 E3611 A3612 L3613 Y3614 F3615 S3616 L3617 VAL
ALA LYS ARG LEU HIS PRO ASP GLU ASP ASP THR LEU VAL GLU SER PRO ALA VAL THR PRO VAL SER ALA ARG VAL PRO ARG VAL ARG PRO PRO HIS GLY PHE ALA LEU PHE LEU
A3657 K3658 E3659 E3660 A3661 R3662 K3663 V3664 K3665 R3666 L3667 H3668 G3669 M3670 L3671 R3672 S3673 L3674 L3675
M3678 L3679
L3685 L3686 Y3689 G3690 D3691 A3692 S3693 C3694 H3695 G3696 H3697 A3698 Y3699 Q3702 I3705 K3706 Q3707 E3708 L3709 H3710 S3711 R3712 A3713 F3714 L3715 A3716 I3717 T3718 R3719 S3720 E3721 E3722 L3723 M3727 Y3734 V3735 H3736 G3737 N3738 Q3739 S3740 S3741 P3742 E3743 L3744 P3747 R3748 L3749 R3750 Q3751 V3752
ARG LEU
GLN GLU ALA LEU TYR PRO ASP PRO PRO PRO GLY PRO ARG VAL HIS THR CYS SER ALA ALA GLY GLY PHE SER THR SER ASP TYR ASP
V3783 G3784 W3785 E3786 S3787 P3788 H3789 N3790 G3791 S3792 G3793 T3794 W3795 A3796 Y3797 S3798 A3799 P3800 D3801 L3802 L3803 G3804 A3805 W3806 S3807 W3808 G3809 S3810 C3811 A3812 V3813 Y3814


D3815 S3816 Y3819 V3820 Q3821 E3822 L3823 G3824 L3825 S3826 E3829 S3830 R3833 L3834 R3835 F3836 L3837 Q3838 L3839 H3840 N3841 W3842 L3843 D3844 N3845 R3846 S3847 R3848 A3849 V3850 F3851 L3852 E3853 R3856 G3862 A3866 V3867 T3868 L3869 R3870 L3871 E3872 A3875 A3876 G3877 R3878 A3879 L3880 A3881 A3882 L3883 S3884 V3885
R3886 L3890 R3891 R3892 L3893 S3894 A3895 G3896 L3897 S3898 L3899 P3900 L3901 L3902 V3905 C3906 L3907 L3908 L3909 F3910 V3916 A3917 E3918 A3919 R3920 H3923 R3924 E3925 W3928 R3929 V3930 L3931 R3932 L3933 G3934 A3935 W3936 A3937 R3938 W3939 L3940 L3941 V3942 T3945 A3946 A3947 T3948 A3949 L3950 V3951 R3952 L3953 A3954 Q3955
L3956 G3957 R3961 R3965 F3966 V3967 R3968 G3969 R3970 P3971 R3972 R3973 F3974 T3975 S3976 F3977 D3978 Q3979 L3983 R3988 G3989 L3990 A3991 A3992 S3993 L3994 L3995 F3996 L3997 L3998 L3999 A4002 A4003 Q4004 Q4005 F4008 V4009 R4010 Q4011 W4012 F4015 L4023 P4024 E4025 L4026 L4027 G4028 V4029 T4030 L4031 G4032
L4036 L4043 A4044 I4045 L4046 L4047 V4048 S4049 S4050 CYS VAL ASP SER LEU TRP SER VAL ALA GLN ALA LEU LEU VAL LEU CYS PRO GLY THR GLY LEU SER THR LEU CYS PRO ALA GLU SER TRP H4081 L4082 S4083 P4084 L4085 L4086 C4087 V4088 G4089 A4092 L4093 R4094 L4095 W4096 G4097 A4098 L4099 R4100 L4101
G4102 A4103 V4104 I4105 L4106 R4107 Y4110 L4113 R4114 G4115 E4116 L4117 Y4118 R4119 P4120 ALA TRP GLU PRO GLN ASP TYR GLU MET VAL GLU LEU PHE LEU ARG ARG LEU ARG LEU TRP MET GLY LEU SER LYS VAL LYS GLU PHE ARG HIS LYS VAL ARG PHE GLU GLY MET GLU PRO LEU PRO SER
ARG SER SER ARG GLY SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27296	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	279.296, 279.296, 279.296	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.34	0/2600	0.52	0/3584
1	F	0.48	0/3860	0.67	6/5247 (0.1%)
1	G	0.51	0/3943	0.67	9/5358 (0.2%)
2	B	0.36	0/5065	0.70	2/6920 (0.0%)
All	All	0.43	0/15468	0.66	17/21109 (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
1	F	0	1
1	G	0	2
2	B	0	7
All	All	0	10

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	460	LEU	CA-CB-CG	8.23	134.23	115.30
1	F	500	LEU	CA-CB-CG	7.90	133.47	115.30
1	F	460	LEU	CA-CB-CG	7.74	133.11	115.30
1	F	395	LEU	CA-CB-CG	7.68	132.97	115.30
1	F	337	LEU	CA-CB-CG	7.37	132.24	115.30
2	B	3686	LEU	CA-CB-CG	6.54	130.34	115.30
1	G	435	LEU	CA-CB-CG	6.44	130.12	115.30
1	G	287	LEU	CA-CB-CG	5.72	128.45	115.30
1	G	435	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	G	315	LEU	CA-CB-CG	5.70	128.40	115.30
1	F	551	LEU	CA-CB-CG	5.49	127.92	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	573	LEU	CA-CB-CG	5.45	127.83	115.30
1	G	510	LEU	CA-CB-CG	5.42	127.76	115.30
1	G	395	LEU	CA-CB-CG	5.33	127.56	115.30
1	G	551	LEU	CA-CB-CG	5.22	127.30	115.30
1	G	536	LEU	CA-CB-CG	5.18	127.23	115.30
2	B	3933	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	3304	ASP	Peptide
2	B	3306	ALA	Peptide
2	B	3699	TYR	Peptide
2	B	3820	VAL	Peptide
2	B	3974	PHE	Peptide
2	B	3975	THR	Peptide
2	B	3976	SER	Peptide
1	F	577	ILE	Peptide
1	G	463	ILE	Peptide
1	G	577	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2579	0	1634	23	0
1	F	3762	0	3656	41	0
1	G	3841	0	3741	43	0
2	B	4960	0	4566	52	0
All	All	15142	0	13597	137	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 5.

All (137) 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:448:THR:HA	1:F:312:GLU:HB3	1.16	1.10
1:A:448:THR:HA	1:F:312:GLU:CB	2.05	0.84
1:A:448:THR:CA	1:F:312:GLU:HB3	2.05	0.82
1:A:573:LEU:O	1:A:577:ILE:N	2.29	0.66
2:B:3702:GLN:OE1	2:B:3706:LYS:NZ	2.28	0.65
2:B:3269:ARG:NH1	2:B:3273:SER:O	2.30	0.65
1:F:319:PRO:HB3	1:F:426:PHE:HB3	1.78	0.64
1:G:319:PRO:HB3	1:G:426:PHE:HB3	1.78	0.64
1:G:380:TRP:HD1	1:G:385:THR:HG22	1.63	0.63
1:A:578:ASN:HA	1:A:583:MET:HB3	1.80	0.63
1:A:677:LEU:HD12	1:F:677:LEU:HD21	1.82	0.62
1:G:229:LEU:HD12	1:G:232:ILE:HD11	1.81	0.62
1:G:492:ILE:HA	1:G:495:ILE:HG22	1.81	0.61
2:B:4028:GLY:HA2	2:B:4031:LEU:HD13	1.83	0.60
2:B:3933:LEU:HA	2:B:3936:TRP:HB3	1.84	0.59
1:A:574:PHE:HA	1:A:577:ILE:CB	2.33	0.59
2:B:3748:ARG:NH1	2:B:3853:GLU:OE1	2.36	0.58
1:F:319:PRO:HG2	1:F:395:LEU:HD11	1.84	0.58
2:B:3970:ARG:HH12	1:G:340:GLU:HG3	1.68	0.58
2:B:3829:GLU:O	2:B:3833:ARG:N	2.39	0.56
1:F:322:ARG:NH1	1:F:387:SER:O	2.40	0.55
2:B:3317:PRO:HB3	2:B:3587:ALA:HB2	1.87	0.55
1:G:313:ASN:OD1	1:G:430:ASN:ND2	2.39	0.55
1:G:227:TYR:OH	1:G:569:VAL:O	2.25	0.54
2:B:3139:GLY:N	2:B:3185:TRP:O	2.40	0.54
2:B:3867:VAL:HG22	2:B:3885:VAL:HG22	1.91	0.53
1:A:573:LEU:O	1:A:577:ILE:CB	2.58	0.52
1:F:674:ASN:HB3	1:G:677:LEU:HD23	1.92	0.51
1:F:278:ASP:HA	1:F:281:LYS:HG2	1.92	0.51
1:F:320:ARG:HH12	1:F:374:LEU:HD21	1.75	0.51
1:A:578:ASN:CA	1:A:583:MET:HB3	2.41	0.51
1:A:449:GLY:N	1:F:312:GLU:OE1	2.44	0.51
1:A:604:PHE:HD1	1:A:672:LEU:HD12	1.76	0.51
2:B:3749:LEU:HA	2:B:3852:LEU:HA	1.93	0.50
1:F:321:ILE:HG12	1:F:424:ILE:HG12	1.92	0.50
2:B:3706:LYS:HE3	2:B:3856:ARG:HD2	1.93	0.50
2:B:3872:GLU:HB2	2:B:3880:LEU:HB2	1.92	0.50
1:A:337:LEU:CB	1:F:539:LEU:HD11	2.41	0.50
2:B:3929:ARG:HE	2:B:3932:ARG:HB2	1.77	0.50
2:B:3263:TRP:HE1	2:B:3284:CYS:HB3	1.77	0.50
1:F:604:PHE:HD1	1:F:672:LEU:HD12	1.76	0.50
2:B:3808:TRP:HB3	2:B:3813:VAL:HG22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3869:LEU:HD23	2:B:3883:LEU:HB2	1.95	0.49
1:G:604:PHE:HD1	1:G:672:LEU:HD12	1.76	0.49
2:B:3705:ILE:HG21	1:G:448:THR:HB	1.94	0.49
1:G:280:TRP:HB3	1:G:410:LYS:HE2	1.95	0.49
2:B:4026:LEU:HD13	2:B:4105:ILE:HD12	1.94	0.49
2:B:3712:ARG:HB3	2:B:3715:LEU:HD23	1.93	0.49
1:A:614:LEU:HD12	1:F:567:PHE:HB2	1.93	0.49
1:G:619:PHE:HZ	1:G:657:GLY:HA2	1.77	0.49
1:A:619:PHE:HZ	1:A:657:GLY:HA2	1.77	0.49
2:B:3599:SER:HA	2:B:3603:TRP:HB2	1.94	0.48
2:B:3751:GLN:O	2:B:3819:TYR:N	2.39	0.48
1:F:624:ASP:OD1	1:G:247:TYR:OH	2.20	0.48
2:B:3138:VAL:HA	2:B:3186:HIS:HA	1.96	0.48
1:F:434:ASN:HD21	1:F:463:ILE:HB	1.78	0.48
1:F:619:PHE:HZ	1:F:657:GLY:HA2	1.77	0.48
1:G:434:ASN:ND2	1:G:463:ILE:O	2.47	0.48
1:F:320:ARG:HH22	1:F:374:LEU:HD11	1.80	0.47
1:G:593:CYS:HB2	1:G:683:THR:HG21	1.96	0.47
1:F:334:PRO:HG3	1:G:463:ILE:HG21	1.96	0.47
2:B:4023:LEU:HG	2:B:4027:LEU:HD23	1.96	0.47
2:B:4110:TYR:OH	2:B:4114:ARG:NH2	2.36	0.47
2:B:3748:ARG:HG2	2:B:3974:PHE:CG	2.49	0.47
1:F:335:GLN:HG3	1:F:338:ARG:NH2	2.29	0.47
1:F:224:LEU:HG	1:F:576:PHE:CZ	2.50	0.46
1:G:328:ASN:ND2	1:G:343:GLU:OE1	2.38	0.46
1:A:340:GLU:CB	1:F:314:LEU:HD13	2.45	0.46
2:B:3284:CYS:SG	2:B:3285:VAL:N	2.89	0.45
1:G:293:TRP:CD1	1:G:309:ILE:HA	2.51	0.45
2:B:3291:PHE:O	2:B:3295:ASN:ND2	2.50	0.45
2:B:3971:PRO:HG2	2:B:3972:ARG:CZ	2.47	0.45
2:B:3996:PHE:HD2	2:B:3997:LEU:HD22	1.82	0.45
1:F:379:HIS:CE1	1:F:386:TYR:HB2	2.51	0.45
1:F:470:ASP:N	1:F:470:ASP:OD1	2.46	0.44
2:B:3140:ILE:HA	2:B:3184:VAL:HA	1.99	0.44
1:A:578:ASN:CB	1:A:583:MET:HB3	2.48	0.44
1:F:440:ARG:NH2	1:F:549:GLU:OE1	2.50	0.44
1:F:592:ARG:NH1	1:F:686:GLU:OE1	2.50	0.44
1:F:623:VAL:HG12	1:F:625:ASP:H	1.83	0.44
1:G:499:LYS:HB2	1:G:502:TYR:HB3	2.00	0.44
2:B:3139:GLY:O	2:B:3185:TRP:N	2.51	0.44
2:B:3705:ILE:O	2:B:3709:LEU:N	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:499:LYS:HB2	1:F:502:TYR:HB3	2.00	0.44
1:G:592:ARG:NH1	1:G:686:GLU:OE1	2.50	0.44
2:B:4027:LEU:O	2:B:4030:THR:OG1	2.34	0.43
1:G:423:PHE:HB3	1:G:442:LEU:HA	2.00	0.43
1:A:592:ARG:NH1	1:A:686:GLU:OE1	2.50	0.43
1:A:623:VAL:HG12	1:A:625:ASP:H	1.83	0.43
1:G:291:LEU:O	1:G:307:SER:OG	2.28	0.43
1:G:326:VAL:HG11	1:G:346:ASP:H	1.84	0.43
1:G:577:ILE:HG23	1:G:578:ASN:H	1.83	0.43
2:B:3269:ARG:NH1	2:B:3274:ARG:O	2.45	0.43
1:G:623:VAL:HG12	1:G:625:ASP:H	1.83	0.43
1:A:514:ILE:O	1:A:518:SER:N	2.51	0.43
1:A:636:GLN:NE2	1:A:660:TYR:OH	2.44	0.43
2:B:3268:ASP:OD1	2:B:3268:ASP:N	2.51	0.43
1:G:423:PHE:HB3	1:G:442:LEU:HD23	2.01	0.43
1:F:326:VAL:HG11	1:F:346:ASP:H	1.84	0.43
1:F:577:ILE:HG23	1:F:578:ASN:H	1.83	0.43
2:B:4099:LEU:HA	1:G:670:PHE:HE1	1.83	0.43
1:F:280:TRP:HB3	1:F:410:LYS:HE2	2.00	0.43
1:A:337:LEU:CB	1:F:539:LEU:CD1	2.96	0.42
1:F:423:PHE:HB3	1:F:442:LEU:HA	2.00	0.42
1:F:503:PHE:CE2	1:F:508:ASN:HB3	2.55	0.42
2:B:3741:SER:O	2:B:3856:ARG:NH2	2.52	0.42
2:B:3799:ALA:HA	2:B:3800:PRO:HD3	1.80	0.42
1:G:501:HIS:O	1:G:501:HIS:ND1	2.52	0.42
2:B:4103:ALA:HA	1:G:674:ASN:HB3	2.00	0.42
2:B:3751:GLN:NE2	2:B:3842:TRP:O	2.52	0.42
1:F:337:LEU:HD11	1:G:429:TYR:CE2	2.55	0.42
1:G:262:VAL:HG12	1:G:282:PHE:HD1	1.85	0.42
2:B:3079:LEU:HD13	2:B:3685:LEU:HG	2.01	0.42
1:G:416:ASP:OD1	1:G:416:ASP:N	2.53	0.42
1:A:578:ASN:HA	1:A:583:MET:CB	2.49	0.42
2:B:4099:LEU:HD13	1:G:669:PHE:CD1	2.55	0.42
1:F:646:PHE:HE1	1:G:638:ARG:HD2	1.85	0.42
2:B:3748:ARG:HH22	2:B:3750:ARG:HD2	1.84	0.41
1:F:595:LYS:HG3	1:G:582:THR:HG21	2.01	0.41
1:A:646:PHE:HB2	1:A:649:ILE:HB	2.02	0.41
2:B:3988:ARG:HG2	1:G:617:LEU:HD12	2.01	0.41
1:G:462:LEU:HD12	1:G:462:LEU:HA	1.86	0.41
1:G:309:ILE:HB	1:G:313:ASN:HB2	2.01	0.41
2:B:4099:LEU:HA	1:G:670:PHE:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:646:PHE:HB2	1:G:649:ILE:HB	2.02	0.41
2:B:3929:ARG:HD2	2:B:3929:ARG:HA	1.94	0.41
2:B:3750:ARG:HD3	2:B:3851:PHE:O	2.21	0.41
2:B:3802:LEU:HD22	2:B:3803:LEU:H	1.86	0.41
1:F:646:PHE:HB2	1:F:649:ILE:HB	2.02	0.41
2:B:3705:ILE:HG13	2:B:3709:LEU:HD23	2.02	0.41
2:B:3335:PRO:O	2:B:3339:ALA:N	2.41	0.40
1:G:383:ILE:HD11	1:G:446:PRO:HG3	2.04	0.40
1:G:510:LEU:HD12	1:G:572:LYS:HE2	2.03	0.40
1:G:580:ASN:HB2	1:G:583:MET:HG2	2.02	0.40
2:B:3286:LEU:HD11	2:B:3565:LEU:HD23	2.02	0.40
1:F:356:ALA:HA	1:F:357:PRO:HD3	1.95	0.40
1:F:605:PHE:HA	1:F:608:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/577 (77%)	398 (90%)	44 (10%)	0	100	100
1	F	459/577 (80%)	438 (95%)	20 (4%)	1 (0%)	47	79
1	G	467/577 (81%)	446 (96%)	20 (4%)	1 (0%)	47	79
2	B	690/1153 (60%)	584 (85%)	105 (15%)	1 (0%)	51	83
All	All	2058/2884 (71%)	1866 (91%)	189 (9%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	578	ASN
1	G	578	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	3788	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	98/508 (19%)	97 (99%)	1 (1%)	76	88
1	F	404/508 (80%)	398 (98%)	6 (2%)	65	84
1	G	413/508 (81%)	407 (98%)	6 (2%)	65	84
2	B	410/946 (43%)	404 (98%)	6 (2%)	65	84
All	All	1325/2470 (54%)	1306 (99%)	19 (1%)	68	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	676	PHE
2	B	3345	ARG
2	B	3750	ARG
2	B	3892	ARG
2	B	3961	ARG
2	B	3965	ARG
2	B	4107	ARG
1	F	320	ARG
1	F	395	LEU
1	F	434	ASN
1	F	495	ILE
1	F	500	LEU
1	F	676	PHE
1	G	256	LEU
1	G	287	LEU
1	G	510	LEU
1	G	525	ASN
1	G	573	LEU
1	G	676	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	613	GLN
2	B	3840	HIS
1	F	434	ASN
1	F	458	GLN
1	F	613	GLN
1	F	681	ASN
1	G	458	GLN
1	G	613	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

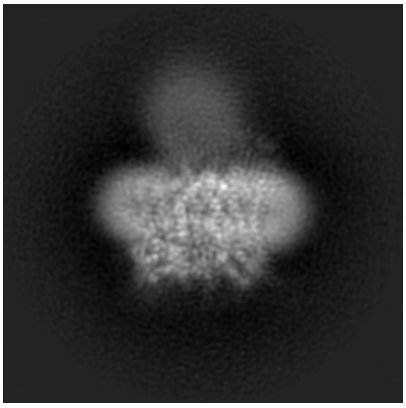
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6991. These allow visual inspection of the internal detail of the map and identification of artifacts.

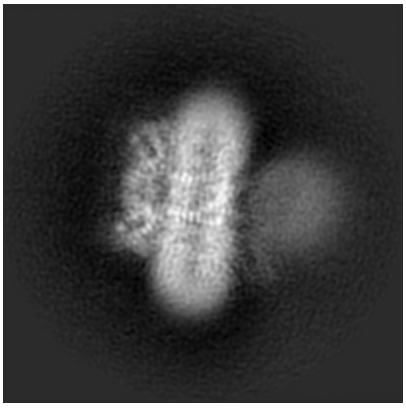
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

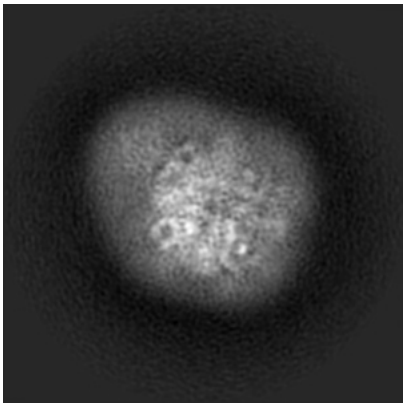
6.1.1 Primary map



X



Y

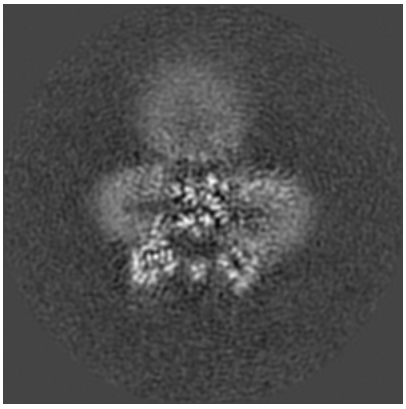


Z

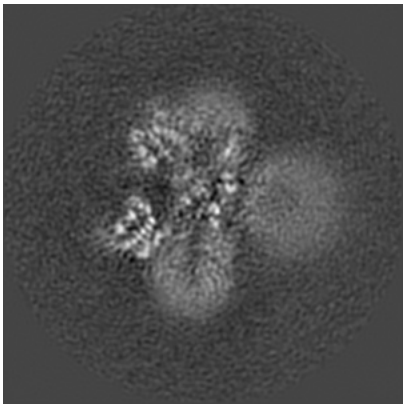
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

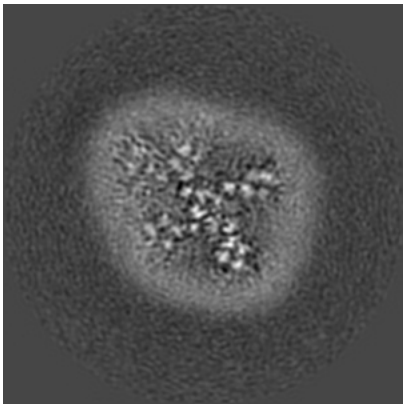
6.2.1 Primary map



X Index: 128



Y Index: 128

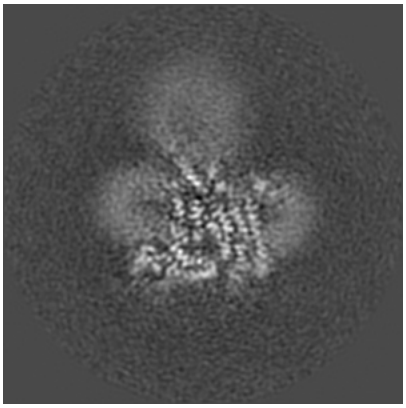


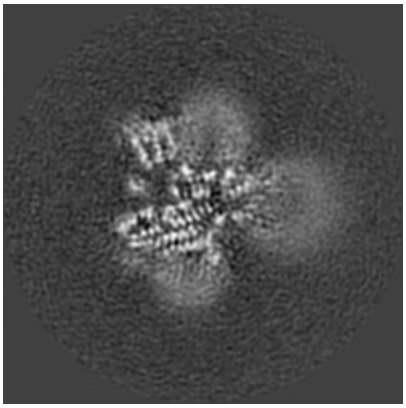
Z Index: 128

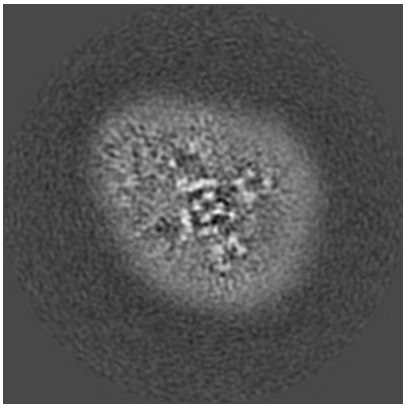
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 121

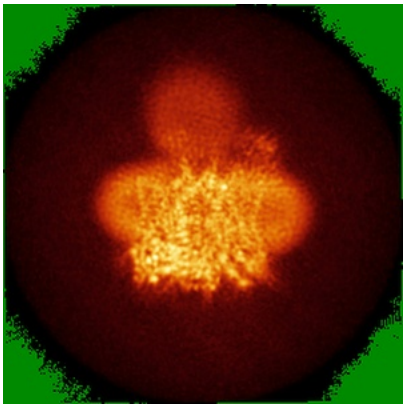

Y Index: 115

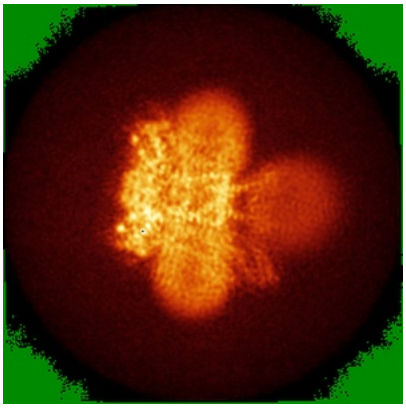

Z Index: 138

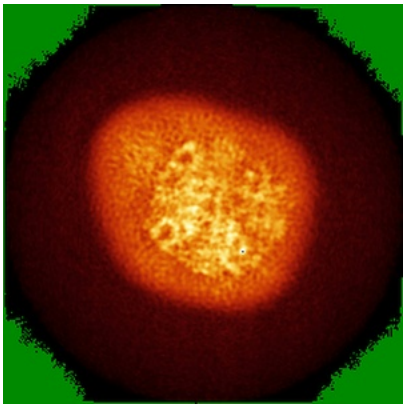
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

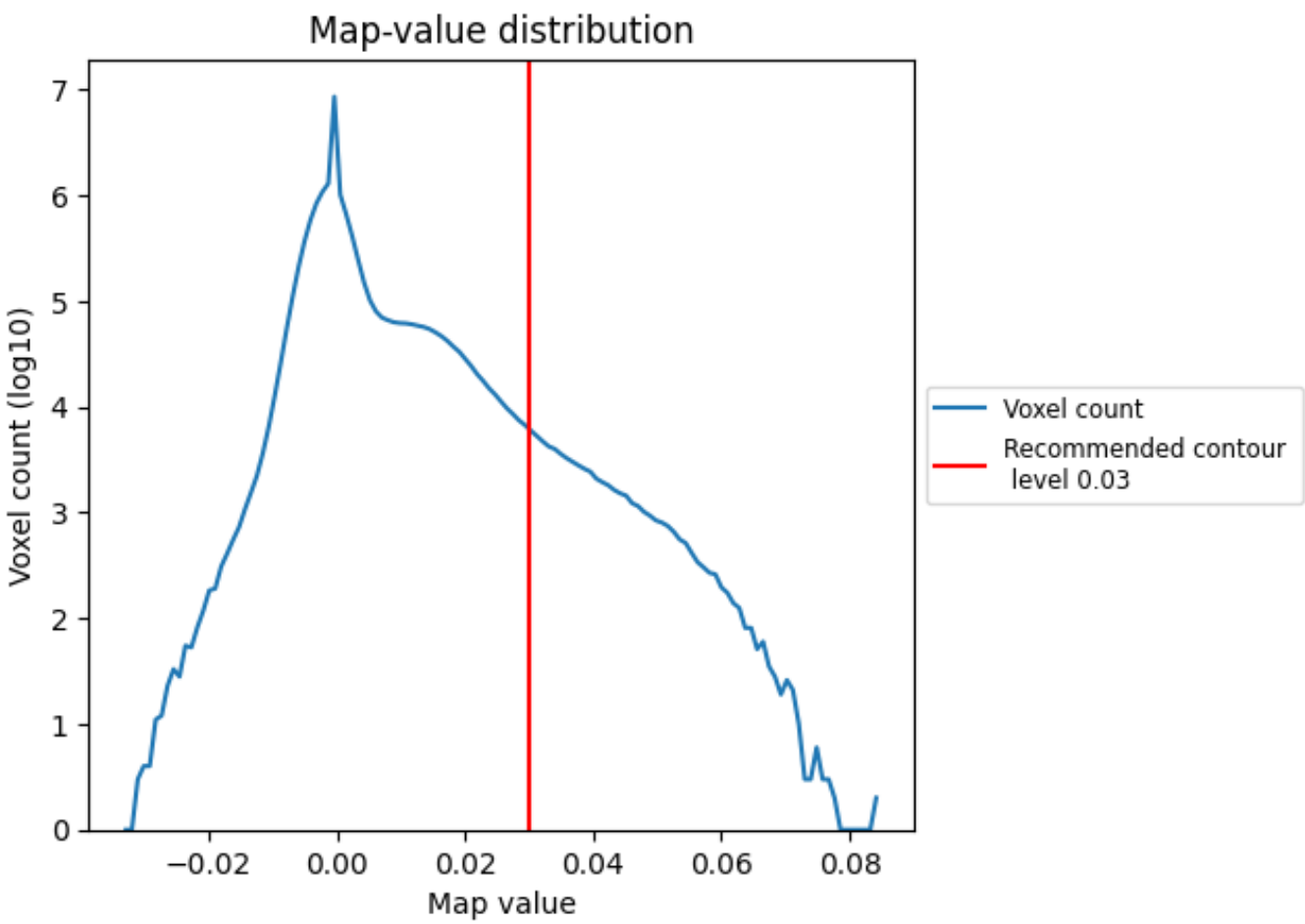
6.6 Mask visualisation (i)

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

7 Map analysis (i)

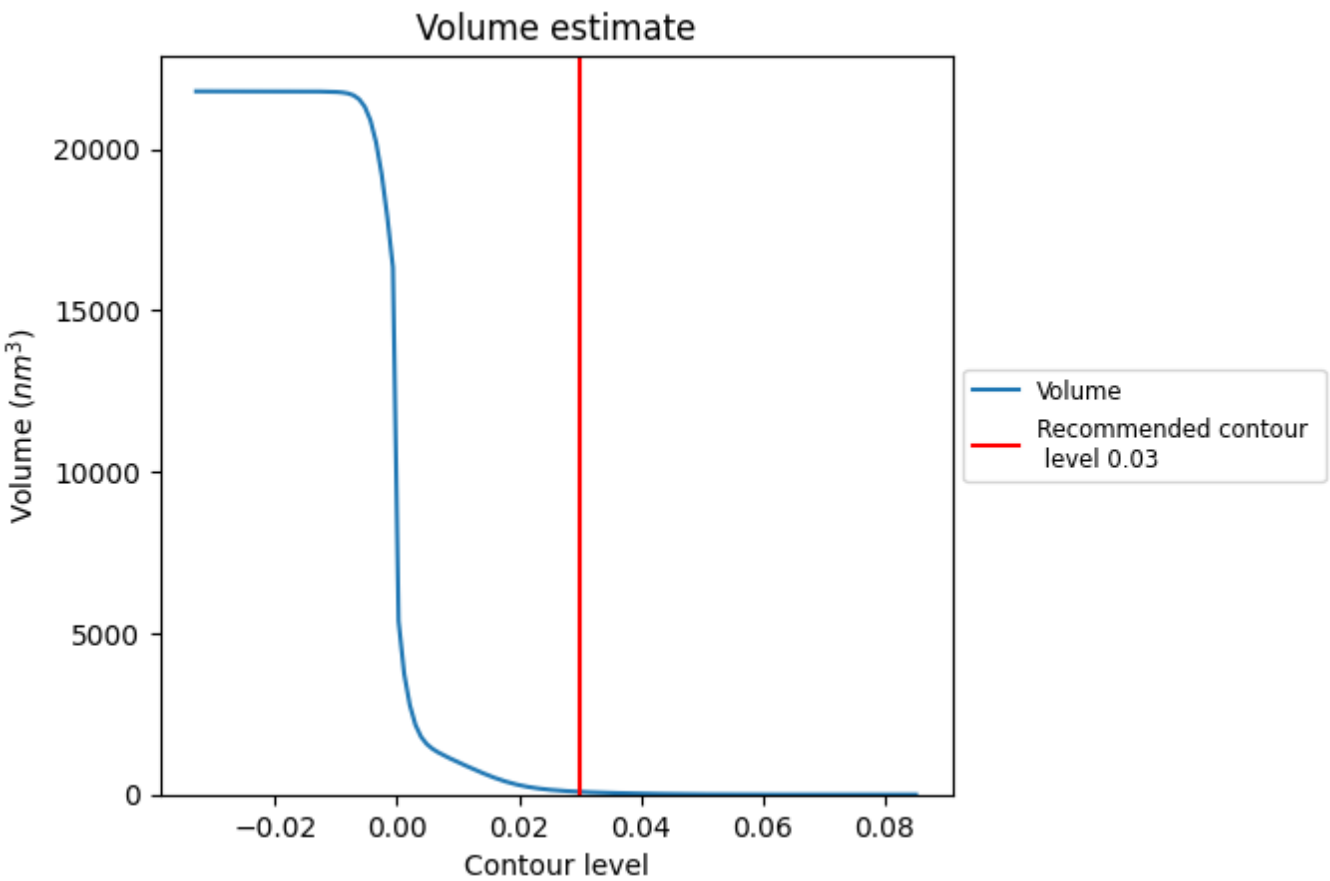
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

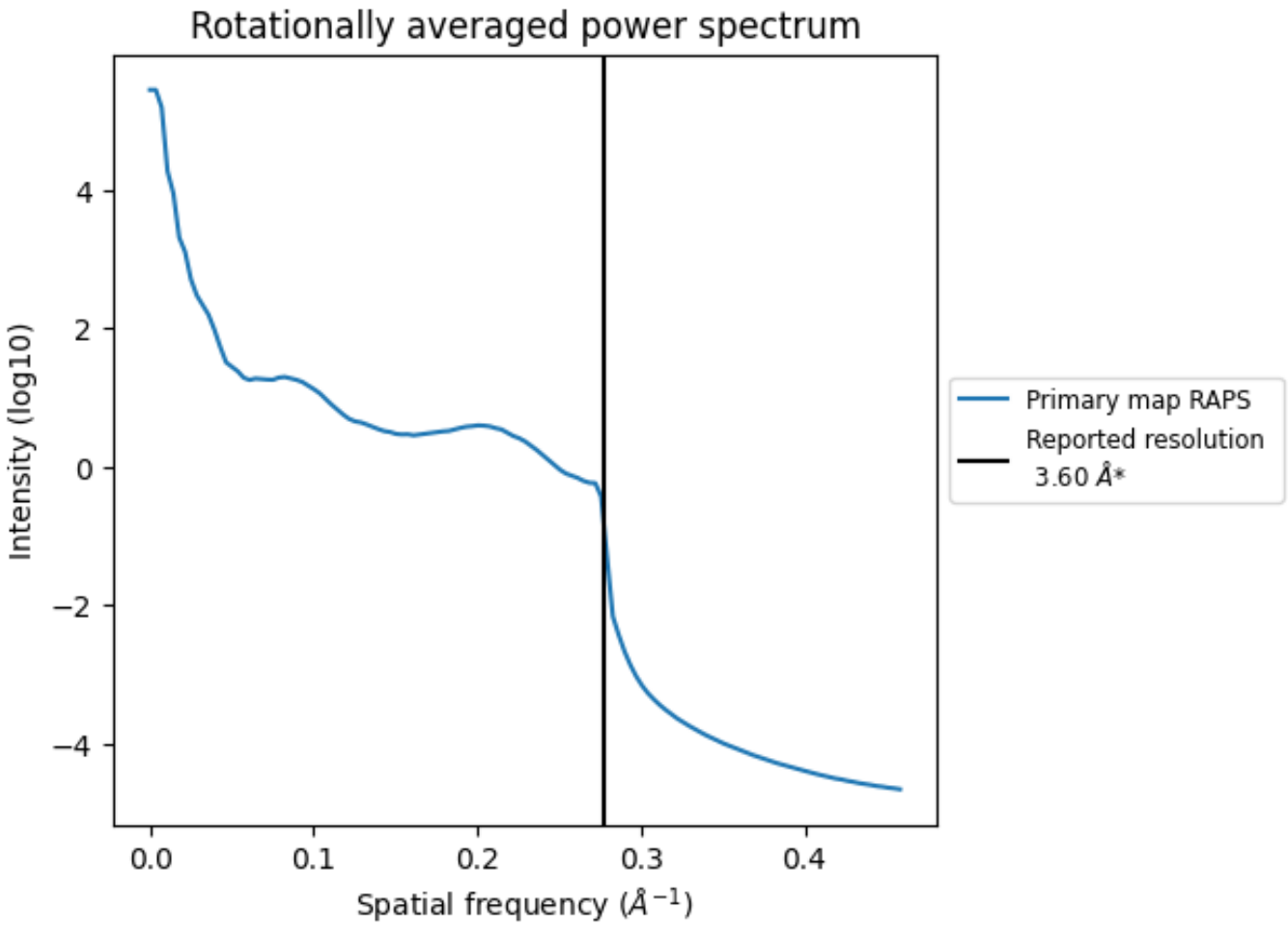
7.2 Volume estimate (i)



The volume at the recommended contour level is 85 nm^3; this corresponds to an approximate mass of 77 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 0.278 Å^{-1}

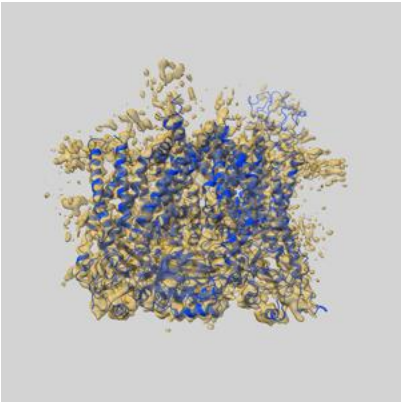
8 Fourier-Shell correlation (i)

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

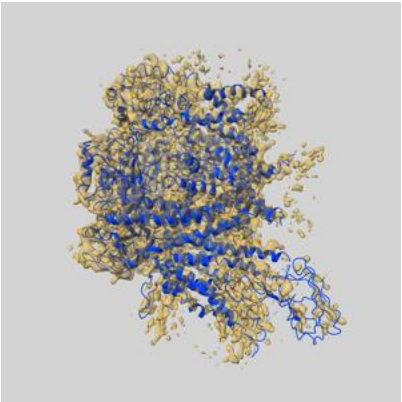
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6991 and PDB model 6A70. Per-residue inclusion information can be found in section 3 on page 8.

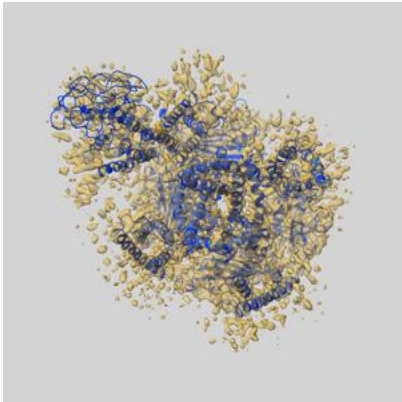
9.1 Map-model overlay (i)



X



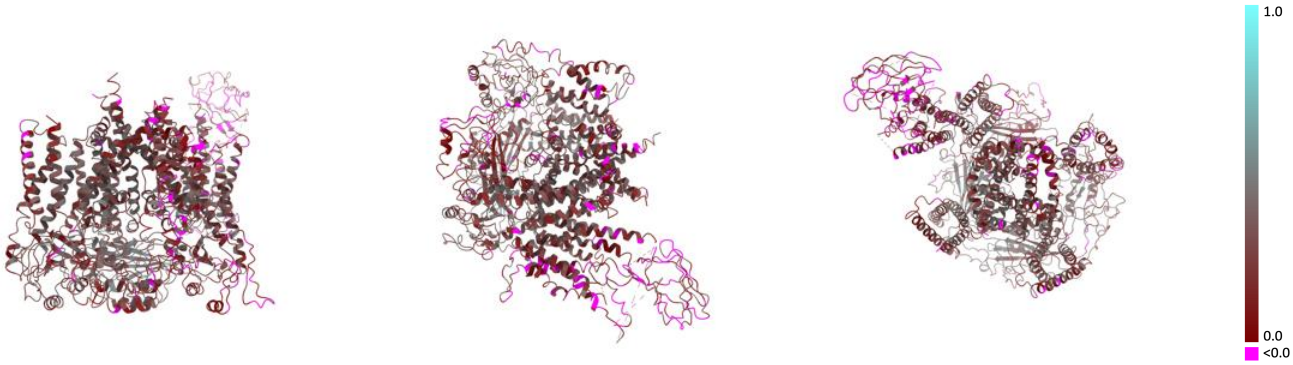
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

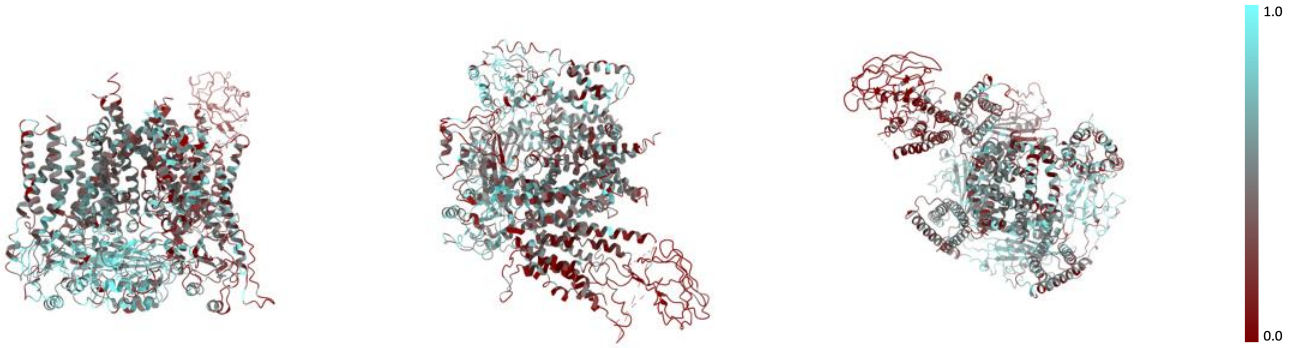
9.2 Q-score mapped to coordinate model (i)



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.

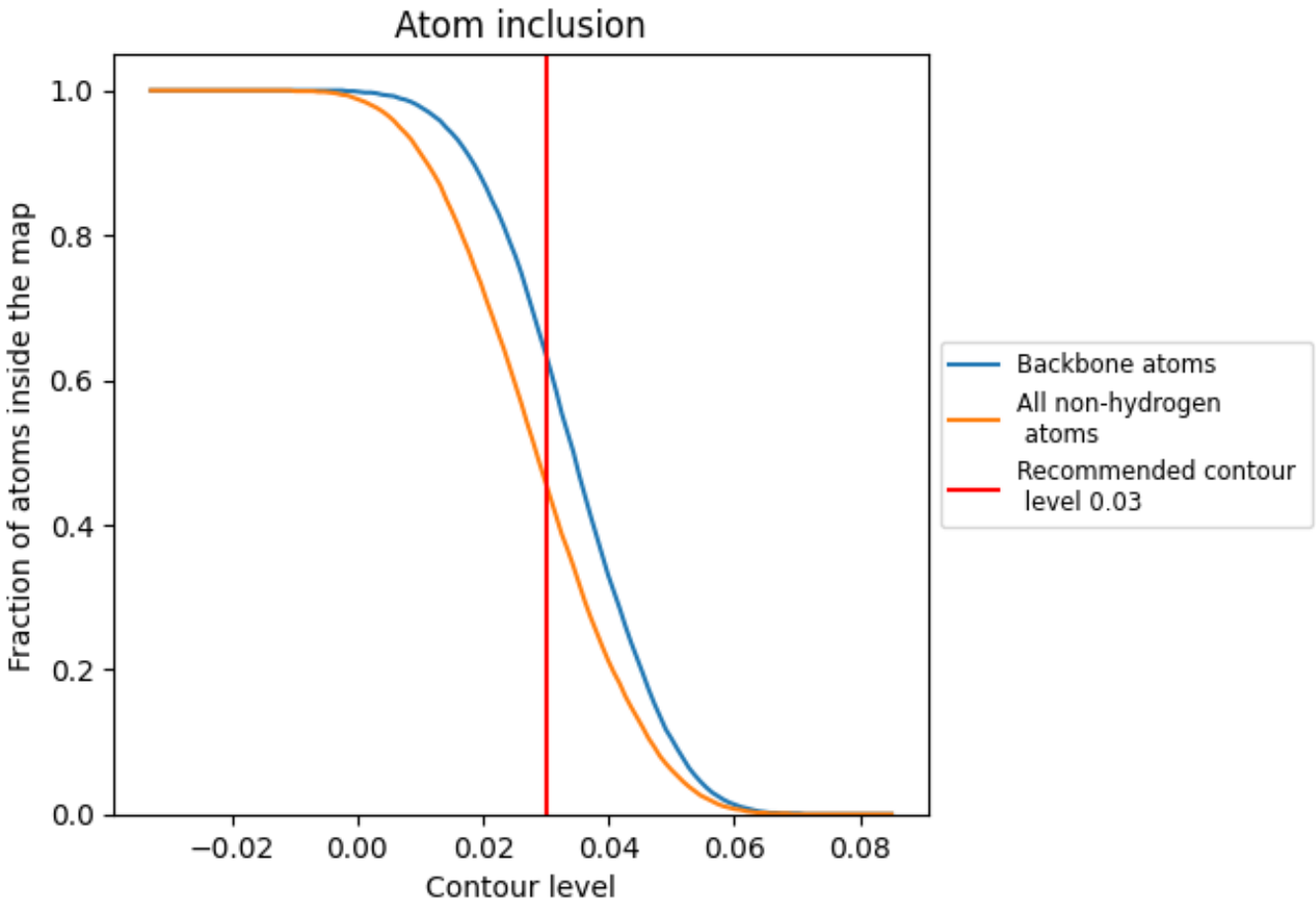
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4580	0.2630
A	0.5200	0.2610
B	0.2900	0.1770
F	0.5560	0.3210
G	0.5370	0.3200